# A User's Guide for the CALPUFF Dispersion Model
## (Version 5)

*Prepared by:*

Joseph S. Scire
David G. Strimaitis
Robert J. Yamartino

Earth Tech, Inc.
196 Baker Avenue
Concord, MA 01742

January 2000

**Table of Contents**

iii

# 1. OVERVIEW

## 1.1     Background

As part of a study to design and develop a generalized non-steady-state air quality modeling system for regulatory use, Sigma Research Corporation (now part of Earth Tech, Inc.), developed the CALPUFF dispersion model and related models and programs, including the CALMET meteorological model.  The original development of CALPUFF and CALMET was sponsored by the California Air Resources Board (CARB).  Systems Application, Inc. (SAI) served as a subcontractor to Sigma Research with the responsibility for developing the original wind field modeling component of the CALMET model.

The original design specifications for the modeling system included:  (1) the capability to treat time-varying point and area sources, (2) suitability for modeling domains from tens of meters to hundreds of kilometers from a source, (3) predictions for averaging times ranging from one-hour to one year, (4) applicability to inert pollutants and those subject to linear removal and chemical conversion mechanisms, and (5) applicability for rough or complex terrain situations.

The modeling system (Scire et al., 1990a, 1990b) developed to meet these objectives consisted of three components:  (1) a meteorological modeling package with both diagnostic and prognostic wind field generators, (2) a Gaussian puff dispersion model with chemical removal, wet and dry deposition, complex terrain algorithms, building downwash, plume fumigation, and other effects, and (3) postprocessing programs for the output fields of meteorological data, concentrations and deposition fluxes.

In July, 1987, CARB initiated a second project with Sigma Research to upgrade and modernize the Urban Airshed Model (UAM) to include state-of-the-science improvements in many of the key technical algorithms including the numerical advection and diffusion schemes, dry deposition, chemical mechanisms, and chemical integration solver.  The new photochemical model, called CALGRID (Yamartino et al., 1992; Scire et al., 1989), was integrated into the CALMET/CALPUFF modeling framework to create a complete modeling system for both reactive and non-reactive pollutants.  A third component of the modeling system, a Lagrangian particle model called the Kinematic Simulation Particle (KSP) model (Strimaitis et al., 1995; Yamartino et al., 1996), was developed under sponsorship of the German Umweldbundesamt.  All three models (CALPUFF, CALGRID, and KSP) are designed to be compatible with the common meteorological model, CALMET, and share preprocessing and postprocessing programs for the display of the modeling results.

In the early 1990s, the Interagency Workgroup on Air Quality Modeling (IWAQM) reviewed various modeling approaches suitable for estimating pollutant concentrations at Class I areas, including the

individual and cumulative impacts of proposed and existing sources on Air Quality Related Values (AQRVs), Prevention of Significant Deterioration (PSD) increments, and National Ambient Air Quality Standards (NAAQS).  IWAQM consists of representatives from the U.S. Environmental Protection Agency (EPA), U.S. Forest Service, National Park Service, and U.S. Fish and Wildlife Service.  IWAQM released a Phase I report (EPA, 1993a) which recommended using the MESOPUFF II dispersion model and MESOPAC II meteorological model on an interim basis for simulating regional air quality and visibility impacts.  These recommendations were to apply until more refined (Phase 2) techniques could be identified and evaluated.  As  part of the development of the Phase 2 recommendations, IWAQM reviewed and intercompared diagnostic wind field models, tested the use of coarse gridded wind fields from the Penn State/NCAR Mesoscale Model with four dimensional data assimilation (MM4) as input into the diagnostic models, and evaluated the MESOPUFF II and CALPUFF modeling systems using tracer data collected during the Cross-Appalachian Tracer Experiment (CAPTEX).  The CAPTEX evaluation results (EPA, 1995) indicated that by using the CALMET/ CALPUFF models with MM4 data, performance could be improved over that obtained with the interim Phase I modeling approach.  The Phase 2 IWAQM report (EPA, 1998) recommends the use of the CALMET and CALPUFF models for estimating air quality impacts relative to the National Ambient Air Quality Standards (NAAQS) and Prevention of Significant Deterioration (PSD) increments.  The U.S. EPA has proposed the CALPUFF modeling system as a *Guideline* ("Appendix A") model for regulatory applications involving long range transport and on a case-by-case basis for near-field applications where non-steady-state effects (situations where factors such as spatial variability in the meteorological fields, calm winds, fumigation, recirculation or stagnation, and terrain or coastal effects) may be important.

The CALMET and CALPUFF models have been substantially revised and enhanced as part of work for IWAQM, U.S. EPA, the U.S.D.A. Forest Service, the Environmental Protection Authority of Victoria (Australia), and private industry in the U.S. and abroad.  The improvements to CALMET included modifications to make it more suitable for regional applications such as the use of a spatially variable initial guess field, an option for using hourly MM4 or MM5 gridded fields as a supplement to observational data, the ability to compute Lambert conformal map factors, a modified mixing height scheme, an option to use similarity theory to vertically extrapolate surface wind observations, an enhanced algorithm to compute the three-dimensional temperature fields over water bodies, improved initialization techniques, a refined slope flow parameterization, and an optional PC-based Graphical User Interface (GUI) to facilitate model setup and execution and to provide access to on-line Help files. Improvements to CALPUFF include new modules to treat buoyant rise and dispersion from area sources (such as forest fires), buoyant line sources, volume sources, an improved treatment of complex terrain, additional model switches to facilitate its use in regulatory applications, enhanced treatment of wind shear through puff splitting, use of a probability density function (pdf) to describe dispersion during convective conditions, and an optional GUI.  CALPUFF has been coupled to the Emissions Production

Model (EPM) developed by the Forest Service through an interface processor.  EPM provides time-dependent emissions and heat release data for use in modeling controlled burns and wildfires.

1.2      Overview of the CALPUFF  Modeling System

The CALPUFF Modeling System includes three main components: CALMET, CALPUFF, and CALPOST and a large set of preprocessing programs designed to interface the model to standard, routinely-available meteorological and geophysical datasets.   In the simplest terms, CALMET is a meteorological model that develops hourly wind and temperature fields on a three-dimensional gridded modeling domain.  Associated two-dimensional fields such as mixing height, surface characteristics, and dispersion properties are also included in the file produced by CALMET.  CALPUFF is a transport and dispersion model that advects "puffs" of material emitted from modeled sources, simulating dispersion and transformation processes along the way.  In doing so it typically uses the fields generated by CALMET, or as an option, it may use simpler non-gridded meteorological data much like existing plume models.  Temporal and spatial variations in the meteorological fields selected are explicitly incorporated in the resulting distribution of puffs throughout a simulation period.  The primary output files from CALPUFF contain either hourly concentrations or hourly deposition fluxes evaluated at selected receptor locations.  CALPOST is used to process these files, producing tabulations that summarize the results of the simulation, identifying the highest and second highest 3-hour average concentrations at each receptor, for example.  When performing visibility-related modeling, CALPOST uses concentrations from CALPUFF to compute extinction coefficients and related measures of visibility, reporting these for selected averaging times and locations.

Most applications of the system are built around these three components.  To enhance their functionality, a PC-based GUI is provided for each major component.  The GUIs can be used to prepare the control file that configures a run, execute the corresponding component model, and conduct file management functions.  The GUIs also contain an extensive help system that makes much of the technical information contained in this manual available to the user on-line.  The modeling system may also be setup and run without the aid of the GUIs.  The control file for each component is simply a text file that is readily edited, and it contains extensive information about model options, default values, and units for each variable.

In addition to CALMET, CALPUFF, CALPOST, and their corresponding GUIs, the modeling system interfaces to several other models, which is facilitated by several preprocessors and utilities.  Figure 1-1 displays the overall modeling system configuration.  Four of the models shown in Figure 1-1 are external models that are not included in the CALPUFF system, but they can be interfaced with CALPUFF modules:
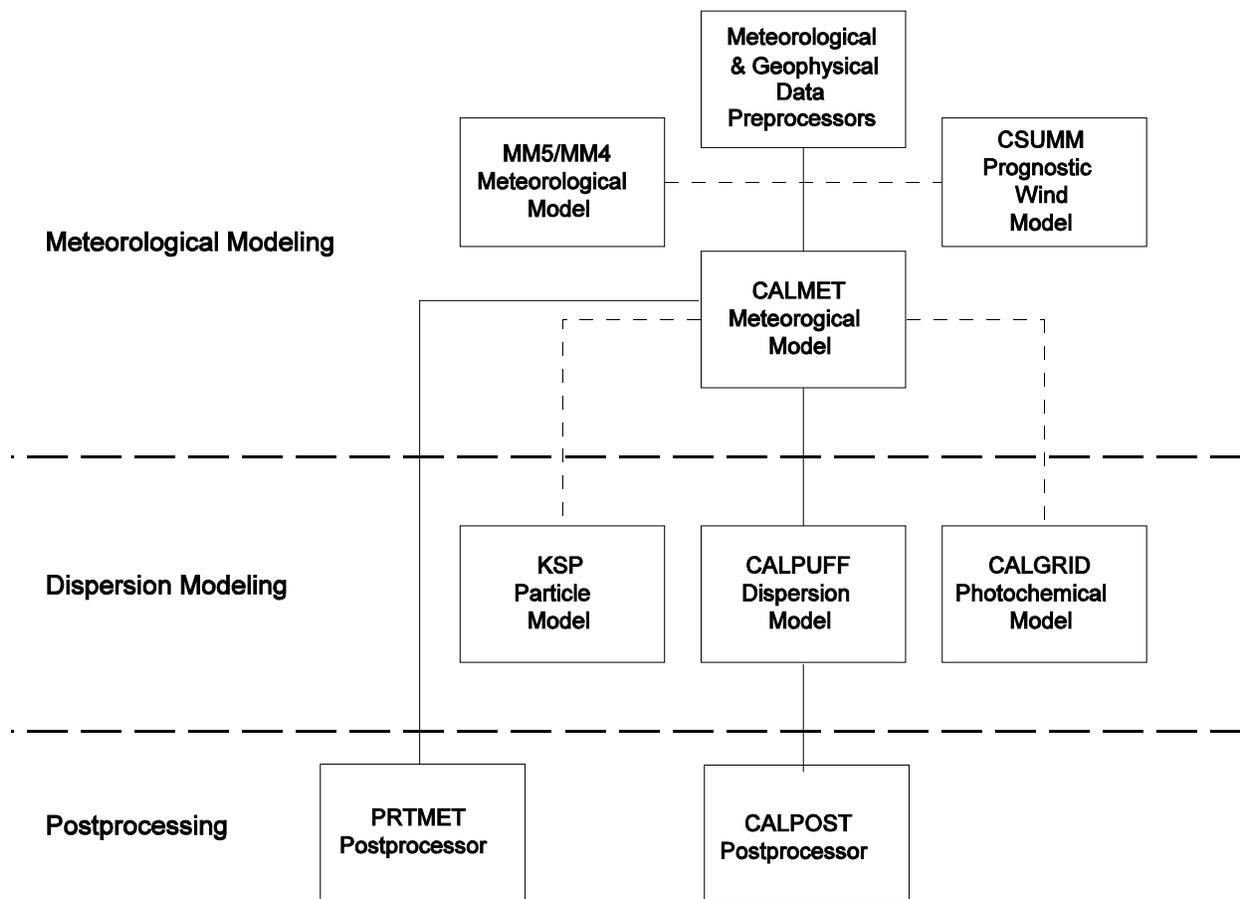
Figure 1-1.    Overview of the program elements in the CALMET/CALPUFF modeling system.  Also shown are the associated CALGRID photochemical model, the KSP particle model, and the MM5/MM4 and CSUMM meteorological models.

**MM5/MM4** (Penn State/NCAR Mesoscale Model) is a prognostic wind field model with four dimensional data assimilation (Anthes et al., 1987; Grell et al., 1996). The diagnostic wind field model within CALMET contains options that allow wind fields produced by MM5 or MM4 to be used as an initial guess field, or pseudo-observations and combined with other data sources as part of the CALMET objective analysis procedure. An interface program (CALMM5) converts the MM5 data into a form compatible with CALMET.

**CSUMM** (a version of the Colorado State University Mesoscale Model) is a primitive equation wind field model (Kessler, 1989) which simulates mesoscale airflow resulting from differential surface heating and terrain effects. Various options for using CSUMM output with CALMET are provided.

The other two external models may use the output file from CALMET for their meteorological fields:

**CALGRID** is an Eulerian photochemical transport and dispersion model which includes modules for horizontal and vertical advection/diffusion, dry deposition, and a detailed photochemical mechanism.

**KSP** is a multi-layer, multi-species Lagrangian particle model that simulates transport, dispersion, and deposition using explicit kinematic simulation (KS) of the larger transportive and dispersive eddies in the atmosphere.

The components in Figure 1-1 that are included in the system are:

**CALMET** is a meteorological model which includes a diagnostic wind field generator containing objective analysis and parameterized treatments of slope flows, kinematic terrain effects, terrain blocking effects, and a divergence minimization procedure, and a micro-meteorological model for overland and overwater boundary layers.

**CALPUFF** is a non-steady-state Lagrangian Gaussian puff model containing modules for complex terrain effects, overwater transport, coastal interaction effects, building downwash, wet and dry removal, and simple chemical transformation.

**CALPOST** is a postprocessing program with options for the computation of time-averaged concentrations and deposition fluxes predicted by the CALPUFF and CALGRID models. CALPOST computes visibility impacts in accordance with IWAQM recommendations and the current Federal Land Managers' Air Quality Related Values Workgroup (FLAG) recommendations.

**PRTMET** is a postprocessing program which displays user-selected portions of the meteorological data file produced by the CALMET meteorological model.

Preprocessors and utilities provided with the modeling system for use with CALMET include:

**METSCAN** is a meteorological preprocessor which performs quality assurance checks on the hourly surface meteorological data in the U.S. National Climatic Data Center (NCDC) CD-144 format which is used as input to the SMERGE program.

**READ62** is a meteorological preprocessor which extracts and processes upper air wind and temperature data from the standard NCDC TD-6201 data format or the NCDC CD-ROM FSL rawinsonde data format.

**SMERGE** is a meteorological preprocessor which processes hourly surface observations from a number of stations in NCDC CD-144 format or NCDC CD-ROM format and reformats the data into a single file with the data sorted by time rather than station. The CD-ROM format contains data in either the Solar and Meteorological Surface Observational Network (SAMSON) format or the Hourly U.S. Weather Observations (HUSWO) format.

**PXTRACT** is a meteorological preprocessor which extracts precipitation data for stations and a time period of interest from a fixed length, formatted precipitation data file in NCDC TD-3240 format.

**PMERGE** is a meteorological preprocessor responsible for reformatting the precipitation data files created by the PXTRACT program. PMERGE resolves "accumulation periods" into hourly values and flags suspicious or missing data. The output file can be formatted or binary, which can be directly input into the CALMET model, containing the precipitation data sorted by hour rather than station.

**TERREL** is a terrain preprocessor which coordinates the allocation of terrain elevation data from several digitized data bases to a user-specified modeling grid.

**CTGCOMP** is a preprocessor used to compress the data file format of a USGS land use CTG data file.

**CTGPROC** is a land use preprocessor which reads the compressed CTG land use data file and computes the fractional land use for each grid cell in the user-specified modeling domain.

**PRLND1** is a land use preprocessor which reads the ARM3 data base of land use data and computes fractional land use for each grid cell in the user-specified modeling domain.

**MAKEGEO** is the final preprocessor which reads the fractional land use data, user inputs which define land use category mapping, and values relating each of the surface parameters to land use, and (optionally) the gridded terrain data file, and produces a GEO.DAT file ready for input to CALMET.

**CALMM5** is a processor that extracts and interprets data in the output file from MM5 (Version 2), and creates a file of meteorological data for direct input to CALMET in either its MM4.DAT format or its MM5.DAT format.

Preprocessors and utilities provided with the modeling system for use with CALPUFF include:

**OPTHILL** is a processor program which uses topographical data (such as terrain maps) to develop hill shape factors that are used in the subgrid scale complex terrain (CTSG) module in CALPUFF.

**EPM2BAEM** is a conversion utility which creates a time-varying emissions file for buoyant forest fire area sources based on the output from the U.S.D.A Forest Service Emissions Production Model (EPM).

The meteorological modeling with the CALMET model is detailed in Figure 1-2. Note that the preprocessors for the raw meteorological data are written to accommodate the U.S. National Climatic Data Center (NCDC) file formats. Figure 1-3 is the schematic of the CALPUFF dispersion model indicating the model input and output files. The postprocessing approach for the meteorological and dispersion modeling results is shown in Figure 1-4.

A series of reports and user's guides describe the components of the modeling system. Documentation for CALPUFF (Version 5) and CALPOST (Version 5) is contained in this report. The technical formulation and user instructions for CALMET (Version 5) and the meteorological and geophysical preprocessing programs are contained in Scire et al. (1999). The CSUMM prognostic wind field model is described in a report by Kessler (1989). A stand-alone version of the Diagnostic Wind Model (DWM) used as the original wind field module in CALMET is discussed by Douglas and Kessler (1988). The CALGRID model is documented in a paper by Yamartino et al. (1992) and reports by Yamartino et al. (1989) and Scire et al. (1989). The KSP model is described by Strimaitis et al., (1995) and Yamartino et al. (1996).
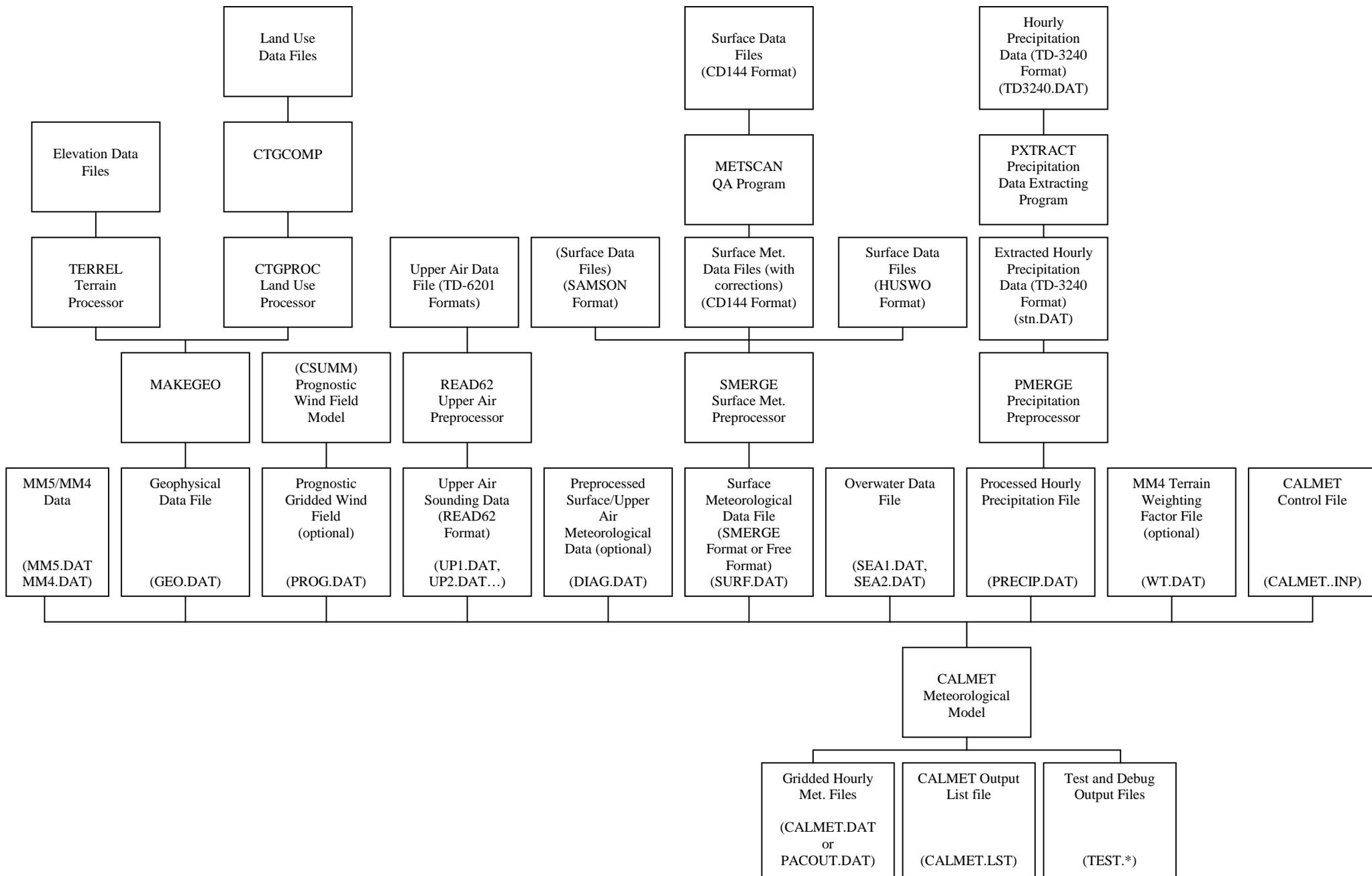
Figure 1-2. Meteorological modeling: CALMET modeling flow diagram.
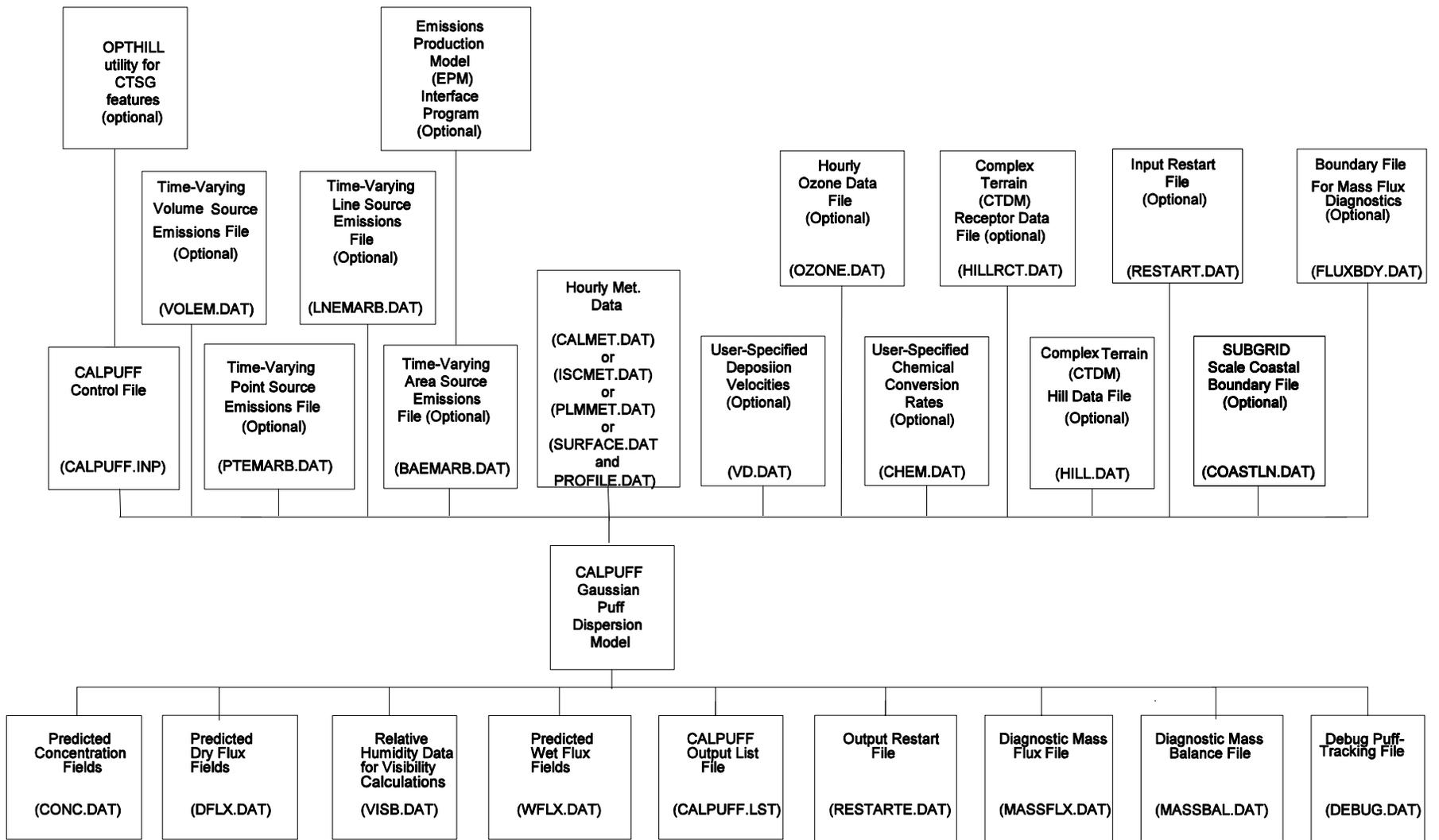
Figure 1-3. Dispersion Modeling: CALPUFF modeling flow diagram.
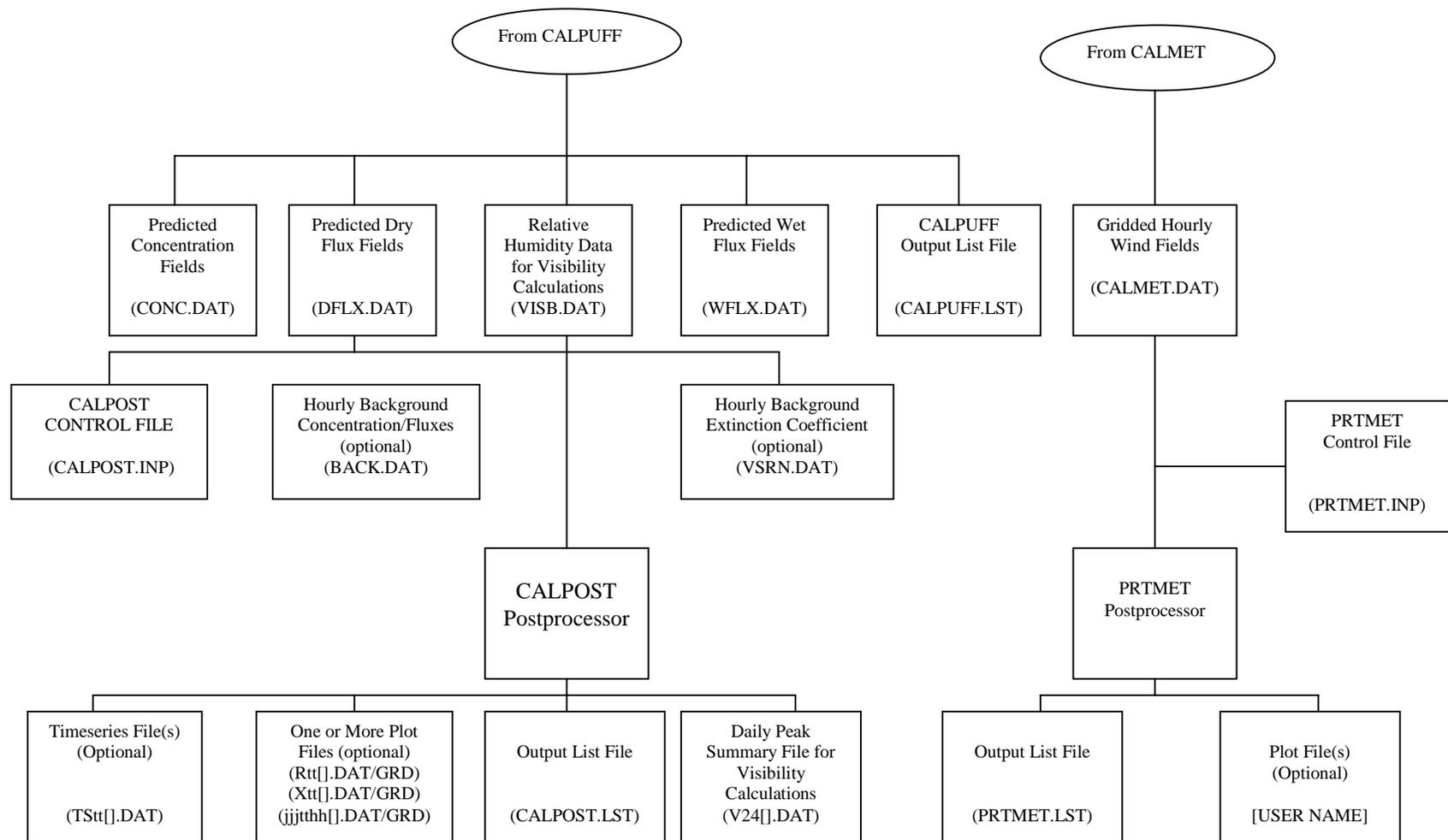
Figure 1-4.  Postprocessing:  CALPOST/PRTMET postprocessing flow diagram.

## 1.3    CALPUFF Features and Options

CALPUFF is a multi-layer, multi-species non-steady-state puff dispersion Model which can simulate the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal.  CALPUFF can use the three dimensional meteorological fields developed by the CALMET model, or simple, single station winds in a format consistent with the meteorological files used to drive the ISCST3 (EPA, 1995), AUSPLUME (Lorimer, 1986), or CTDMPLUS (Perry et al., 1989) steady-state Gaussian models.  However, single-station ISCST3, CTDMPLUS, or AUSPLUME winds should be used with caution, because they do not allow CALPUFF to take advantage of its capabilities to treat spatially-variable meteorological fields.

CALMET includes a diagnostic wind field generator, and overland and overwater boundary layer modules.  CALMET has the ability to combine the wind fields generated by the CSUMM prognostic wind field model or the MM5/MM4 model with observational data through an objective analysis procedure.

CALPUFF contains algorithms for near-source effects such as building downwash, transitional plume rise, partial plume penetration, subgrid scale terrain interactions as well as longer range effects such as pollutant removal (wet scavenging and dry deposition), chemical transformation, vertical wind shear, overwater transport and coastal interaction effects.  It can accommodate arbitrarily-varying point source and gridded area source emissions.  Most of the algorithms contain options to treat the physical processes at different levels of detail depending on the model application.

The major features and options of the CALPUFF model are summarized in Table 1-1.  Some of the technical algorithms are briefly described below.

> **Dry Deposition:**  A full resistance model is provided in CALPUFF for the computation of dry deposition rates of gases and particulate matter as a function of geophysical parameters, meteorological conditions, and pollutants species.  Options are provided to allow user-specified, diurnally varying deposition velocities to be used for one or more pollutants instead of the resistance model (e.g., for sensitivity testing) or to bypass the dry deposition model completely.

> **Wet Deposition:**  An empirical scavenging coefficient approach is used in CALPUFF to compute the depletion and wet deposition fluxes due to precipitation scavenging.  The scavenging coefficients are specified as a function of the pollutant and precipitation type (i.e., frozen vs. liquid precipitation).

Table 1-1

Major Features of the CALPUFF Model

- **Source types**
  - · Point sources (constant or variable emissions)
  - · Line sources (constant or variable emissions)
  - · Volume sources (constant or variable emissions)
  - · Area sources (constant or variable emissions)

- **Non-steady-state emissions and meteorological conditions**
  - · Gridded 3-D fields of meteorological variables (winds, temperature)
  - · Spatially-variable fields of mixing height, friction velocity, convective velocity scale, Monin-Obukhov length, precipitation rate
  - · Vertically and horizontally-varying turbulence and dispersion rates
  - · Time-dependent source and emissions data

- **Efficient sampling functions**
  - · Integrated puff formulation
  - · Elongated puff (slug) formulation

- **Dispersion coefficient ($\sigma_y$, $\sigma_z$) options**
  - · Direct measurements of $\sigma_v$ and $\sigma_w$
  - · Estimated values of $\sigma_v$ and $\sigma_w$ based on similarity theory
  - · Pasquill-Gifford (PG) dispersion coefficients (rural areas)
  - · McElroy-Pooler (MP) dispersion coefficients (urban areas)
  - · CTDM dispersion coefficients (neutral/stable)

- **Vertical wind shear**
  - · Puff splitting
  - · Differential advection and dispersion

- **Plume rise**
  - · Partial penetration
  - · Buoyant and momentum rise
  - · Stack tip effects
  - · Vertical wind shear
  - · Building downwash effects

- **Building downwash**
  - · Huber-Snyder method
  - · Schulman-Scire method

(Continued)

Table 1-1 (Concluded)

Major Features of the CALPUFF Model

- **Subgrid scale complex terrain**
  - Dividing streamline, $H_d$:
    - Above $H_d$, puff flows over the hill and experiences altered diffusion rates
    - Below $H_d$, puff deflects around the hill, splits, and wraps around the hill

- **Interface to the Emissions Production Model (EPM)**
  - Time-varying heat flux and emissions from controlled burns and wildfires

- **Dry Deposition**
  - Gases and particulate matter
  - Three options:
    - Full treatment of space and time variations of deposition with a resistance model
    - User-specified diurnal cycles for each pollutant
    - No dry deposition

- **Overwater and coastal interaction effects**
  - Overwater boundary layer parameters
  - Abrupt change in meteorological conditions, plume dispersion at coastal boundary
  - Plume fumigation
  - Option to introduce subgrid scale Thermal Internal Boundary Layers (TIBLs) into coastal grid cells

- **Chemical transformation options**
  - Pseudo-first-order chemical mechanism for $SO_2$, $SO_4^=$, $NO_x$, $HNO_3$, and $NO_3^-$ (MESOPUFF II method)
  - User-specified diurnal cycles of transformation rates
  - No chemical conversion

- **Wet Removal**
  - Scavenging coefficient approach
  - Removal rate a function of precipitation intensity and precipitation type

- **Graphical User Interface**
  - Point-and-click model setup and data input
  - Enhanced error checking of model inputs
  - On-line Help files

**Chemical Transformation:** CALPUFF includes options for parameterizing chemical transformation effects using the five species scheme ($SO_2$, $SO_4^=$, $NO_x$, $HNO_3$, and $NO_3^-$) employed in the MESOPUFF II model, a modified six-species scheme ($SO_2$, $SO_4^=$, $NO$, $NO_2$, $HNO_3$, and $NO_3^-$) adapted from the RIVAD/ARM3 method, or a set of user-specified, diurnally-varying transformation rates.

**Subgrid Scale Complex Terrain:** The complex terrain module in CALPUFF is based on the approach used in the Complex Terrain Dispersion Model (CTDMPLUS) (Perry et al., 1989). Plume impingement on subgrid scale hills is evaluated using a dividing streamline ($H_d$) to determine which pollutant material is deflected around the sides of a hill (below $H_d$) and which material is advected over the hill (above $H_d$). Individual puffs are split into up to three sections for these calculations.

**Puff Sampling Functions:** A set of accurate and computationally efficient puff sampling routines are included in CALPUFF which solve many of the computational difficulties with applying a puff model to near-field releases. For near-field applications during rapidly-varying meteorological conditions, an elongated puff (slug) sampling function is used. An integrated puff approached is used during less demanding conditions. Both techniques reproduce continuous plume results exactly under the appropriate steady state conditions.

**Wind Shear Effects:** CALPUFF contains an optional puff splitting algorithm that allows vertical wind shear effects across individual puffs to be simulated. Differential rates of dispersion and transport occur on the puffs generated from the original puff, which under some conditions, can substantially increase the effective rate of horizontal growth of the plume.

**Building Downwash:** The Huber-Snyder and Schulman-Scire downwash models are both incorporated into CALPUFF. An option is provided to use either model for all stacks, or make the choice on a stack-by-stack and wind sector-by-wind sector basis. Both algorithms have been implemented in such a way as to allow the use of wind direction specific building dimensions.

**Overwater and Coastal Interaction Effects:** Because the CALMET meteorological model contains both overwater and overland boundary layer algorithms, the effects of water bodies on plume transport, dispersion, and deposition can be simulated with CALPUFF. The puff formulation of CALPUFF is designed to handle spatial changes in meteorological and dispersion conditions, including the abrupt changes which occur at the coastline of a major body of water.

**Dispersion Coefficients:** Several options are provided in CALPUFF for the computation of dispersion coefficients, including the use of turbulence measurements ($\sigma_v$ and $\sigma_w$), the use of

similarity theory to estimate $\sigma_v$ and $\sigma_w$ from modeled surface heat and momentum fluxes, or the use of Pasquill-Gifford (PG) or McElroy-Pooler (MP) dispersion coefficients, or dispersion equations based on the Complex Terrain Dispersion Model (CDTM).  Options are provided to apply an averaging time correction or surface roughness length adjustments to the PG coefficients.

1.4     Summary of CALPUFF Data and Computer Requirements

The input data sets used by CALPUFF are summarized in Table 1-2 (also see the modeling system flow diagram, Figure 1-1).  CALPUFF reads user inputs from a "control file" with a default name of CALPUFF. INP.  This file contains the user's selections for the various model options, technical input variables, output options, and other user-controllable options.

A meteorological data file (CALMET.DAT) contains hourly gridded fields of micro-meteorological parameters and three-dimensional wind and temperature fields.  The meteorological data file also contains geophysical data such as terrain heights and land use which are required by both the meteorological model (e.g., for terrain adjustment of the wind fields) and by the CALPUFF model.  The contents of the CALMET.DAT input file and the other input data bases are summarized in Table 1-3.  Options also exist for using single-station meteorological data in ISCST3, CTDMPLUS, or AUSPLUME data format.

Five files are provided for the input of emissions data.  The control file, CALPUFF.INP includes point, line, volume and area source data for sources with constant emission parameters or those that can be described by a cycle based on time of day (24 factors), month (12 factors), hour and season (24 x 4 factors), wind speed and stability class (6 x 6 factors), or temperature (12 factors).  Separate scaling factors can be specified for each source-species combination.  Arbitrarily-varying source data may be provided in files for point sources (default name PTEMARB.DAT), area sources (default name AREMARB.DAT), line sources (default name LNEMARB.DAT), and gridded volume sources (default name VOLEM.DAT).

Hourly observations of ozone data are used in the calculation of $SO_2$ and $NO_x$ transformation rates if either the MESOPUFF II or the RIVAD/ARM3 chemical transformation scheme is selected.  The hourly ozone data for one or more ozone stations are read from a data file called OZONE.DAT.

Because of the similarity between CTDMPLUS and the CTSG option with CALPUFF, an input option is provided for hill data and the associated receptor data in files produced for CTDMPLUS.  These files, HILL.DAT and HILLRCT.DAT can be read by CALPUFF without modification, to specify all CTSG input requirements.

Table 1-2

Summary of CALPUFF Input Files

| Default File Name | Contents | Unit* Number | Type |
|---|---|---|---|
| RESTARTB.DAT | Input restart file containing a dump of all puff parameters sufficient to allow a model run to continue (optional) | IO3 | Unformatted |
| CALPUFF.INP | Control file inputs | IO5 | Formatted |
| CALMET.DAT | Geophysical and hourly meteorological data, created by the CALMET meteorological model | IO7 | Unformatted |
| or ISCMET.DAT | Single-station ASCII meteorological data in ISCST3-format | IO7 | Formatted |
| or PLMMET.DAT | Single-station ASCII meteorological data in AUSPLUME format | IO7 | Formatted |
| PTEMARB.DAT | Source and emissions data for point sources with arbitrarily-varying emission parameters (optional) | IO16 | Formatted or unformatted |
| BAEMARB.DAT | Emissions data for area sources with arbitrarily-varying emission parameters. Can be derived from EPM model files (optional) | IO17 | Formatted |
| VOLEM.DAT | Emissions data for gridded volume sources with arbitrarily-varying emission parameters (optional) | IO18 | Formatted or unformatted |
| LNEMARB.DAT | Emission data for line sources with arbitrarily-varying line source emissions (optional) | I019 | Formatted |
| VD.DAT | User-specified deposition velocities (optional) | IO20 | Formatted |
| OZONE.DAT | Hourly ozone measurements at one or more ozone stations (optional) | IO22 | Formatted |
| CHEM.DAT | User-specified chemical transformation rates (optional) | IO24 | Formatted |
| COASTLN.DAT | Subgrid scale coastal boundary file (optional) | IO25 | Formatted |
| HILL.DAT | Hill specifications from CTDMPLUS terrain processor (optional) | IO28 | Formatted |
| HILLRCT.DAT | CTSG Receptors from CTDMPLUS processor (optional) | IO29 | Formatted |
| PROFILE.DAT | Single-station ASCII meteorological tower data as prepared for CTDMPLUS (optional) | IO31 | Formatted |
| SURFACE.DAT | CTDMPLUS surface layer parameters (optional) | IO32 | Formatted |
| FLUXBDY.DAT | Boundary Data for Mass flux (optional) | IO35 | Formatted |

---

* Variable shown is the parameter controlling the FORTRAN unit number associated with the file. Usually, the value assigned to the parameter is consistent with the name (i.e., IO7 = 7). However, the value can be easily changed in the parameter file to accommodate reserved unit numbers on a particular system.

Table 1-3

Summary of Input Data Used by CALPUFF

**Geophysical Data (CALMET.DAT)**

Gridded fields of:
- surface roughness lengths ($z_o$)
- land use categories
- terrain elevations
- leaf area indices

**Meteorological Data (CALMET.DAT)**

Gridded fields of:
- u, v, w wind components (3-D)
- air temperature (3-D)
- surface friction velocity ($u_*$)
- convective velocity scale ($w_*$)
- mixing height ($z_i$)
- Monin-Obukhov length (L)
- PGT stability class
- Precipitation rate

Hourly values of the following parameters at surface met. stations:
- air density ($\rho_a$)
- air temperature
- short-wave solar radiation
- relative humidity
- precipitation type

**Meteorological Data (ISCMET.DAT)**

Hourly values (standard records)
- wind speed, flow direction
- temperature, stability class
- mixing height ($z_i$) for rural/urban

Hourly values (extended records)
- surface friction velocity ($u_*$), Monin-Obukhov length (L)
- surface roughness ($z_o$)
- precipitation code and rate
- potential temperature gradient
- wind speed profile power-law exponent
- short-wave solar radiation
- relative humidity

(Continued)

Table 1-3 (Continued)
Summary of Input Data Used by CALPUFF

**Meteorological Date (PLMMET.DAT)**

Hourly values (standard records)
- wind speed, wind direction
- temperature, stability class
- mixing height ($z_i$)
- turbulence ($\sigma_\theta$)
- wind speed profile power-law exponent
- potential temperature gradient

Hourly values (extended records)
- precipitation code and rate
- short-wave solar radiation
- relative humidity

**Meteorological Data (SURFACE.DAT, PROFILE.DAT)**

Hourly values (SURFACE.DAT - standard records)
- mixing height ($z_i$)
- surface friction velocity ($u_*$), Monin-Obukhov length (L)
- surface roughness ($z_o$)

Hourly values (SURFACE.DAT - extended records)
- precipitation code and rate
- short-wave solar radiation
- relative humidity

Hourly values at multiple levels (PROFILE.DAT)
- height
- wind speed (scalar, vector)
- wind direction
- temperature
- turbulence ($\sigma_v/\sigma_\theta$, $\sigma_w$)

**Restart Data (RESTARTB.DAT)**

Model puff data generated from a previous run (allows continuation of a previous model run)

(Continued)

Table 1-3 (Concluded)
Summary of Input Data Used by CALPUFF

**Emissions Data (CALPUFF.INP, PTEMARB.DAT, BAEMARB.DAT, VOLEM.DAT, LNEMARB.DAT)**

  Point source emissions:
- Source and emissions data for point sources with constant or cyclical emission parameters (CALPUFF.INP)
- Source and emissions data for point sources with arbitrarily-varying emission parameters (PTEMARB.DAT)

  Area source emissions
- Emissions and initial size, height, and location for area sources with constant or cyclical emission parameters (CALPUFF.INP)
- Gridded emissions data for buoyant area sources with arbitrarily-varying emission parameters (BAEMARB.DAT)

  Volume source emissions
- Emissions, height, size, and location of volume sources with constant or cyclical emission parameters (CALPUFF.INP)
- Emissions data for volume sources with arbitrarily-varying emission parameters (VOLEM.DAT)

  Line source emissions
- Source and emissions data, height, length, location, spacing, and orientation of buoyant line sources with constant or cyclical emission parameters (CALPUFF.INP)
- Emissions data for buoyant line sources with arbitrarily-varying emission parameters (LNEMARB.DAT)

**Deposition Velocity Data (VD.DAT)**
- Deposition velocity for each user-specified species for each hour of a diurnal cycle

**Ozone Monitoring Data (OZONE.DAT)**
- Hourly ozone measurements at one or more monitoring stations

**Chemical Transformation Data (CHEM.DAT)**
- Species-dependent chemical transformation rates for each hour of a diurnal cycle

**Hill Data (HILL.DAT)**
- Hill shape and height parameters in CTDMPLUS format for use in the subgrid-scale complex terrain module (CTSG)

**CTSG Receptors (HILLRCT.DAT)**
- Receptor locations and associated hill ID in CTDMPLUS format

**Subgrid Scale Coastal Boundary Data (COASTLN.DAT)**
- File containing X,Y coordinates of subgrid scale coastlines to be treated by CALPUFF

**Boundary Data for Diagnostic Mass Flux Option (FLUXBDY.DAT)**
- File containing X,Y coordinates of boundaries used to evaluate hourly mass transport

Two additional input files, VD.DAT and CHEM.DAT, contain diurnal cycles of user-specified deposition velocities and chemical transformation rates, respectively. These files are necessary only if the user wishes to substitute the values normally computed internally by the deposition and chemical models with sets of time-varying but spatially-uniform externally specified values.

The optional input file, PROFILE.DAT in the CTDMPLUS format can also be used to provide vertical profiles of hourly observations of $\sigma_v$ and $\sigma_w$. These parameters can be used to compute the plume dispersion coefficients $\sigma_v$ and $\sigma_z$. The strength of a temperature inversion at the top of a convective boundary layer can also be provided in the PROFILE.DAT file, as an option, at the end of the record for the first level in the profile.

CALPUFF can continue a previous simulation using an optional restart file (RESTARTB.DAT). The restart file contains all of the puff variables at the end of the previous run needed to allow the model to continue the simulation. The restart file used as input of a continuation run must be generated as the output restart file in the previous CALPUFF simulation. The restart file is an optional file.

CALPUFF contains a subgrid scale coastal effects module that allows a parameterization of the Thermal Internal Boundary Layer (TIBL) at scales smaller than the grid spacing. The user inputs the X,Y coordinates of one or more coastlines in an optional file called COASTLN.DAT.

The CALPUFF output files are summarized in Table 1-4. The list file contains a copy of the inputs used in the run, optional output fields of gridded and discrete receptor concentrations, wet deposition fluxes, and dry deposition fluxes and other run data. The CONC.DAT, WFLX.DAT, and DFLX.DAT files contain the output concentrations, wet and dry fluxes, respectively, in an unformatted form suitable for further processing by the postprocessing program, CALPOST. The VISB.DAT file contains relative humidity information which is required by CALPOST in order to perform certain visibility-related computations. The model can generate an optional output restart file (RESTARTE.DAT) containing all the puff parameters needed to continue the CALPUFF simulation. The output restart file can be generated at regular intervals of the simulation to protect against loss of the simulation resulting from power failures or other interruptions. The output restart file of a run serves as the input restart file of the next (continuation) run.

### Computer Requirements

The memory management scheme used in CALMET and CALPUFF is designed to allow the maximum array dimensions in the model to be easily adjusted to match the requirements of a particular application. An external parameter file contains the maximum array size for all of the major arrays. A re-sizing of the program can be accomplished by modifying the appropriate variable or variables in the parameter file and re-compiling the program. All appropriate arrays in the model will be automatically re-sized by the updated

Table 1-4

Summary of CALPUFF Output Files

| Default File Name | Contents | Unit* Number | Type |
|---|---|---|---|
| RESTARTE.DAT | Output restart file containing a dump of all puff parameters sufficient to allow a model run to continue (optional) | IO4 | Unformatted |
| CALPUFF.LST | List file produced by CALPUFF | IO6 | Formatted |
| CONC.DAT | One-hour averaged concentrations ($g/m^3$) at the gridded and discrete receptors for species selected by the user in the control file (optional) | IO8 | Unformatted |
| DFLX.DAT | One-hour averaged dry deposition fluxes ($g/m^2/s$) at the gridded and discrete receptors for species selected by the user in the control file (optional) | IO9 | Unformatted |
| WFLX.DAT | One-hour averaged wet deposition fluxes ($g/m^2/s$) at the gridded and discrete receptors for species selected by the user in the control file (optional) | IO10 | Unformatted |
| VISB.DAT | Relative humidity data required for visibility-related postprocessing (optional) | IO11 | Unformatted |
| DEBUG.DAT | Tables of detailed puff/slug data useful for debugging (optional) | IO30 | Formatted |
| MASSFLX.DAT | Hourly report of mass flux into and out of regions defined by the boundaries in the FLUXBDY.DAT file | IO36 | Formatted |
| MASSBAL.DAT | Hourly report of changes in mass of all species modeled | IO37 | Formatted |

---

\*      Variable shown is the parameter controlling the FORTRAN unit number associated with the file. Usually, the value assigned to the parameter is consistent with the name (i.e., IO8 = 8). However, the value can be easily changed in the parameter file to accommodate reserved unit numbers on a particular system.

parameter values. For example, the maximum number of horizontal grid cells allowed in the model, MXNX and MXNY, are two of the variables which can be adjusted within the parameter file. However, no change to the parameter file is necessary if a particular application requires a smaller array size than the maximum values specified in the parameter file.

The memory required by CALPUFF will be a strong function of the specified maximum array dimensions in the parameter file. However, as an example, CALPUFF required approximately 300 K bytes of memory for a test run with a 10 x 10 horizontal grid, with 5 vertical layers, and a maximum number of puffs of 100. This type of configuration may be suitable for ISC-mode simulations of a small number of point sources. For more typical studies, memory requirements will typically be at least 32 megabytes, with more required for simulations involving large numbers of sources.

The run time of CALPUFF will vary considerably depending on the model application. Variations of factors of 10-100 are likely depending of the size of the domain, the number of sources, selection of technical options, and meteorological variables such as the mean wind speed. Because each puff is treated independently, any factor which influences the number and residence time of puffs on the computational grid, and the model sampling time step will affect the run time of the model. As an example of the range of runtimes, an annual simulation of CALPUFF in ISC-mode for 2 sources and 64 receptors required less than one minute on a 500 MHz PC. A visibility application involving 218 sources and 425 receptors for an annual period required approximately 9 hours of runtime for CALMET and 95 hours for CALPUFF.

Three additional files may be produced for diagnostic purposes. When CALPUFF is run with the debug switch set to true, much information about specific puffs is written to the list file for specific sampling steps. Summary information for these puffs is also written to the file DEBUG. DAT. Because of the volume of information written to the list file, the debug option is generally used for very short periods. Options to characterize hourly charges in pollutant mass report results to the files MASSFLX.DAT and MASSBAL.DAT. MASSFLX.DAT reports the mass of selected species that cross into and out of regions defined by the user in the file FLUXBDY.DAT. MASSBAL.DAT reports changes in the mass of all modeled species throughout the modeling domain.

**Program Execution**

CALPUFF (Version 4.0 and above) can be executed with the following DOS command line:

CALPUFF filename

where it is assumed that the executable file is called CALPUFF.EXE and the "filename" is the name of the control file and path (up to 70 characters in length) containing the input information defining the run. The default input file name is CALPUFF.INP. The "filename" can be omitted if using the default control file name for a run. The first input group in CALPUFF.INP contains all of the other input and output (I/O) filenames used in the run. Within this group the user can change the name of any of the input and output files from their default names, and change the directory from which the files will be accessed by specifying the file's full pathname.

# 2. TECHNICAL DISCUSSION

2.1     Solution of the Puff Equations

Puff models represent a continuous plume as a number of discrete packets of pollutant material.  Most puff models (e.g., Ludwig et al., 1977; van Egmond and Kesseboom, 1983; Peterson, 1986) evaluate the contribution of a puff to the concentration at a receptor by a "snapshot" approach.  Each puff is "frozen" at particular time intervals (sampling steps).  The concentration due to the "frozen" puff at that time is computed (or sampled).  The puff is then allowed to move, evolving in size, strength, etc., until the next sampling step.  The total concentration at a receptor is the sum of the contributions of all nearby puffs averaged for all sampling steps within the basic time step.  Depending on the model and the application, the sampling step and the time step may both be one hour, indicating only one "snapshot" of the puff is taken each hour.

A traditional drawback of the puff approach has been the need for the release of many puffs to adequately represent a continuous plume close to a source.  Ludwig et al. (1977) have shown that if the distance between puffs exceeds a maximum of about 2 $\sigma_y$, inaccurate results may be obtained (see Figure 2-1).  Better results are obtained if the puff separation is reduced to no more than one $\sigma_y$.  If the puffs do not overlap sufficiently, the concentrations at receptors located in the gap between puffs at the time of the "snapshot" are underestimated, while those at the puff centers are overestimated.

Ludwig et al. (1977) recommend spacing puffs uniformly in space rather than in time with a puff merging/purging scheme to reduce the total number of puffs.  Zannetti (1981) suggests tracking fewer puffs than necessary for adequate sampling, but then saturating the area near a receptor with artificially generated puffs to provide the required puff overlap (see Figure 2-2).  Although both schemes act to reduce the number of puffs carried by the model, the snapshot sampling method still requires that an uneconomically large number of puffs be generated near the source.  For example, at a receptor 100 meters from a source, and assuming PGT dispersion rates, puffs at a density corresponding to a release rate of over 1300 puffs/hour are required to meet the 2 $\sigma_y$ criterion for F stability, 3 m/s wind conditions.  During high wind speed, neutral conditions (10 m/s, D stability), nearly 2200 puffs/hour are needed.  The more stringent one $\sigma_y$ criterion would double the number of puffs required.

Two alternatives to the conventional snapshot sampling function are discussed below.  Both are based on the integrated sampling function in the MESOPUFF II model (Scire et al., 1984a,b), with modifications for near-field applications.  The first sampling scheme employs radially symmetric Gaussian puffs.  The second scheme uses a non-circular puff (a "slug"), elongated in the direction of the wind during release, to eliminate the need for frequent releases of puffs.  CALPUFF allows either of these sampling schemes to be selected, and also allows a hybrid simulation that takes advantage of the strengths of each algorithm (slugs in the near-field transition to puffs in the far-field).
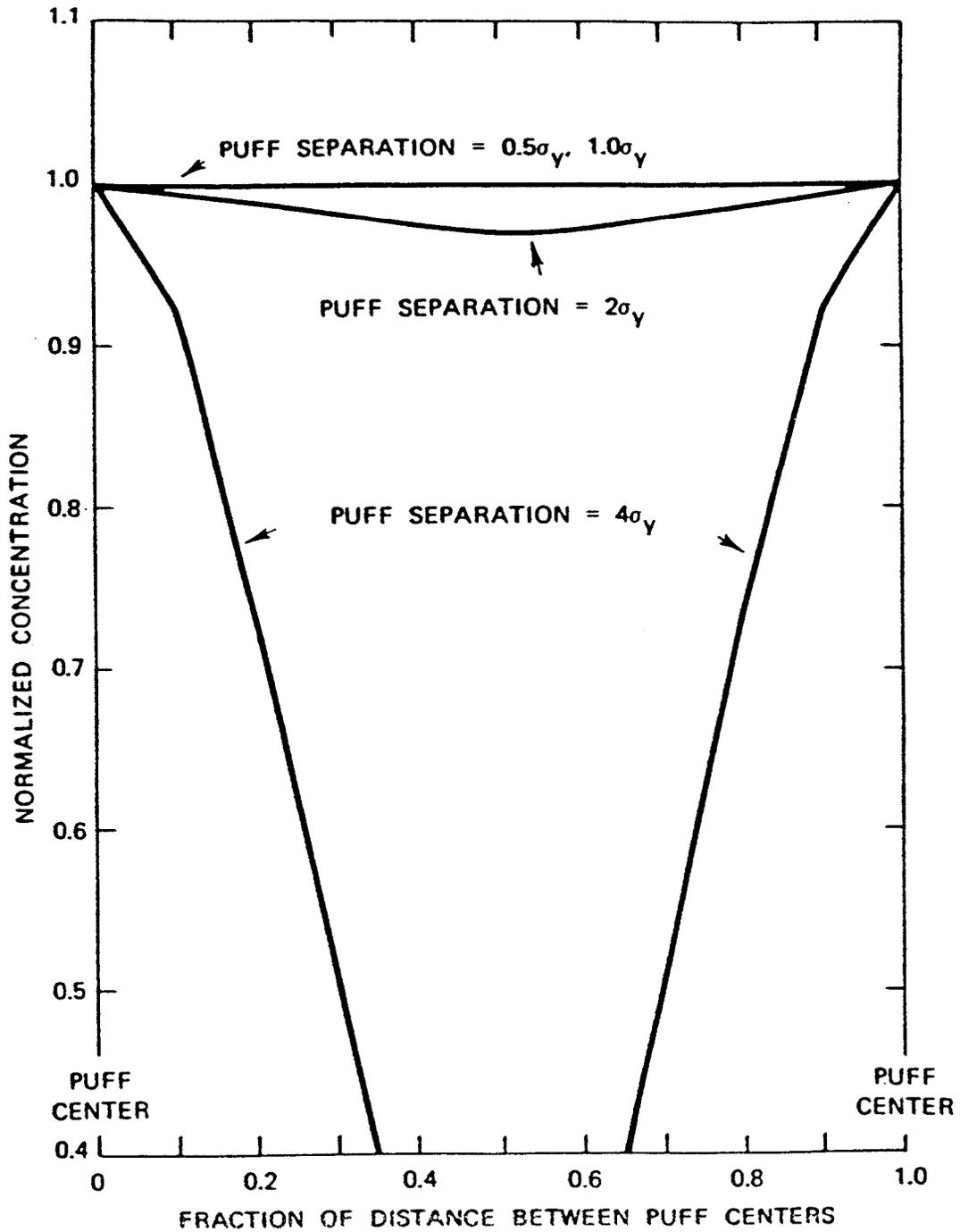
Figure 2-1.    Normalized concentration between two puffs in a string of puffs of equal size and spacing.(From Ludwing et al. (1977).
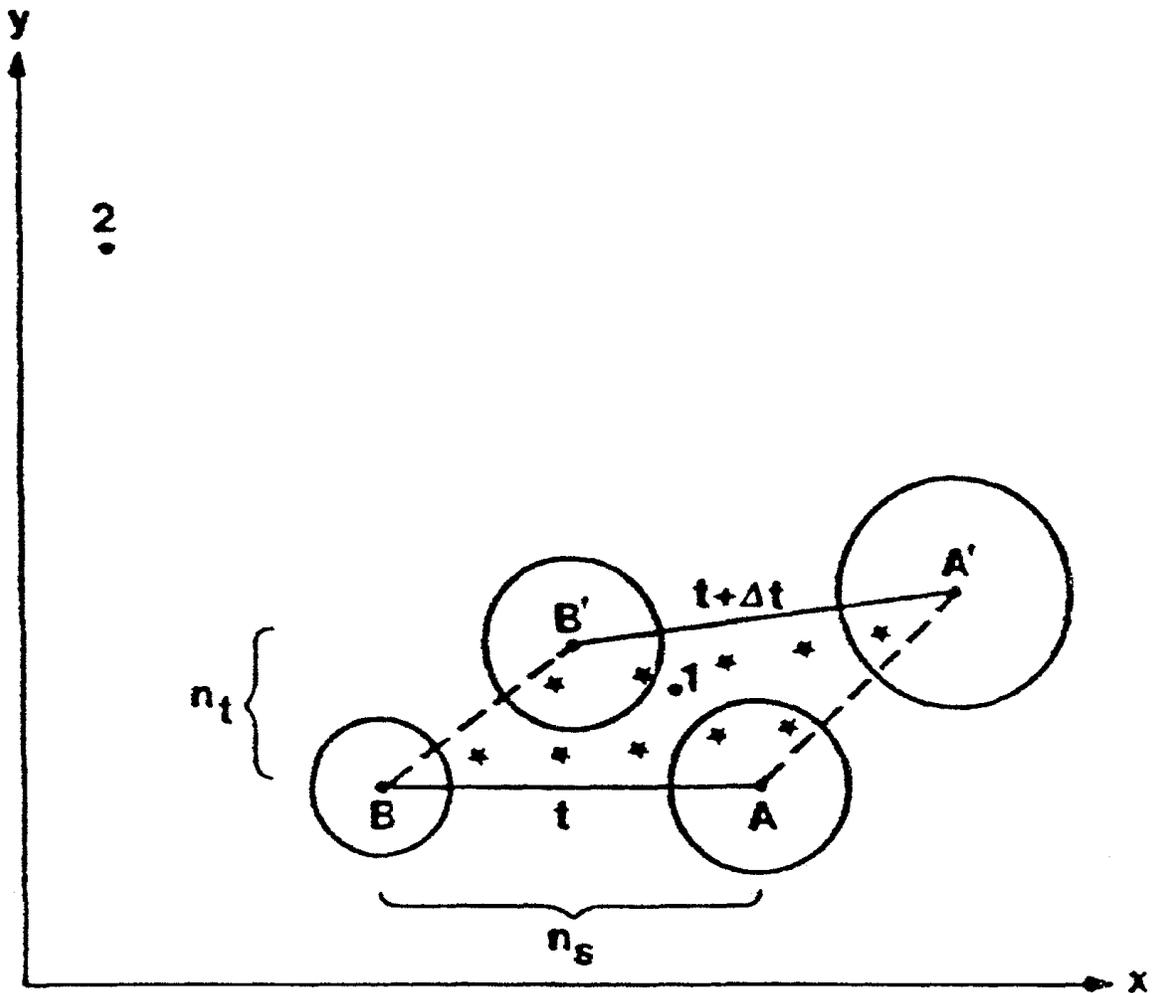
Figure 2-2.　Illustrations of the puff generation scheme of Zannetti (1981).  The advected puffs (A → A$'$, B → B$'$) in the vicinity of Receptor 1 are not sufficient to resolve the plume.  The mass from the original puffs is redistributed into $n_s \times n_s$ new puffs (asterisks) for sampling purposes. [From Zannetti (1981)].

## 2.1.1 Integrated Puff Sampling Function Formulation

The basic equation for the contribution of a puff at a receptor is:

$$C = \frac{Q}{2\pi\sigma_x\sigma_y}\ g\ \exp\left[-d_a^2/\left(2\sigma_x^2\right)\right]\exp\left[-d_c^2/\left(2\sigma_y^2\right)\right]$$ (2-1)

$$g = \frac{2}{(2\pi)^{1/2}\sigma_z}\sum_{n=-\infty}^{\infty}\exp\left[-\left(H_e + 2nh\right)^2/\left(2\sigma_z^2\right)\right]$$ (2-2)

where, C     is the ground-level concentration (g/m$^3$),

       Q     is the pollutant mass (g) in the puff,

       $\sigma_x$     is the standard deviation (m) of the Gaussian distribution in the along-wind direction,

       $\sigma_y$     is the standard deviation (m) of the Gaussian distribution in the cross-wind direction,

       $\sigma_z$     is the standard deviation (m) of the Gaussian distribution in the vertical direction,

       $d_a$     is the distance (m) from the puff center to the receptor in the along-wind direction,

       $d_c$     is the distance (m) from the puff center to the receptor in the cross-wind direction,

       g     is the vertical term (m) of the Gaussian equation,

       H     is the effective height (m) above the ground of the puff center, and

       h     is the mixed-layer height (m).

The summation in the vertical term, g, accounts for multiple reflections off the mixing lid and the ground. It reduces to the uniformly mixed limit of 1/h for $\sigma_z > 1.6\ h$. In general, puffs within the convective boundary layer meet this criterion within a few hours after release.

For a horizontally symmetric puff, with $\sigma_x = \sigma_y$, Eqn. (2-1) reduces to:

$$C(s) = \frac{Q(s)}{2\pi\sigma_y^2(s)}\ g(s)\ \exp\left[-R^2(s)/\left(2\sigma_y^2(s)\right)\right]$$ (2-3)

where, R is the distance (m) from the center of the puff to the receptor, and,

       s is the distance (m) traveled by the puff.

The distance dependence of the variables in Eqn. (2-3) is indicated (e.g., C(s), $\sigma_y$(s), etc.). Integrating Eqn. (2-3) over the distance of puff travel, ds, during the sampling step, dt, yields the time averaged concentration, $\overline{C}$ .

$$\overline{C} = \frac{1}{ds}\int_{s_o}^{s_o+ds} \frac{Q(s)}{2\pi\sigma_y^{\,2}(s)}\, g(s)\, \exp\left[-R^2(s)/2\sigma_y^2(s))\right]ds \tag{2-4}$$

where $s_o$ is the value of s at the beginning of the sampling step.

An analytical solution to this integral can be obtained if it is assumed that the most significant s-dependencies during the sampling step are in the R(s) and Q(s) terms. Figure 2-3 illustrates the movement of a puff from coordinates $(x_1, y_1)$ to $(x_2, y_2)$. Assuming the trajectory segment is a straight line, and transforming s to a dimensionless trajectory variable, p, the radial distance to the receptor at $(x_r, y_r)$ is:

$$R(s) = \left[(x_1 - x_r + p\ dx)^2 + (y_1 - y_r + p\ dy)^2\right]^{1/2} \tag{2-5}$$

where,  p       is zero at the beginning of the trajectory segment (i.e., at $(x_1, y_1)$),
        p       is one at the end of the trajectory segment (i.e., at $(x_2, y_2)$), and
        dx, dy   are the incremental X and Y distances traveled by the puff (i.e., $dx = x_2 - x_1$,
        and $dy = y_2 - y_1$).

The exponential variation of Q due to removal and chemical transformation processes is expressed as a linear function of the sampling interval:

$$Q(s) = Q(s_o) + p\left[Q(s_o + ds) - Q(s_o)\right] \tag{2-6}$$

Using Eqn. (2-6), and transforming to p coordinates, Eqn. (2-4) becomes:

$$
\begin{aligned}
C = \frac{g}{2\pi\ \sigma_y^2} &\left\{ Q(s_o)\int_0^1 \exp\left[-R^2(p)/(2\sigma_y^2)\right] dp\ + \right.\\
&\left. \left[Q(s_o + ds) - Q(s_o)\right]\int_0^1 p\ \exp\left[-R^2(p)/(2\sigma_y^2)\right] dp \right\}
\end{aligned}
\tag{2-7}
$$

The solution of the integrals in Eqn. (2-7) is expressed in terms of error functions and exponentials:

$$\overline{C} = \frac{g}{2\pi\sigma_y^2}\left\{ Q(s_o)\ I_1 + \left[Q(s_o + ds) - Q(s_o)\right] I_2 \right\} \tag{2-8}$$

$$I_1 = \left[\frac{\pi}{2a}\right]^{1/2} \exp\left[\frac{b^2}{2a} - \frac{c}{2}\right]\left\{ erf\left[\frac{a+b}{(2a)^{1/2}}\right] - erf\left[\frac{b}{(2a)^{1/2}}\right]\right\} \tag{2-9}$$
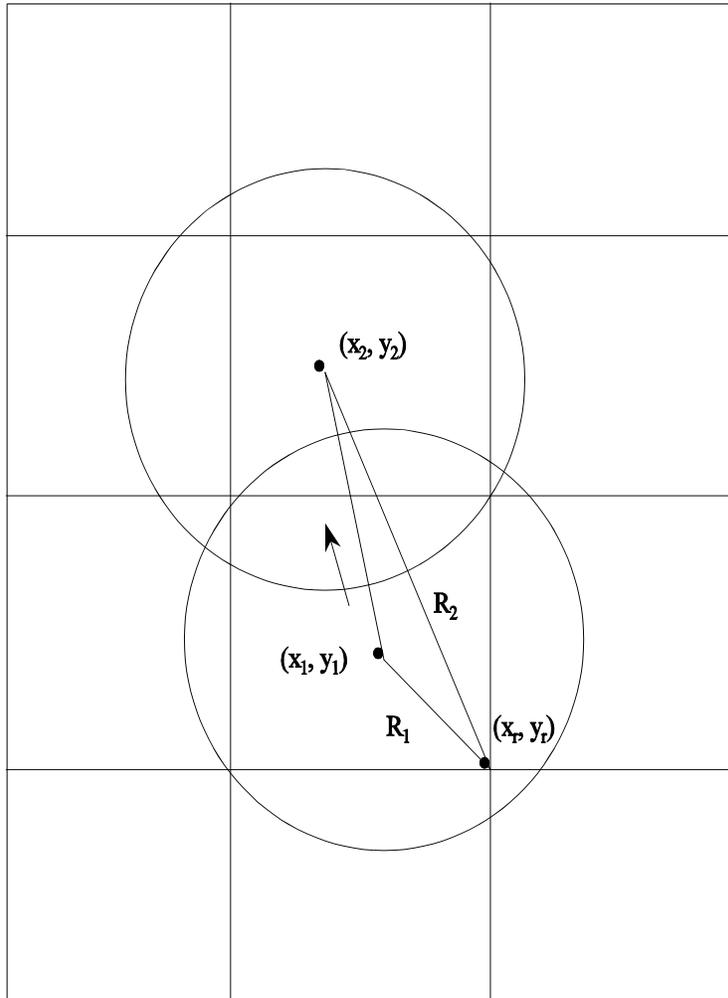
Figure 2-3.    Illustration of the puff movement during the sampling step and the associated changes in the puff receptor distance.

$$I_2 = \frac{-b\,I_1}{a} + \frac{1}{a}\,\exp\left[\frac{b^2}{2a} - \frac{c}{2}\right]\left\{\exp\left[\frac{-b^2}{2a}\right] - \exp\left[\frac{-1}{2}\left(a + 2b + \frac{b^2}{a}\right)\right]\right\} \tag{2-10}$$

$$a = \left(dx^2 + dy^2\right)/\sigma_y^2 \tag{2-11}$$

$$b = \left[dx\left(x_1 - x_r\right) + dy\left(y_1 - y_r\right)\right]/\sigma_y^2 \tag{2-12}$$

$$c = \left[\left(x_1 - x_r\right)^2 + \left(y_1 - y_r\right)^2\right]/\sigma_y^2 \tag{2-13}$$

The horizontal dispersion coefficient, $\sigma_y$, and the vertical term, g, are evaluated and held constant throughout the trajectory segment. In MESOPUFF II, $\sigma_y$ and g are computed at the mid-point of the trajectory segment (p = 0.5). At mesoscale distances, the fractional change in the puff size during the sampling step is usually small, and the use of the mid-point values of $\sigma_y$ and g is adequate. This assumption reduces the number of times that the dispersion coefficients and vertical reflection terms need be computed to one per sampling step (independent of the number of receptors). This optimization for mesoscale distances, however, may not be appropriate in the near-field, where the fractional puff growth rate can be rapid and plume height may vary. For this reason, the integrated sampling function has been implemented with receptor-specific values of $\sigma_y$ and g, evaluated at the point of closest approach of the puff to each receptor.

2.1.2    Slug Formulation and Sampling Functions

In the slug model, the "puffs" consist of Gaussian packets of pollutant material stretched in the along-wind direction. A slug can be visualized as a group of overlapping circular puffs having very small puff separation distances. In fact, the slug represents the continuous emission of puffs, each containing the infinitesimal mass q dt. The length of the main body of the slug is u $\Delta t_e$, where u is the wind speed and $\Delta t_e$ is the time of emission of the pollutant. The concentration due to the presence of a slug can be described as:

$$C(t) = \frac{Fq}{(2\pi)^{1/2}\,u'\sigma_y}\,g\,\exp\left[\frac{-d_c^2}{2\sigma_y^2}\,\frac{u^2}{u'^2}\right] \tag{2-14}$$

$$F = \frac{1}{2}\left\{erf\left[\frac{d_{a2}}{\sqrt{2}\,\sigma_{y2}}\right] - erf\left[\frac{-d_{a1}}{\sqrt{2}\,\sigma_{y1}}\right]\right\} \tag{2-15}$$

where, $u$      is the vector mean wind speed (m/s),

$u'$      is the scalar wind speed (defined as $u' = (u^2 + \sigma_v^2)^{1/2}$ with $\sigma_v$ = wind speed variance),

$q$      is the source emission rate (g/s),

$F$      is a "causality" function, and

$g$      is the vertical coupling factor of Eqn. 2-2.

The quantities $d_c$ and $d_a$ are cross-slug (i.e., perpendicular to the slug axis) and along-slug distances, respectively, to the receptor. In particular, $d_{a2}$ is the distance from slug end 2 (with $d_{a2} > 0$ in the direction of end 1), whereas the distance from slug end 1 is defined as $-d_{a1} \equiv d_{a2} - \ell_{xy}$, with $\ell_{xy}$ being the length of the slug projection in the x-y plane. The subscripts 1 and 2 on the dispersion coefficients refer to values at the oldest and youngest ends of the slug, respectively. The absence of a numerical subscript indicates a value defined at the receptor.

This "slug" formulation retains many of the important properties of the circular puff model, while significantly reducing puff overlap problems associated with snapshot sampling of circular puffs. The concentration distribution within the body of the slug, away from the slug endpoints, approaches that of the Gaussian plume result under the appropriate steady-state conditions. The concentrations near the endpoints of the slug (both inside and outside of the body of the slug) fall off in such a way that if adjacent slugs are present, the plume predictions will be reproduced when the contributions of those slugs are included (again, during steady-state conditions). Eqn. (2-14) can be explicitly shown to conserve mass. As with circular puffs, each slug is free to evolve independently in response to the local effects of dispersion, chemical transformation, removal, etc.

The "causality" function, $F$, accounts for edge effects near the endpoints of the slug. For long emission times such that $u \, \Delta t_e \gg \sigma_x$, and points well inside the body of the slug, evaluation of the error functions in Eqn. (2-15) produces $F = 0.5(1 - (-1)) = 1$ (i.e., no edge effects). For receptors well outside the slug, $F$ becomes zero, indicating that the pollutant material has not yet reached the receptor or has already passed it by. Near the endpoints, the causality factor produces a leading/trailing Gaussian tail on the distribution.

The factor $(u/u')$ allows low wind speed and calm conditions to be properly treated. As $u$ approaches zero, the exponential crosswind term becomes unity and $F$ approaches $-\mathrm{erf}\{d_a/[(\sqrt{2}\,\sigma_y]\}$. Under these conditions, the radial concentration dependence of the distribution is determined by the causality factor. For $u$ greater than a few meters per second, $(u/u')$ is very close to one, so that this ratio becomes unimportant. The factors $(u/u')$ and $F$ make the slug model more "puff-like" than segmented plume models (e.g., Hales et al., 1977; Benkley and Bass, 1979). Unlike the slug model, segmented plume models generally do not properly treat low wind speed conditions or segment edge effects.

Eqn. (2-14) represents a "snapshot" description of the elongated puff at time t. Figure 2-4 displays the concentration isopleths of two such slug snapshots. As with the "snapshot" puff equation, Eqn. (2-14) must be integrated during the sampling step to produce a time-averaged concentration. In the case where the emission rate and meteorological conditions do not vary during the sampling step, a generalized analytical solution to the integral can be obtained for "emitting" slugs (i.e., the endpoint of the "youngest" end of the slug is at the source):

$$\overline{C} = \frac{\overline{F}q}{\sqrt{2\pi}u'\sigma_y} \ g \ \exp\left[\frac{-d^2}{2\sigma_y^2}\frac{u^2}{u'^2}\right] \tag{2-16}$$

$$\overline{F} = \frac{1}{2} \ erf\left(\phi_2\right) + \frac{1}{2} \ \frac{\sqrt{2}\ \sigma_y}{u\Delta t_s}\left\{\left[\ \xi_e \ erf\left(\xi_e\right) - \xi_b \ erf\left(\xi_b\right)\right] + \frac{1}{2} \ \left[\exp\left(\xi_e^2\right) - \exp\left(\xi_b^2\right)\right]\right\} \tag{2-17}$$

where
$$\xi_e = \frac{d_{a2} - u\Delta t_s}{\sqrt{2}\sigma_y} \tag{2-18}$$

represents the situation at the <u>end</u> of the time step $\Delta t_s$.

$$\xi_b = \frac{d_{a2}}{\sqrt{2}\sigma_y} \tag{2-19}$$

represents the situation at the <u>beginning</u> of the time step,

$$\phi_2 = \frac{d_{a2}}{\sqrt{2}\sigma_{y2}} \tag{2-20}$$

represents the steady state conditions at the source, and where $\Delta t_s$ is the duration of the sampling step.

For Eqn. (2-16) to apply, the sampling interval must correspond to the emission interval, as is normally the case for fresh emissions. The value of $\sigma_{y2}$ used is the initial lateral spread (if any) of the emissions at the source. For older slugs, the endpoint of the slug is no longer fixed at the source and the long axis of the slug is not likely to be along the advecting wind direction. An analytical integration of Eqn. (2-14) is not possible for these slugs unless restrictive conditions are imposed on the form of the puff growth equations. Because of the importance of generality in the puff growth equations, the time-averaged concentrations of older/ slugs are determined by numerical integration of Eqn. (2-14). This integration
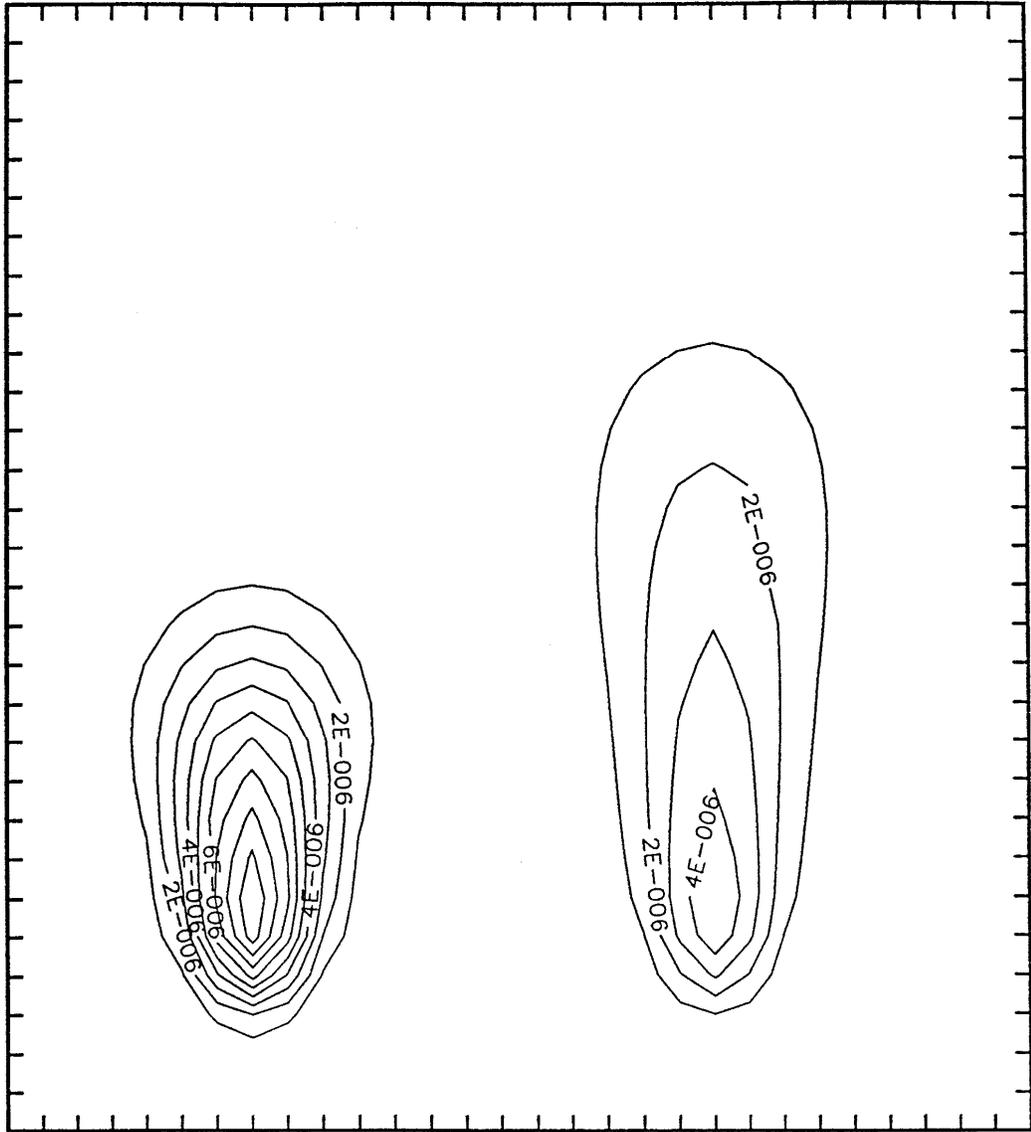
Figure 2-4.    Isopleths of two slug "snapshots." The slug snapshot at left represents the slug at the beginning of a time step whereas the snapshot at right shows the instantaneous distribution at the end of the time step. During the time step, the slug experienced advection (to the right), diffusion, and some along-slug stretching due to wind shear.

Figure 2-5.    Receptor-time averaged concentrations resulting from the transport and evolution of the slug depicted in Figure 2-4 from its initial (left "snapshot") to final (right "snapshot") state.  The tickmarks on the border suggest the 2-d mesh of receptors considered.

can be accomplished at reasonable computation cost.  Figure 2-5 shows the result of such integral averaging for the situation where the Figure 2-4 "snapshots" depict the start and end slug states of the averaging period.

The above development also ignores the effect of loss or production mechanisms; however, this can be handled in much the same "linearized" manner that MESOPUFF II invokes.  This is accomplished by allowing the effective emission rate, q, to vary linearly over time as:

$$q(t) = q_b + (q_e - q_b) \cdot (t / \Delta t_s) \qquad (2\text{-}21)$$

where,  $q_b$   is the effective emission rate for the slug at the beginning of the time step (n.b., $q_b = q$ for fresh emissions),

$q_e$   is the effective emission rate including loss or production which occurs during the time step,

and

$\Delta t_s$   is the duration of the time step.

The variable $\xi$ is also the function

$$\xi = \frac{d_{a2} - u\Delta t_s \cdot (t / \Delta t_s)}{\sqrt{2}\sigma_y} \qquad (2\text{-}22)$$

of the dimensionless time variable $t/\Delta t_s$, where $0 \le t/\Delta t_s \le 1$, such that

$$\xi = \xi_b + (\xi_e - \xi_b) \cdot (t / \Delta t_s) \qquad (2\text{-}23)$$

and the causality function becomes

$$F(\xi) = \frac{1}{2} \left\{ erf(\varphi_2) - erf(\xi) \right\} \qquad (2\text{-}24)$$

Thus, the time averaging process yields

$$\overline{C} = \frac{g}{\sqrt{2\pi}u'\sigma_y} \left\{ \exp\left[ \frac{-d_c^2}{2\sigma_y^2} \frac{u^2}{u'^2} \right] \right\} \left\{ q_b F_o + (q_e - q_b) F_1 \right\} \qquad (2\text{-}25)$$

where $F_o$ is just $\overline{F}$ from Eqn. (2-17) and

$$F_1 = \int_0^{\Delta t_s} \frac{dt}{\Delta t_s} (t / \Delta t_s) F(t) = \frac{1}{\Delta\xi} \int_{\xi_b}^{\xi_e} d\xi \frac{\xi - \xi_b}{\Delta\xi} F(\xi) \qquad (2\text{-}26)$$

with $\Delta\xi \equiv \xi_e - \xi_b = \dfrac{-u\Delta t_s}{\sqrt{2}\sigma_y}$

Substituting in Eqn. (2-24) then yields

$$F_1 = \frac{1}{4} erf(\varphi_2) - \frac{1/2}{(\Delta\xi)^2}\left\{\int_\xi^{\xi_e} d\xi\, \xi\, erf(\xi) - \xi_b \int_\xi^{\xi_e} d\xi\, erf(\xi)\right\} \qquad (2\text{-}27)$$

where $\displaystyle\int dx\, erf(x) = x\, erf(x) + \frac{1}{\sqrt{\pi}} \exp(-x^2)$ $\qquad\qquad\qquad\qquad\qquad$ (2-28)

has already been used to obtain Eqn. (2-17) and where

$$\int dx\, x\, erf(x) = \frac{1}{2}x^2\, erf(x) + \frac{1}{2}\frac{x}{\sqrt{\pi}}\exp(-x^2) - \frac{1}{4} erf(x) \qquad (2\text{-}29)$$

is a special case of the more general expression developed by Geller and Ng (1971) in terms of the generalized hypergeometric function $_2F_2$.

Generalizing the problem of dealing with older slugs is trivial if one deals with a numerical integration (i.e., time average) of Eqn. (2-14). The time dependent expression q(t) given by Eqn. (2-21) simply replaces q and the numerical integration proceeds.

This numerical integration process has itself received special attention because it greatly influences the computing time needs of the slug model. First, all receptors lying outside of the slug's $\pm 3\sigma_y$ envelope during the entire averaging time interval are eliminated from consideration. Second, for those receptors remaining, integration time limits are computed such that sampling is not performed when the receptor is outside of the $\pm 3\sigma_y$ envelope.

Invocation of the "frozen $\sigma$" methodology (i.e., $\sigma_y$ and $\sigma_z$ are fixed at receptor-specific values throughout the averaging time period) creates another class of situations which can be integrated analytically; however, the most general case involves indefinite integrals of the form

$$\int dt\, \exp(-\beta^2 t^2) erf(a + bt), \qquad\qquad\qquad (2\text{-}30)$$

which defy solution except in a few simple cases (e.g., $a = 0$ and $b = \beta$). In fact, integrability has proven not to be the sole criteria in these slug sampling problems. For example, the preceding work on linear time variation of loss (or production) mechanisms can also be evaluated for the more realistic exponential process; however, the analytic forms are found to be very volatile on a computer because subtraction of large numbers to obtain small numbers is required.

One tractable case involves the quite physical scenario of a slug passing rapidly over a receptor and with slug endpoints sufficiently far away that the along-slug causality factor, F(t), is time independent. In this case the causality factor also becomes fixed and can be taken outside the integral and approximated as

$$\overline{F} = \frac{1}{2} \left( F_b + F_e \right) , \tag{2-31}$$

which is just the average of values at the beginning and end of the time step. This approximation is, however, made only if $F_b$ and $F_e$ are within a specified fractional tolerance of each other. A similar procedure enables one to move the vertical coupling factor, g, outside the integral and replace it with the mean value $\overline{g}$. The tolerance factor for both causality and vertical coupling coefficient variation is currently set at a conservative 0.02 (i.e., 2%).

Finally the variability of the lateral coupling term,

$$Y(t) = \exp \left( -\eta (t)^2 \right) , \tag{2-32}$$

where $\eta(t) = \dfrac{d_c(t)}{\sqrt{2}\sigma_y} \cdot \dfrac{u}{u'}$ and $d_c(t)$ is the time dependent crosswind distance, is checked and the

integrals

$$I_m = \int_0^{\Delta t_s} \frac{dt}{\Delta t_s} \left( t/\Delta t_s \right)^m Y(t) \tag{2-33}$$

evaluated for m = 0 and 1. These integrals can be solved to yield

$$I_0 = \frac{\sqrt{\pi}}{2} \left[ erf \left( \eta_e \right) - erf \left( \eta_b \right) \right] / \left( \eta_e - \eta_b \right) \tag{2-34}$$

and

$$I_1 = \frac{1}{2} \left[ \exp \left( -\eta_b^2 \right) - \exp \left( -\eta_e^2 \right) \right] / \left( \eta_e - \eta_b \right)^2 \\ - \eta_b I_0 / \left( \eta_e - \eta_b \right) \tag{2-35}$$

so that the final time-averaged concentrations can be written as

$$\overline{C} = \frac{\overline{g} \, \overline{F}}{\sqrt{2\pi}u'\sigma_y} \left\{ q_b I_0 + \left( q_e - q_b \right) I_1 \right\} \tag{2-36}$$

as an alternative to numerical integration for the older slugs.

Computations are also performed for the vertically integrated counterparts to Eqns. (2-25 and 2-36) as these are required for evaluation of wet removal and wet fluxes at a ground level receptor; however, Gaussian normalization dictates that this is accomplished simply by replacing g with 1.0 in Eqn. (2-25) or with 1.0 in Eqn. (2-36).

2.1.3    Sampling Function Testing

The slug model and two versions of the integrated (circular) puff model have been subjected to several sensitivity tests in order to:

· 	evaluate the performance of each formulation in reproducing the known steady-state plume solution under the appropriate emission and meteorological conditions;

· 	demonstrate and intercompare the models' capabilities under non-steady conditions;

· 	assess the cost-effectiveness of the different algorithms;

· 	demonstrate the consistency of the circular puff/elongated slug models.

The two versions of the circular puff model differ in that one uses local puff-specific properties (height, sigmas are evaluated at the mid-point of a step) for each sampling step, and the other uses receptor-specific properties (this is the one employed in CALPUFF). In the discussion below, we denote the first model as the "local" puff model, and the second is identified as the CALPUFF integrated puff model.

Tables 2-1 and 2-2 present the plume, puff, and slug results for two sets of steady-state emission and meteorological conditions. Plume centerline values are presented at receptors from 100 m to 10 km from the source. A constant emission rate of 1 g/s from a 10 m high source is assumed. The first set of results assume neutral (D class) stability conditions with 10 m/s winds. Stable (F class) conditions with 3 m/s winds are applied in the second set of runs. The local puff model results reported in Tables 2-1 (a) and 2-2 (a) are obtained for puff release rates and sampling rates that varied from 100/hr to 500/hr. Results for the CALPUFF integrated puff model reported in Tables 2-1 (b) and 2-2 (b) are obtained for a puff release rate and sampling rate of 1/hr. Operationally, the slug model would employ the efficient time-integrated relationship (Eqn. 2-16) for the slug originating at the source, but this form is not used here in order to assess the performance of the more general sampling algorithms. The slug model was evaluated by considering the slugs as being "old", and both the numerical integration technique of Eqn. (2-14) and the approximate, factored form of Eqn. (2-36) were considered. Both of these "old" slug methods gave predictions identical to the plume model for the four significant digits displayed. (It should be noted that numerical integration was not necessary in this special case of steady-state conditions, but was performed anyway to demonstrate the more general technique and allow its evaluation in terms of its consistency with the plume solution and its cost effectiveness.)

Table 2-1 (a)

Comparison of Plume, Puff, and Slug Models for Steady-State Conditions

(Wind Speed: 10 m/s, Stability Class: D, Stack Height: 10 m,
Unlimited Mixing Height, Emission Rate: 1 g/s)

| Distance (m) | Plume Model $(g/m^3)$ | Local Puff Model | | |
| --- | --- | --- | --- | --- |
| | | 100 puffs/hr 100 samp./hr | 300 puffs/hr 300 samp./hr | 500 puffs/hr 500 samp./hr |
| 100 | $8.273 \times 10^{-5}$ | $1.266 \times 10^{-4}$ | $1.749 \times 10^{-4}$ | $9.618 \times 10^{-5}$ |
| 200 | $1.204 \times 10^{-4}$ | $1.266 \times 10^{-4}$ | $1.295 \times 10^{-4}$ | $1.306 \times 10^{-4}$ |
| 300 | $8.270 \times 10^{-5}$ | $1.288 \times 10^{-4}$ | $8.341 \times 10^{-5}$ | $7.929 \times 10^{-5}$ |
| 400 | $5.711 \times 10^{-5}$ | $3.164 \times 10^{-5}$ | $5.183 \times 10^{-5}$ | $5.682 \times 10^{-5}$ |
| 500 | $4.145 \times 10^{-5}$ | $3.693 \times 10^{-5}$ | $3.976 \times 10^{-5}$ | $4.176 \times 10^{-5}$ |
| 600 | $3.144 \times 10^{-5}$ | $3.733 \times 10^{-5}$ | $3.212 \times 10^{-5}$ | $3.145 \times 10^{-5}$ |
| 700 | $2.469 \times 10^{-5}$ | $3.189 \times 10^{-5}$ | $2.529 \times 10^{-5}$ | $2.467 \times 10^{-5}$ |
| 800 | $1.995 \times 10^{-5}$ | $1.559 \times 10^{-5}$ | $2.002 \times 10^{-5}$ | $1.995 \times 10^{-5}$ |
| 900 | $1.648 \times 10^{-5}$ | $1.658 \times 10^{-5}$ | $1.644 \times 10^{-5}$ | $1.648 \times 10^{-5}$ |
| 1000 | $1.387 \times 10^{-5}$ | $1.654 \times 10^{-5}$ | $1.394 \times 10^{-5}$ | $1.393 \times 10^{-5}$ |
| 2000 | $4.863 \times 10^{-6}$ | $4.871 \times 10^{-6}$ | $4.853 \times 10^{-6}$ | $4.856 \times 10^{-6}$ |
| 3000 | $2.616 \times 10^{-6}$ | $2.613 \times 10^{-6}$ | $2.614 \times 10^{-6}$ | $2.612 \times 10^{-6}$ |
| 4000 | $1.702 \times 10^{-6}$ | $1.704 \times 10^{-6}$ | $1.699 \times 10^{-6}$ | $1.698 \times 10^{-6}$ |
| 5000 | $1.219 \times 10^{-6}$ | $1.219 \times 10^{-6}$ | $1.217 \times 10^{-6}$ | $1.217 \times 10^{-6}$ |
| 6000 | $9.284 \times 10^{-7}$ | $9.280 \times 10^{-7}$ | $9.270 \times 10^{-7}$ | $9.268 \times 10^{-7}$ |
| 7000 | $7.374 \times 10^{-7}$ | $7.372 \times 10^{-7}$ | $7.364 \times 10^{-7}$ | $7.359 \times 10^{-7}$ |
| 8000 | $6.040 \times 10^{-7}$ | $6.029 \times 10^{-7}$ | $6.023 \times 10^{-7}$ | $6.022 \times 10^{-7}$ |
| 9000 | $5.066 \times 10^{-7}$ | $5.060 \times 10^{-7}$ | $5.055 \times 10^{-7}$ | $5.053 \times 10^{-7}$ |
| 10000 | $4.329 \times 10^{-7}$ | $4.326 \times 10^{-7}$ | $4.324 \times 10^{-7}$ | $4.321 \times 10^{-7}$ |
| Relative CPU time | 1.0 | 249.4 | 2054.3 | 5592.4 |

Table 2-1 (b)

Comparison of Plume, Puff, and Slug Models for Steady-State Conditions

(Wind Speed: 10 m/s, Stability Class: D, Stack Height: 10 m,
Unlimited Mixing Height, Emission Rate: 1 g/s)

| | | — CALPUFF MODULES — | |
| Distance (m) | Plume Model $(g/m^3)$ | Integrated Puff Model* $(g/m^3)$ | Slug Model* $(g/m^3)$ |
|---|---|---|---|
| 100 | $8.273 \times 10^{-5}$ | $8.273 \times 10^{-5}$ | $8.273 \times 10^{-5}$ |
| 200 | $1.204 \times 10^{-4}$ | $1.204 \times 10^{-4}$ | $1.204 \times 10^{-4}$ |
| 300 | $8.270 \times 10^{-5}$ | $8.270 \times 10^{-5}$ | $8.270 \times 10^{-5}$ |
| 400 | $5.711 \times 10^{-5}$ | $5.711 \times 10^{-5}$ | $5.711 \times 10^{-5}$ |
| 500 | $4.145 \times 10^{-5}$ | $4.145 \times 10^{-5}$ | $4.145 \times 10^{-5}$ |
| 600 | $3.144 \times 10^{-5}$ | $3.144 \times 10^{-5}$ | $3.144 \times 10^{-5}$ |
| 700 | $2.469 \times 10^{-5}$ | $2.469 \times 10^{-5}$ | $2.469 \times 10^{-5}$ |
| 800 | $1.995 \times 10^{-5}$ | $1.995 \times 10^{-5}$ | $1.995 \times 10^{-5}$ |
| 900 | $1.648 \times 10^{-5}$ | $1.648 \times 10^{-5}$ | $1.648 \times 10^{-5}$ |
| 1000 | $1.387 \times 10^{-5}$ | $1.387 \times 10^{-5}$ | $1.387 \times 10^{-5}$ |
| 2000 | $4.863 \times 10^{-6}$ | $4.863 \times 10^{-6}$ | $4.863 \times 10^{-6}$ |
| 3000 | $2.616 \times 10^{-6}$ | $2.616 \times 10^{-6}$ | $2.616 \times 10^{-6}$ |
| 4000 | $1.702 \times 10^{-6}$ | $1.702 \times 10^{-6}$ | $1.702 \times 10^{-6}$ |
| 5000 | $1.219 \times 10^{-6}$ | $1.219 \times 10^{-6}$ | $1.219 \times 10^{-6}$ |
| 6000 | $9.284 \times 10^{-7}$ | $9.284 \times 10^{-7}$ | $9.284 \times 10^{-7}$ |
| 7000 | $7.374 \times 10^{-7}$ | $7.374 \times 10^{-7}$ | $7.374 \times 10^{-7}$ |
| 8000 | $6.040 \times 10^{-7}$ | $6.040 \times 10^{-7}$ | $6.040 \times 10^{-7}$ |
| 9000 | $5.066 \times 10^{-7}$ | $5.066 \times 10^{-7}$ | $5.066 \times 10^{-7}$ |
| 0000 | $4.329 \times 10^{-7}$ | $4.329 \times 10^{-7}$ | $4.329 \times 10^{-7}$ |
| Relative CPU time | 1.0 | 1.8 | 1.2-5.7 |

* Same as plume model to four places of accuracy.

Table 2-2 (a)

Comparison of Plume, Puff, and Slug Models for Steady-State Conditions

(Wind Speed:  5 m/s, Stability Class:  F, Stack Height:  10 m,
Unlimited Mixing Height, Emission Rate:  1 g/s)

| Distance (m) | Plume Model $(g/m^3)$ | ——— Local Puff Model ——— | | |
|---|---|---|---|---|
| | | 100 puffs/hr 100 samp./hr | 300 puffs/hr 300 samp./hr | 500 puffs/hr 500 samp./hr |
| 100 | $6.495 \times 10^{-7}$ | $1.379 \times 10^{-7}$ | $1.379 \times 10^{-7}$ | $5.814 \times 10^{-5}$ |
| 200 | $1.017 \times 10^{-4}$ | $1.823 \times 10^{-4}$ | $1.159 \times 10^{-4}$ | $1.018 \times 10^{-4}$ |
| 300 | $2.075 \times 10^{-4}$ | $1.869 \times 10^{-4}$ | $2.033 \times 10^{-4}$ | $2.046 \times 10^{-4}$ |
| 400 | $2.255 \times 10^{-4}$ | $2.171 \times 10^{-4}$ | $2.313 \times 10^{-4}$ | $2.242 \times 10^{-4}$ |
| 500 | $2.076 \times 10^{-4}$ | $2.234 \times 10^{-4}$ | $2.027 \times 10^{-4}$ | $2.078 \times 10^{-4}$ |
| 600 | $1.816 \times 10^{-4}$ | $1.733 \times 10^{-4}$ | $1.818 \times 10^{-4}$ | $1.813 \times 10^{-4}$ |
| 700 | $1.567 \times 10^{-4}$ | $1.736 \times 10^{-4}$ | $1.575 \times 10^{-4}$ | $1.566 \times 10^{-4}$ |
| 800 | $1.357 \times 10^{-4}$ | $1.337 \times 10^{-4}$ | $1.351 \times 10^{-4}$ | $1.355 \times 10^{-4}$ |
| 900 | $1.184 \times 10^{-4}$ | $1.197 \times 10^{-4}$ | $1.185 \times 10^{-4}$ | $1.183 \times 10^{-4}$ |
| 1000 | $1.042 \times 10^{-4}$ | $1.062 \times 10^{-4}$ | $1.041 \times 10^{-4}$ | $1.040 \times 10^{-4}$ |
| 2000 | $4.154 \times 10^{-5}$ | $4.135 \times 10^{-5}$ | $4.153 \times 10^{-5}$ | $4.154 \times 10^{-5}$ |
| 3000 | $2.397 \times 10^{-5}$ | $2.401 \times 10^{-5}$ | $2.398 \times 10^{-5}$ | $2.394 \times 10^{-5}$ |
| 4000 | $1.644 \times 10^{-5}$ | $1.644 \times 10^{-5}$ | $1.641 \times 10^{-5}$ | $1.641 \times 10^{-5}$ |
| 5000 | $1.224 \times 10^{-5}$ | $1.224 \times 10^{-6}$ | $1.223 \times 10^{-5}$ | $1.222 \times 10^{-5}$ |
| 6000 | $9.612 \times 10^{-6}$ | $9.609 \times 10^{-6}$ | $9.592 \times 10^{-6}$ | $9.594 \times 10^{-6}$ |
| 7000 | $7.830 \times 10^{-6}$ | $7.832 \times 10^{-6}$ | $7.822 \times 10^{-6}$ | $7.818 \times 10^{-6}$ |
| 8000 | $6.596 \times 10^{-6}$ | $6.584 \times 10^{-6}$ | $6.581 \times 10^{-6}$ | $6.580 \times 10^{-6}$ |
| 9000 | $5.669 \times 10^{-6}$ | $5.661 \times 10^{-6}$ | $5.659 \times 10^{-6}$ | $5.658 \times 10^{-6}$ |
| 10000 | $4.950 \times 10^{-6}$ | $4.945 \times 10^{-6}$ | $4.939 \times 10^{-6}$ | $4.940 \times 10^{-6}$ |
| Relative CPU time | 1.0 | 282 | 2333 | 6409 |

Table 2-2 (b)

Comparison of Plume, Puff, and Slug Models for Steady-State Conditions

(Wind Speed:  5 m/s, Stability Class:  F, Stack Height:  10 m,
Unlimited Mixing Height, Emission Rate:  1 g/s)

| | | —— CALPUFF MODULES —— | |
| Distance (m) | Plume Model $(g/m^3)$ | Puff Model* $(g/m^3)$ | Integrated Slug Model* $(g/m^3)$ |
| --- | --- | --- | --- |
| 100 | $6.495 \times 10^{-7}$ | $6.495 \times 10^{-7}$ | $6.495 \times 10^{-7}$ |
| 200 | $1.017 \times 10^{-4}$ | $1.017 \times 10^{-4}$ | $1.017 \times 10^{-4}$ |
| 300 | $2.075 \times 10^{-4}$ | $2.075 \times 10^{-4}$ | $2.075 \times 10^{-4}$ |
| 400 | $2.255 \times 10^{-4}$ | $2.255 \times 10^{-4}$ | $2.255 \times 10^{-4}$ |
| 500 | $2.076 \times 10^{-4}$ | $2.076 \times 10^{-4}$ | $2.076 \times 10^{-4}$ |
| 600 | $1.816 \times 10^{-4}$ | $1.816 \times 10^{-4}$ | $1.816 \times 10^{-4}$ |
| 700 | $1.567 \times 10^{-4}$ | $1.567 \times 10^{-4}$ | $1.567 \times 10^{-4}$ |
| 800 | $1.357 \times 10^{-4}$ | $1.357 \times 10^{-4}$ | $1.357 \times 10^{-4}$ |
| 900 | $1.184 \times 10^{-4}$ | $1.184 \times 10^{-4}$ | $1.184 \times 10^{-4}$ |
| 1000 | $1.042 \times 10^{-4}$ | $1.042 \times 10^{-4}$ | $1.042 \times 10^{-4}$ |
| 2000 | $4.154 \times 10^{-6}$ | $4.154 \times 10^{-6}$ | $4.154 \times 10^{-6}$ |
| 3000 | $2.397 \times 10^{-6}$ | $2.397 \times 10^{-6}$ | $2.397 \times 10^{-6}$ |
| 4000 | $1.644 \times 10^{-6}$ | $1.644 \times 10^{-6}$ | $1.644 \times 10^{-6}$ |
| 5000 | $1.224 \times 10^{-6}$ | $1.224 \times 10^{-6}$ | $1.224 \times 10^{-6}$ |
| 6000 | $9.612 \times 10^{-6}$ | $9.613 \times 10^{-8}$ | $9.613 \times 10^{-8}$ |
| 7000 | $7.830 \times 10^{-6}$ | $7.830 \times 10^{-6}$ | $7.830 \times 10^{-6}$ |
| 8000 | $6.596 \times 10^{-6}$ | $6.596 \times 10^{-6}$ | $6.596 \times 10^{-6}$ |
| 9000 | $5.669 \times 10^{-6}$ | $5.669 \times 10^{-6}$ | $5.669 \times 10^{-6}$ |
| 10000 | $4.950 \times 10^{-6}$ | $4.950 \times 10^{-6}$ | $4.950 \times 10^{-6}$ |
| Relative CPU time | 1.0 | 1.4 | 1.2-5.2 |

* Same as plume model to four places of accuracy.

The results indicate that a large number of puffs/samples is necessary to adequately reproduce the plume solution at near-field receptors when the local puff model assumption is employed. The errors are associated with the use of the trajectory mid-point values of $\sigma_y$ and g. This model is optimized for source-receptor distances on scales from tens to hundreds of kilometers, and is not cost effective for application close to the source. The CALPUFF integrated puff model, using receptor-specific dispersion coefficients and the integrated sampling function, reproduces the plume solution exactly with a computational cost less than 1% of that required for the local puff model. In fact, its CPU requirements are competitive with those needed to solve the steady-state plume equation. The CPU costs of the slug model are comparable to the plume model when the analytic form is used, but is somewhat more costly than the corresponding integrated puff model when the 40 iteration, numerical solver is selected. Additional test runs of the puff and slug models under a range of different meteorological conditions produced similar results.

The CALPUFF slug and puff models were also used to simulate a case of non-steady emissions. An emission rate of 1 g/s for a duration of one hour was modeled. Although a one-hour release was used in this demonstration run, either formulation is intrinsically capable of handling arbitrary variations in emission rates, including those on time scales of less than one hour. B stability, 1 m/s winds were the assumed meteorological conditions. The results are presented in Figures 2-6 and 2-7 along with the steady-state plume solution. The puff and slug model results intercompare well (within a few percent, except at the tails of the distribution with very low concentration values). The puff/slug predictions approach the steady-state results when the center of the pollutant cloud passes the receptor, but clearly show the causality and edge effects of the approaching/passing distribution. The puff model lumps the pollutant mass into n packets (puffs), each with 1/n of the total emission (n = 100 in this test). The mass actually released from time t = 0 to t = dt/n is packaged into the puff released at t = 0. The puff lumping effect tends to result in a slightly premature arrival/departure of the pollutant, which is not seen in the case of steady emissions. In the non-steady runs, because the correct puff causality is obtained by increasing the puff release rate, the slug model is more computationally efficient.

In order to provide a cost-effective sampling scheme for a range of meteorological, emission, and source-receptor configurations, CALPUFF allows a hybrid circular puff/elongated slug approach. The model stores information on the trailing endpoint of the emission cloud (required for the slug model) in addition to the data describing the leading edge (used in both the puff and slug models), at least initially, when the ratio $\sigma_y/(u \, dt_e)$ is small. This ratio compares the spread of the cloud at each end-point of the slug to the length of the slug. In the far-field, the initial elongation of the slug can become unimportant relative to the growth in the cloud $\sigma_y$ due to diffusion, and puff sampling can then represent the impact of the cloud. For near-field receptors, however, if the emission rate changes rapidly, or if a large wind direction change results in advection of a slug segment at a large angle to its long axis, the slug model provides a more cost effective simulation. The user invokes this hybrid treatment by selecting the slug sampling method, and by specifying the ratio $\sigma_y/(u \, dt_e)$ at which slugs are transformed to puffs.
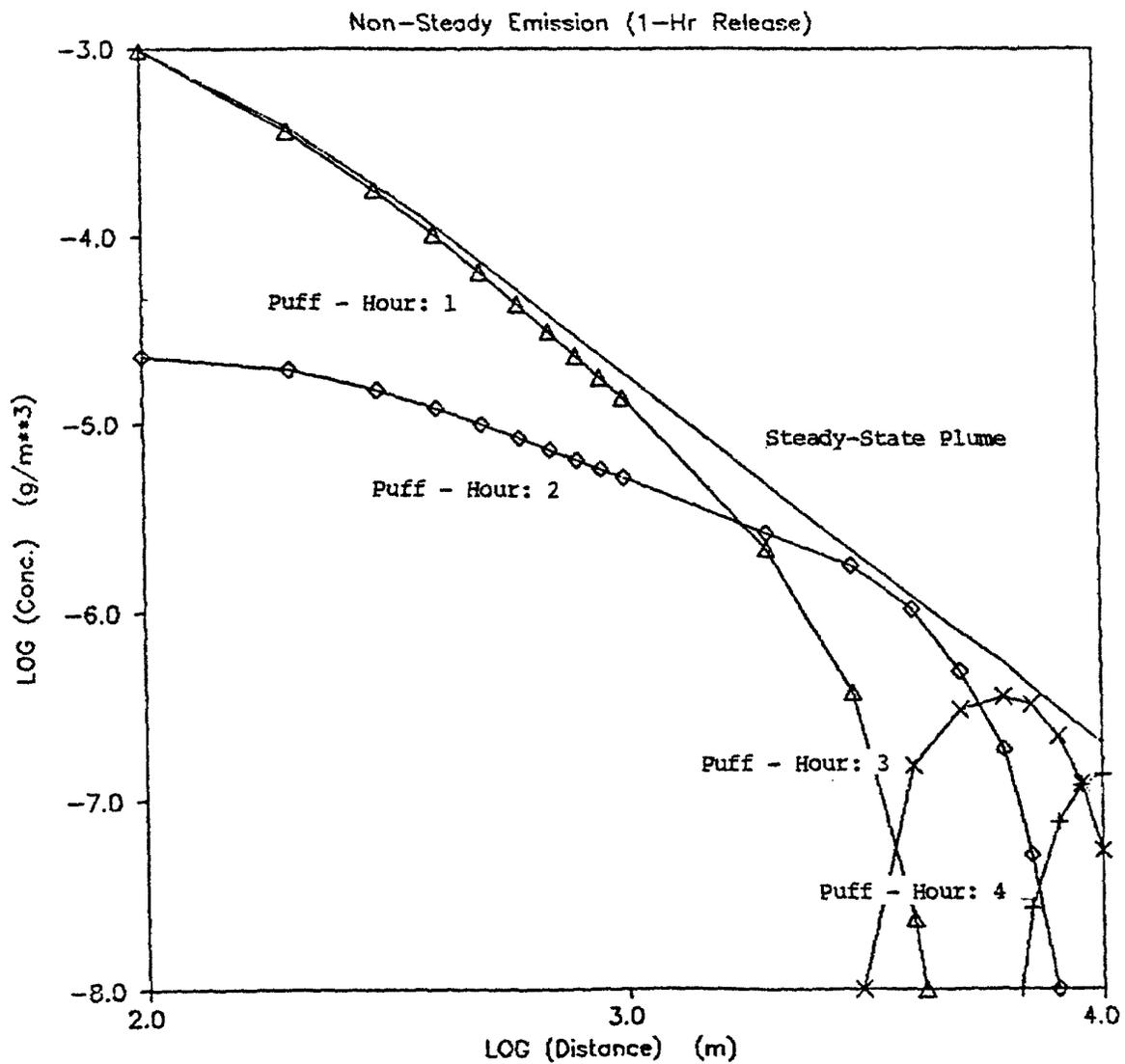
Figure 2-6.    Concentration predictions of puff model with receptor-specific sigmas for non-steady emission conditions. Emission rate: 1 g/s, Emission duration: 1 hour, Wind speed: 1 m/s, Stability class: B, Stack height: 10m, Mixing height: unlimited.
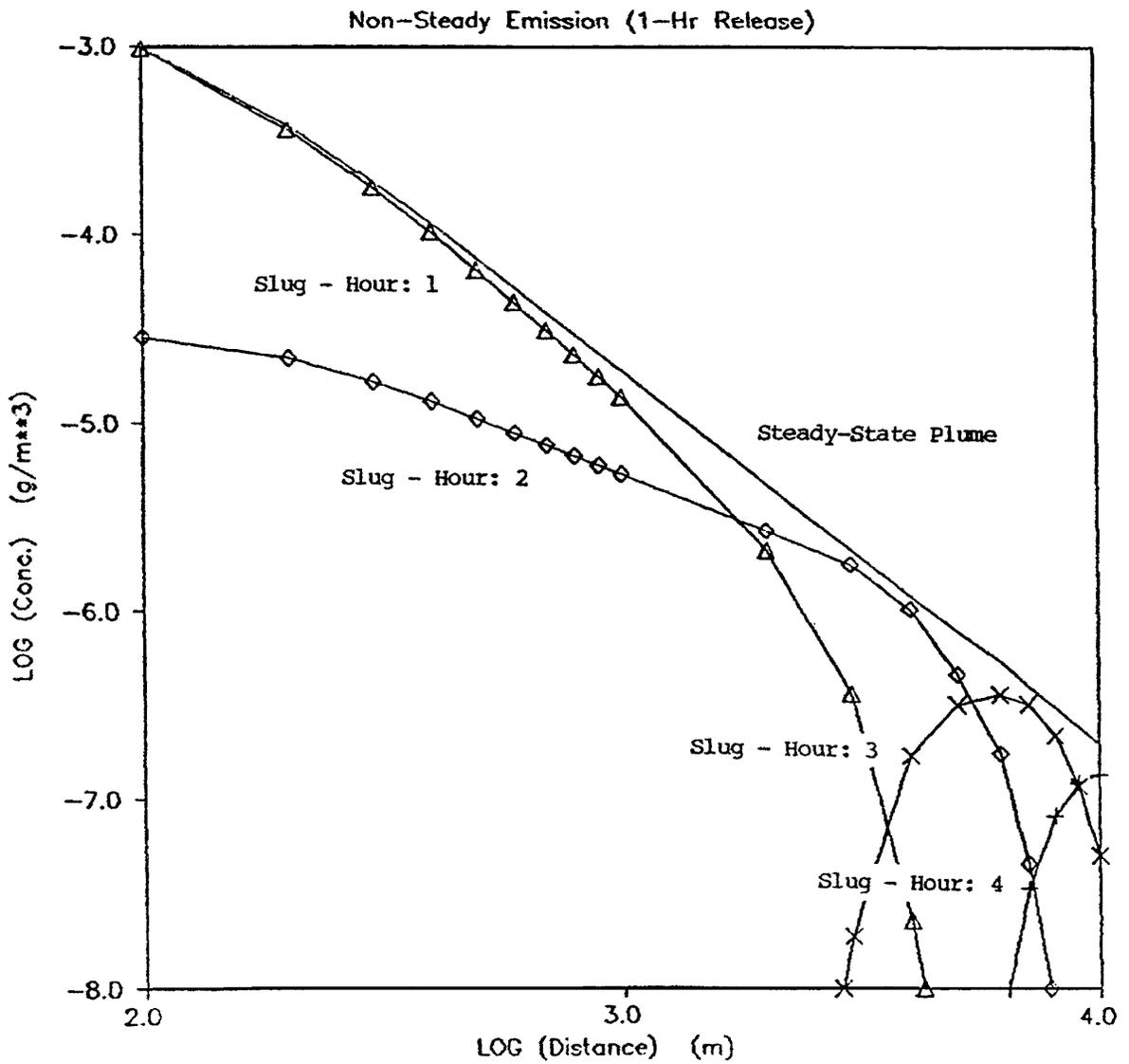
Figure 2-7.    Concentration predictions of slug model with receptor-specific sigmas for non-steady emission conditions. Emission rate: 1 g/s, Emission duration: 1 hour, Wind speed: 1 m/s, Stability class: B, Stack height: 10m, Mixing height: unlimited.

## 2.2    Dispersion

A key modeling consideration in CALPUFF is the specification of the horizontal and vertical Gaussian dispersion coefficients, $\sigma_y$ and $\sigma_z$, for a puff (or each end of a slug) at the start and end of a sampling step, and also for each receptor at which the cloud has a computed contribution during the step (the receptor-specific sigmas referred to in Section 2.1). The coefficients for the puff location at the start of a step are equal to those found at the end of the preceding sampling step, because cloud-size is continuous between sampling steps. Those at the end of the step, or at nearby receptors during the step, are computed according to an ambient turbulence growth relationship (for the current dispersion conditions!) and possibly a source-related constant variance. The growth due to ambient turbulence may be formulated as either a function of time, or as a function of distance, so we shall use a generic metric $\xi$ which stands for either one.

The dispersion coefficients for an incremental "position" $\Delta\xi$ relative to the beginning of sampling step n are :

$$\sigma_{y,n}^2 \left(\Delta\xi_y\right) = \sigma_{yt}^2 \left(\xi_{yn} + \Delta\xi_y\right) + \sigma_{ys}^2 + \sigma_{yb}^2 \tag{2-37}$$

and

$$\sigma_{z,n}^2 \left(\Delta\xi_z\right) = \sigma_{zt}^2 \left(\xi_{zn} + \Delta\xi_z\right) + \sigma_{zb}^2 \tag{2-38}$$

where $\xi_{yn}$ and $\xi_{zn}$ are the virtual-source metrics (time; distance) that are defined implicitly by the requirement that the sigmas match those at the end of the previous step when $\Delta\xi = 0$, and

$\sigma_{y,n}, \sigma_{z,n}$     are the total horizontal and vertical dispersion coefficients (m) at some position during sampling step n,

$\sigma_{yt}, \sigma_{zt}$     are the functional forms of the dispersion coefficients (m) of $\sigma_y$ and $\sigma_z$ due to atmospheric turbulence,

$\sigma_{yb}, \sigma_{zb}$     are the components (m) of $\sigma_y$ and $\sigma_z$ due to plume buoyancy at the time of release, and

$\sigma_{ys}$     is the component of the horizontal dispersion coefficient (m) due to the lateral (cross-wind) scale of an area-source.

The increment $\Delta\xi$ is positive when describing the growth of the puff during the sampling step, but can be either positive or negative for receptor-specific sigmas. For example, $\Delta\xi$ would be negative for a receptor located just upwind of the puff at the start of a sampling step. This allows CALPUFF to reproduce plume-like features during steady meteorological conditions, using very few puffs. Negative $\Delta\xi$ 's could also drive the argument of $\sigma_{yt}$ and $\sigma_{zt}$ through zero if a lower limit on the size of the sigmas at the source were not enforced. So there is an initial $\xi_0$ imposed, defined implicitly by the relations

$\sigma_{yt}^2(\xi_{oy}) = \sigma_{yo}^2$ and $\sigma_{zt}^2(\xi_{oz}) = \sigma_{zo}^2$ where

| | |
|---|---|
| $\sigma_{yo}, \sigma_{zo}$ | are the initial values (m) of $\sigma_y$ and $\sigma_z$ due to the nature of the source (e.g., volume source) or the rapid initial dilution associated with building downwash of point sources, and |
| $\xi_o$ | is the initial virtual-source metric and is defined implicitly and separately for y and z. |

Thus, quadratic addition of initial dispersion components for buoyant rise effects and for the lateral size of an area source are assumed, but other initial cloud dimensions and the subsequent growth of the puff or slug are accomplished using the virtual-distance or virtual-transport time approach. This virtual-source approach is necessary if current puff growth is to be dependent only on the current size of the puff and not on how it reached that size. Note that the concept of a virtual source is particularly important when a puff can move between substantially different dispersion regimes in just one sampling step. For example, land use varies by grid cell, so a puff may go from an overwater cell with weak dispersion into an overland cell with substantial vertical convection. Or a young puff in the late afternoon mixed layer may see the turbulence decay rapidly. In both cases, CALPUFF computes subsequent growth during the step using the appropriate turbulence (actual or parameterized), and the growth rate appropriate to its size.

2.2.1    Atmospheric Turbulence Components

The basic strategy in the design of the dispersion module is to allow the use of the most refined data available in the calculation of $\sigma_{yt}$ and $\sigma_{zt}$ while providing for backup algorithms not requiring specialized data for situations in which these data are not available. Three levels of input data are provided, depending on which of five dispersion options is selected. The five dispersion options are:

| | |
|---|---|
| 1 | dispersion coefficients computed from measured values of turbulence, $\sigma_v$ and $\sigma_w$ |
| 2 | dispersion coefficients from internally calculated $\sigma_v$ and $\sigma_w$ using micrometeorological variables ($u_*$, $w_*$, L, etc.) |
| 3 | PG dispersion coefficients for RURAL areas (computed using the ISCST multi-segment approximation) and McElroy-Pooler coefficients in urban areas |
| 4 | same as 3 except PG coefficients computed using the MESOPUFF II eqns. |
| 5 | CTDM sigmas used for stable and neutral conditions (assumes that measured $\sigma_v$ and $\sigma_w$ are read). For unstable conditions, sigmas are computed as in Dispersion Option 3. |

The three levels of input data are:

- direct measurements of turbulence, $\sigma_v$ and $\sigma_w$, (Dispersion Options 1 and 5-neutral/stable)

- micrometeorological scaling parameters $u_*$, $w_*$, $L$, and $h$, from CALMET or other meteorological model yielding internally computed estimates of the crosswind and vertical components of turbulence based on similarity theory, (Dispersion Option 2), or
- Pasquill-Gifford-Turner (PGT) class and user choice of either ISCST implementation of the dispersion coefficients (Dispersion Options 3 and 5-unstable) or the MESOPUFF II implementation of PGT rural dispersion coefficients (Dispersion Option 4).

The general forms of $\sigma_{yt}$ and $\sigma_{zt}$ (Hanna et al., 1977) for Dispersion Options 1, 2, and 5 are:

$$\sigma_{yt} = \sigma_v \, t \, f_y\left(t / t_{ly}\right) \tag{2-39}$$

$$\sigma_{zt} = \sigma_w \, t \, f_z\left(t / t_{lz}\right) \tag{2-40}$$

where, $\sigma_v$    is the standard deviation (m/s) of the horizontal crosswind component of the wind,

$\sigma_w$    is the standard deviation (m/s) of the vertical component of the wind,

$t$    is the travel time (s) of the plume to the receptor, and

$t_{ly}, t_{lz}$    are the horizontal and vertical Lagrangian time scales (s).

Eqns. (2-39) and (2-40) can be expressed in terms of the horizontal and vertical components ($i_y$ and $i_z$) of the turbulence intensity using the following relationships.

$$i_y = \sigma_v / u \simeq \sigma_\theta \tag{2-41}$$

$$i_z = \sigma_w / u \simeq \sigma_\varphi \tag{2-42}$$

where, $u$    is the wind speed (m/s),

$\sigma_\theta$    is the standard deviation radians of the horizontal wind angle, and

$\sigma_\varphi$    is the standard deviation radians of the vertical wind angle.

The most desirable approach is to relate the dispersion coefficients directly to the measured turbulence velocity variances ($\sigma_v$ and $\sigma_w$) or intensity components ($i_y$ and $i_z$). However, it is important that the quality of the observational data be considered in the selection of the method for computing the dispersion coefficients. For example, inaccurate observations of $i_z$, which is difficult to measure, may lead to less accurate modeling results that predictions based on more routine data. It is recommended that the default selection be Dispersion Option 2, which uses similarity theory and micrometeorological variables derived from routinely available meteorological observations and surface characteristics. Many laboratory experiments, field studies, and numerical simulations (e.g., Deardorff and Willis, 1975; Caughey, 1981; Lamb, 1981) have shown the importance and utility of convective scaling in the convective boundary layer. Convective scaling has been successfully applied to data collected at a wide variety of sites, including oceans, rural land surfaces (e.g., Hicks, 1985) and urban areas (Ching et al., 1983). Similarly, in

the stable boundary layer, local scaling has been shown to apply (e.g., Hunt, 1982; Nieuwstadt, 1984). The micrometeorological model, (see Section 4) explicitly relates the aerodynamic and thermal characteristics of the surface to the sensible heat flux and momentum transfer rates that are used in the computation of the dispersion coefficients.

Weil (1985) and Briggs (1985) provide reviews on the use of similarity theory in diffusion models.  In the convective boundary layer, Weil describes the turbulence characteristics in three layers:

(1)     Surface layer - z ≤ 0.1 h;              $\sigma_v$ ~ constant with height,
                                                $\sigma_w$ increases with height

(2)     Mixed layer - 0.1h < z < 0.8h;          $\sigma_v$ ~ constant with height,
                                                $\sigma_w$ ~ constant with height

(3)     Entrainment layer - z > 0.8h;           $\sigma_v$ decreases with height,
                                                $\sigma_w$ decreases with height.

In the surface layer, Panofsky et al. (1977) propose the following relations.

$$\sigma_v = u_* \left[ 4 + 0.6 \left(-h/L\right)^{2/3} \right]^{1/2} \tag{2-43}$$

$$\sigma_w = u_* \left[ 1.6 + 2.9 \left(-z/L\right)^{2/3} \right]^{1/2} \tag{2-44}$$

where,  $u_*$      is the surface friction velocity (m/s), and
        L        is the Monin-Obukhov length (m).

Hicks (1985) suggests the following for the mixed layer (0.1 to 0.8 h):

$$\sigma_v = \left( 3.6 \, u_*^2 + 0.35 \, w_*^2 \right)^{1/2} \tag{2-45}$$

$$\sigma_w = \left( 1.2 \, u_*^2 + 0.35 \, w_*^2 \right)^{1/2} \tag{2-46}$$

In the neutral boundary layer, Arya (1984) reports monotonically decreasing values of $\sigma_v$ and $\sigma_w$ throughout the mixed layer.  Using Blackadar and Tennekes (1968) relationship for the neutral boundary layer height, Arya's results can be expressed as:

$$\sigma_v = 1.8 \, \exp \left(-0.9 \, z/h\right) \tag{2-47}$$

$$\sigma_w = 1.3 \, \exp \left(-0.9 \, z/h\right) \tag{2-48}$$

In the stable boundary layer, Nieuwstadt (1984) finds that $\sigma_v$ and $\sigma_w$ bear constant ratios with the local friction velocity.

$$\sigma_v / u_{*\ell} = C_v \tag{2-49}$$

$$\sigma_w / u_{*\ell} = C_w \tag{2-50}$$

where, $u_{*\ell}$ is the local friction velocity (m/s), and $C_v$ and $C_w$ are constants.

Hanna et al. (1986) suggest that $C_v \approx 1.6$. $C_w$ has a value $\approx 1.3$ (Nieuwstadt, 1984). The local friction velocity, $u_{*\ell}$, can be expressed (Nieuwstadt, 1984) as:

$$u_{*\ell} = u_* \left(1 - z/h\right)^{3/4} \tag{2-51}$$

The modeling requires a formulation that yields the proper values and vertical variations for $\sigma_v$ and $\sigma_w$ in the convective, neutral, and stable limits, and one that provides a mechanism for interpolating the results for intermediate conditions without physically unrealistic discontinuities. The following equations for the neutral-convective boundary layer are based on the data discussed above and satisfy these conditions. The formulation for the entrainment layer is based on data reported by Caughey (1981).

Surface Layer: $z \leq 0.1\ h$          $(L \leq 0)$

$$\sigma_v = \left[4\ u_*^2\ a_n^2 + 0.35\ w_*^2\right]^{1/2} \tag{2-52}$$

$$\sigma_w = \left[1.6\ u_*^2\ a_n^2 + 2.9\ u_*^2\ (-z/L)^{2/3}\right]^{1/2} \tag{2-53}$$

$$a_n = \exp\left[-0.9\ (z/h)\right] \tag{2-54}$$

Mixed-Layer: $z = 0.1\text{-}0.8\ h$          $(L \leq 0)$

$$\sigma_v = \left[4\ u_*^2\ a_n^2 + 0.35\ w_*^2\right]^{1/2} \tag{2-55}$$

$$\sigma_w = \left[1.15\ u_*^2\ a_n^2 + 0.35\ w_*^2\right]^{1/2} \tag{2-56}$$

Entrainment Layer: $z > 0.8\ h$          $(L \leq 0)$

$$\sigma_v = \left[4\ u_*^2\ a_n^2 + 0.35\ w_*^2\right]^{1/2} \tag{2-57}$$

for $z = 0.8$ to $1.0\ h$

$$\sigma_w = \left[1.15\ u_*^2\ a_n^2 + a_{cl}\ 0.35\ w_*^2\right]^{1/2} \tag{2-58}$$

$$a_{c1} = \left[ 1/2 + (h - z) / (0.4h) \right] \qquad (2\text{-}59)$$

for z = 1.0 to 1.2 h

$$\sigma_w = \left[ 1.15 \; u_*^2 \; a_n^2 + a_{c2} \; 0.35 \; w_*^2 \right]^{1/2} \qquad (2\text{-}60)$$

$$a_{c2} = \left[ 1/3 + (1.2h - z) / (1.2h) \right] \qquad (2\text{-}61)$$

In the neutral-stable boundary layer, the following equations can be used to interpolate vertical profiles of $\sigma_v$ and $\sigma_w$ as a function of stability. As with the neutral-convective equations, they provide the proper values in the appropriate stability limits.

$$\sigma_v = u_* \left[ \left( 1.6 \; C_s \; (z/L) + 1.8 \; a_n \right) / (1 + z/L) \right] \qquad (L > 0) \qquad (2\text{-}62)$$

$$\sigma_w = 1.3 \; u_* \left[ \left( C_s \; (z/L) + a_n \right) / (1 + z/L) \right] \qquad (L > 0) \qquad (2\text{-}63)$$

$$C_s = (1 - z/h)^{3/4} \qquad (L > 0) \qquad (2\text{-}64)$$

It is assumed that the similarity-based values of $\sigma_v$, $\sigma_w$ from which $\sigma_y$, $\sigma_z$ are derived, are representative of one-hour average values. In order to provide for non-zero plume growth rates above the mixing height and to prevent numerical problems associated with near-zero plume dimensions, minimum $\sigma_v$ and $\sigma_w$ values are applied. Hanna et al. (1986) suggest an appropriate minimum one-hour average $\sigma_v$ value is $\approx$ 0.5 m/s. This is significantly higher than $\sigma_v$ expected based on PGT E and F stability curves. Appropriate default minimum values for $\sigma_v$ and $\sigma_w$ can be input by the user.

Eqns. (2-52) to (2-61) have been tested with the original data providing the basis for the Panofsky et al. (1977) and Hicks (1985) formulations. The results (summarized in Table 2-3) indicate that the modified equations compare well with the original equations and the observational data. The modified equations have the advantage of allowing a smooth and continuous transition to the neutral stability results of Arya (1984).

Irwin (1983) evaluated several schemes for determining the $f_y$ and $f_z$ functions. It was concluded that a parameterization suggested by Draxler (1976) performed best overall.

$$f_y = \left[ 1 + 0.9 \; (t/1000)^{1/2} \right]^{-1} \qquad (2\text{-}65)$$

$$f_z = \left[ 1 + 0.9 \; (t/500)^{1/2} \right]^{-1} \qquad L < 0 \qquad (2\text{-}66)$$

$$f_z = \left[ 1 + 0.945 \; (t/100)^{.806} \right]^{-1} \qquad L > 0 \qquad (2\text{-}67)$$

These are used in CALPUFF for Dispersion Options 1 and 2.  When Dispersion Option 5 is selected, and the Monin-Obukhov length is positive (neutral to stable), the $f_y$ and $f_z$ functions are from CTDMPLUS (Perry et al., 1989):

$$f_y = \left[ 1 + \frac{u\ t}{20000} \right]^{-1/2} \qquad L < 0 \tag{2-68}$$

$$f_z = \left[ 1 + \sigma_w\ t \left( \frac{1}{.72z} + \frac{N}{.54\sigma_w} \right) \right]^{-1/2} \qquad L > 0 \tag{2-69}$$

where z is the height above ground, and N is the Brunt-Vaisala frequency.

At longer transport distances, an option is provided to switch to the Heffter (1965) equations (i.e., $\sigma_{yt} \simeq t$, $\sigma_{zt} \simeq t^{1/2}$).  The transition from distance-dependent to time-dependent (i.e., Heffter) dispersion coefficients occurs in CALPUFF when the lateral dimension of the plume reaches a critical size, defined by the variable SYTDEP in Input Group 12 of the control file.  The default value of SYTDEP is 550 m.  Assuming PG dispersion rates under neutral conditions, a plume's $\sigma_y$ will reach 550 m after approximately 10 km of travel distance.  The use of the Hefter equation for $\sigma_z$ along with $\sigma_y$ is optional.

The user may also wish to have puff growth determined on the basis of gridded input fields of PGT class.  The approach is particularly useful if one is trying to compare the modeling results with steady-state regulatory model predictions or attempting to achieve compatibility with regulatory requirements.  The user may select either ISC3 model (U.S. EPA, 1992) dispersion methodology (Dispersion Option 3) or the MESOPUFF II (Scire et al., 1984b) implementation of the PGT dispersion curves (Dispersion Option 4).

Dispersion Option 3 also requires the specification of gridded land use type, which in turn determines whether the ISC "rural" or "urban" dispersion curves are used.  The "rural" dispersion equations and parameters are presented in Tables 2-4 and 2-5 for $\sigma_y$ and $\sigma_z$ respectively and are based on parameterizations of the PGT curves.

The "urban" dispersion equations and parameter values are based on Briggs' (as reported in Gifford, 1976) parameterizations of the St. Louis dispersion data analyzed by McElroy and Pooler (1968) and are presented in Tables 2-6 and 2-7 for $\sigma_y$ and $\sigma_z$ respectively.

Table 2-3

Comparison of Panofsky et al. (1977)/Hicks (1985)

$\sigma_v$, $\sigma_w$ Formulations with Eqns. (2-52) to (2-61)

| Panofsky et al. data | Observed $\sigma_v$ vs. Panofsky | Observed $\sigma_v$ vs. Eqns. (2-52) to (2-61) | Panofsky $\sigma_v$ vs. Eqns. (2-52) to (2-61) |
|---|---|---|---|
| Average | (1.14, 1.20) | (1.14, 1.21) | (1.20, 1.21) |
| Corr. Coef. | .81 | .84 | .992 |
| Average Bias | .07 | .07 | .00 |
| Average Abs. Error | .10 | .09 | .02 |
| RMSE | .13 | .12 | .02 |

| Hicks 1985 data | Observed $\sigma_v$ vs. Hicks | Observed $\sigma_v$ vs. Eqns. (2-52) to (2-61) | Hicks $\sigma_v$ vs. Eqns. (2-52) to (2-61) |
|---|---|---|---|
| Average | (1.17, 1.12) | (1.17, 1.06) | (1.12, 1.06) |
| Corr. Coef. | .79 | .77 | .998 |
| Average Bias | -.05 | -.11 | .06 |
| Average Abs. Error | .20 | .23 | .06 |
| RMSE | .27 | .30 | .08 |

| Hicks 1985 data | Observed $\sigma_w$ vs. Hicks | Observed $\sigma_w$ vs. Eqns. (2-52) to (2-61) | Hicks $\sigma_w$ vs. Eqns. (2-52) to (2-61) |
|---|---|---|---|
| Average | (.98, 1.01) | (.98, .98) | (1.01, .98) |
| Corr. Coef. | .91 | .91 | .998 |
| Average Bias | .03 | .00 | -.03 |
| Average Abs. Error | .12 | .11 | .03 |
| RMSE | .15 | .14 | .04 |

Table 2-4

Parameters Used to Calculate Pasquill-Gifford $\sigma_y$

| Pasquill Stability Class | $\sigma_y = 465.11628 \, (x) \tan (\theta)$**  $\theta = 0.017453293 \, (c\text{-}d \ln x)$ | |
| | c | d |
| --- | --- | --- |
| A | 24.1670 | 2.5334 |
| B | 18.3330 | 1.8096 |
| C | 12.5000 | 1.0857 |
| D | 8.3330 | 0.72382 |
| E | 6.2500 | 0.54287 |
| F | 4.1667 | 0.36191 |

\*       Source: U.S. EPA (1992)

\**     Where $\sigma_y$ is in meters and x is in kilometers

Table 2-5
Parameters Used to Calculate Pasquill-Gifford $\sigma_z$*

| Pasquill Stability Class | x (km) | $\sigma_z$ (meters) = a x$^b$ | |
| --- | --- | --- | --- |
| | | a | b |
| A** | < .10 | 122.800 | 0.94470 |
| | 0.10 - 0.15 | 158.080 | 1.05420 |
| | 0.16 - 0.20 | 170.220 | 1.09320 |
| | 0.21 - 0.25 | 179.520 | 1.12620 |
| | 0.26 - 0.30 | 217.410 | 1.26440 |
| | 0.31 - 0.40 | 258.890 | 1.40940 |
| | 0.41 - 0.50 | 346.750 | 1.72830 |
| | 0.51 - 3.11 | 453.850 | 2.11660 |
| | > 3.11 | ** | ** |
| B** | < .20 | 90.673 | 0.93198 |
| | 0.21 - 0.40 | 98.483 | 0.98332 |
| | > 0.40 | 109.300 | 1.09710 |
| C** | All | 61.141 | 0.91465 |
| D | < .30 | 34.459 | 0.86974 |
| | 0.31 - 1.00 | 32.093 | 0.81066 |
| | 1.01 - 3.00 | 32.093 | 0.64403 |
| | 3.01 - 10.00 | 33.504 | 0.60486 |
| | 10.01 - 30.00 | 36.650 | 0.56589 |
| | > 30.00 | 44.053 | 0.51179 |
| E | < .10 | 24.260 | 0.83660 |
| | 0.10 - 0.30 | 23.331 | 0.81956 |
| | 0.31 - 1.00 | 21.628 | 0.75660 |
| | 1.01 - 2.00 | 21.628 | 0.63077 |
| | 2.01 - 4.00 | 22.534 | 0.57154 |
| | 4.01 - 10.00 | 24.703 | 0.50527 |
| | 10.01 - 20.00 | 26.970 | 0.46713 |
| | 20.01 - 40.00 | 35.420 | 0.37615 |
| | > 40.00 | 47.618 | 0.29592 |
| F | < .20 | 15.209 | 0.81558 |
| | 0.21 - 0.70 | 14.457 | 0.78407 |
| | 0.70 - 1.00 | 13.953 | 0.68465 |
| | 1.01 - 2.00 | 13.953 | 0.63227 |
| | 2.01 - 3.00 | 14.823 | 0.54503 |
| | 3.01 - 7.00 | 16.187 | 0.46490 |
| | 7.01 - 15.00 | 17.836 | 0.41507 |
| | 15.01 - 30.00 | 22.651 | 0.32681 |
| | 30.01 - 60.00 | 27.074 | 0.27436 |
| | > 60.00 | 34.219 | 0.21716 |

*  Source:  U.S. EPA (1992)

** If the calculated value of $\sigma_z$ exceeds 5000 m, $\sigma_z$ is set equal to 5000 m

Table 2-6

Briggs Formulas Used to Calculate McElroy-Pooler $\sigma_{y*}$

| Pasquill Stability Category | $\sigma_y$ (meters)** |
|:---:|:---:|
| A | $0.32 \, x \, (1.0 + 0.0004 \, x)^{-\frac{1}{2}}$ |
| B | $0.32 \, x \, (1.0 + 0.0004 \, x)^{-\frac{1}{2}}$ |
| C | $0.22 \, x \, (1.0 + 0.0004 \, x)^{-\frac{1}{2}}$ |
| D | $0.16 \, x \, (1.0 + 0.0004 \, x)^{-\frac{1}{2}}$ |
| E | $0.11 \, x \, (1.0 + 0.0004 \, x)^{-\frac{1}{2}}$ |
| F | $0.11 \, x \, (1.0 + 0.0004 \, x)^{-\frac{1}{2}}$ |

\* Source: U.S. EPA (1992)
\*\* where x is in meters

Table 2-7

Briggs Formulas Used to Calculate McElroy-Pooler $\sigma_{z*}$

| Pasquill Stability Category | $\sigma_z$ (meters)** |
|:---:|:---:|
| A | $0.24 \, x \, (1.0 + 0.001 \, x)^{+\frac{1}{2}}$ |
| B | $0.24 \, x \, (1.0 + 0.001 \, x)^{+\frac{1}{2}}$ |
| C | $0.20 \, x$ |
| D | $0.14 \, x \, (1.0 + 0.0003 \, x)^{-\frac{1}{2}}$ |
| E | $0.08 \, x \, (1.0 + 0.0015 \, x)^{-\frac{1}{2}}$ |
| F | $0.08 \, x \, (1.0 + 0.0015 \, x)^{-\frac{1}{2}}$ |

\* Source: U.S. EPA (1992)
\*\* where x is in meters

Table 2-8

MESOPUFF II Growth Rate Coefficients $a_y$, $b_y$, $a_z$, $b_z$[*]

| Stability Class | $a_y$ | $b_y$ | $a_z$ | $b_z$ |
|---|---|---|---|---|
| A | 0.36 | 0.9 | 0.00023 | 2.10 |
| B | 0.25 | 0.9 | 0.058 | 1.09 |
| C | 0.19 | 0.9 | 0.11 | 0.91 |
| D | 0.13 | 0.9 | 0.57 | 0.58 |
| E | 0.096 | 0.9 | 0.85 | 0.47 |
| F | 0.063 | 0.9 | 0.77 | 0.42 |

_____

* Source:  Scire et al. (1984b)

If the MESOPUFF II form of the PGT stability-dependent dispersion curves is selected (Dispersion Option 4), the puff growth functions are of the form:

$$\sigma_y = a_y \, x^{b_y} \tag{2-70}$$
$$\sigma_z = a_z \, x^{b_z} \tag{2-71}$$

where $a_y$, $b_y$, $a_z$, $b_z$ are the stability dependent coefficients presented in Table 2-8.

The regulatory modeling guidance from the US EPA indicates that the PG dispersion curves, as defined above, are suitable for predicting one-hour average concentrations. The EPA of Victoria (Australia) bases the PG dispersion curves on a 3-minute averaging time and a surface roughness length ($z_o$) of 0.03 m. CALPUFF has the option to scale the PG dispersion coefficients for different averaging times or

$$\sigma_y(\tau_{ave}) = \sigma_y(\tau_{base}) \left( \frac{\tau_{ave}}{\tau_{base}} \right)^{0.2} \tag{2-72}$$

surface roughness lengths. The averaging time adjustment applies only to $\sigma_y$ and is of the form where

$\tau_{base}$     is the averaging time (minutes) assumed for the standard PG curves (e.g., 60 minutes by U.S. EPA, 3 minutes in Australia),

$\tau_{ave}$     is the averaging time (minutes) of the concentrations predicted by CALPUFF ($\tau_{ave} \leq 60$ minutes), and

$\sigma_y(\tau_{base})$, $\sigma_y(\tau_{ave})$ are the values of $\sigma_y$ assumed for averaging times of $\tau_{base}$ and $\tau_{ave}$ minutes, respectively.

The value of $\tau_{base}$ is defined as 60 minutes in CALPUFF. The $\tau_{ave}$ variable is specified by the user in Input Group 1 of the control file (see the variable AVET). The value of $\tau_{ave}$ should not exceed 60 minutes because multi-hour average concentrations are computed explicitly by time-averaging hourly values in CALPUFF.

A roughness length adjustment to the PG $\sigma_z$ curves is an option in CALPUFF and is based on Smith (1972), as implemented in the AUSPLUME model (Lorimer, 1986). This adjustment is most appropriate for near-surface releases and is not recommended for tall stack emissions (e.g., sources above 100 m). The value of $\sigma_z$ with this adjustment is given by:

$$\sigma_z' = a' x^{b'} \tag{2-73}$$

where

$$a' = a \cdot \left\{ 1.585 (1000)^{\beta} z_o^{0.1301} \right\} \tag{2-74}$$

$$b' = b - \beta \tag{2-75}$$

$$\beta = 0.0777 + 0.0215 \quad \ln(z_o) \tag{2-76}$$

and     $z_o$ is the surface roughness length (m),

        x is the downwind distance (m), and

        a, b are the PG dispersion curve parameters (see Table 2-5).

For $\sigma_y$, the roughness length adjustments is:

$$\sigma_y' = \sigma_y \, (z_o / z_{o(ref)})^{0.2} \tag{2-77}$$

where the reference roughness length ($z_{o(ref)}$) is 0.03 meters, and the prime indicates the roughness length adjusted value of $\sigma_y$.

It is recommended that the surface correction be limited to surface roughness lengths no greater than one meter. The time average and surface roughness adjustments can be applied to either the ISC3 or MESOPUFF II PG rural dispersion curves. Adjustments are not made to the McElroy-Pooler urban curves or the similarity-based dispersion curves, which have the effects of roughness implicitly included.

## 2.2.2    Buoyancy - Induced Dispersion

The effect of plume buoyancy on the dispersion coefficients are parameterized in terms of the plume rise (Pasquill, 1976; Irwin, 1979):

$$\sigma_{yb} = \Delta H / 3.5 \tag{2-78}$$

$$\sigma_{zb} = \Delta H / 3.5 \tag{2-79}$$

where $\Delta H$ is the plume rise (m). Buoyancy-induced dispersion (BID) is automatically included for all the dispersion coefficient options described in Section 2.2.1. CALPUFF uses the convention in the ISC3 model for BID. This includes the use of transition plume rise in the BID equation, even if the option for only final rise is selected for the plume height in the basic concentration equation (i.e., Eqn. (2-1)) and the _non-use_ of BID when the Schulman-Scire building downwash algorithm is used (see Section 2.3).

## 2.2.3  Initial Plume Size

The initial size of puffs emitted by volume sources is determined by user-specified initial dispersion coefficients, $\sigma_{yo}$ and $\sigma_{zo}$.  The volume source option allows the emissions from a number of smaller sources in a given area (e.g., a grid cell) to be combined into a single source.  The volume source emissions are immediately spread over a volume described by $\sigma_{yo}$ and $\sigma_{zo}$.  The subsequent growth of the volume source puff is computed in the same manner as the point source puffs, using a virtual source to match the initial values of $\sigma_y$ and $\sigma_z$.

Point source emissions subject to building downwash effects experience a rapid initial growth due to the high building-induced turbulence intensity in the lee of the building.  A building downwash model (described in Section 2.3) is used to internally compute initial plume dimensions for downwashed point source emissions as a function of building dimensions, stack height, momentum flux, and meteorological conditions.

## 2.2.4  Puff Splitting (Vertical Wind Shear)

Vertical wind shear can sometimes be an important factor affecting plume transport and dispersion.  The change of wind speed and wind direction with height causes a differential advection of pollutant material emitted at different heights.  Even for material emitted at a given height, when plumes become large enough, across-plume shear may transport the upper portion of a plume in a different direction than the lower portion.  When vertical mixing brings the entire plume to the ground, the effective horizontal dispersion of the plume may be significantly enhanced as a result of the differential transport.  CALPUFF explicitly models wind shear effects on <u>different</u> puffs by allowing each puff to be independently advected by its *local* average wind speed and direction, and independently mixed vertically to the ground. The average wind for a puff is obtained from profiles of wind speed and direction (available when using CALMET winds or PROFILE winds) from the top to the bottom of the puff.  For example, puffs emitted from two sources co-located in the horizontal, but with different release heights will be transported in CALPUFF in different directions and at different speeds if the wind fields indicate such a shear exists.

Shear across a <u>single</u> puff is handled in CALPUFF by allowing a well-mixed puff to split into two or more pieces when across-puff shear becomes important.  Each portion of the puff is then independently transported and dispersed.  This is illustrated in Figure 2-8.  A single puff may be split multiple times if it remains in the modeling domain long enough.  A puff that is still Gaussian in the vertical will not be split.  Because across-puff wind shear effects are not likely to be important in all applications, and because puff splitting increases computational requirements, the puff splitting feature is an option that can be modified or turned off.

Across-puff shear is likely to be important for well-mixed puffs after stable surface flows develop in the evening.  The mixing height switches from convective to mechanical, so that the current height is small

# CALPUFF PUFF-SPLITTING

Side
View



Top View
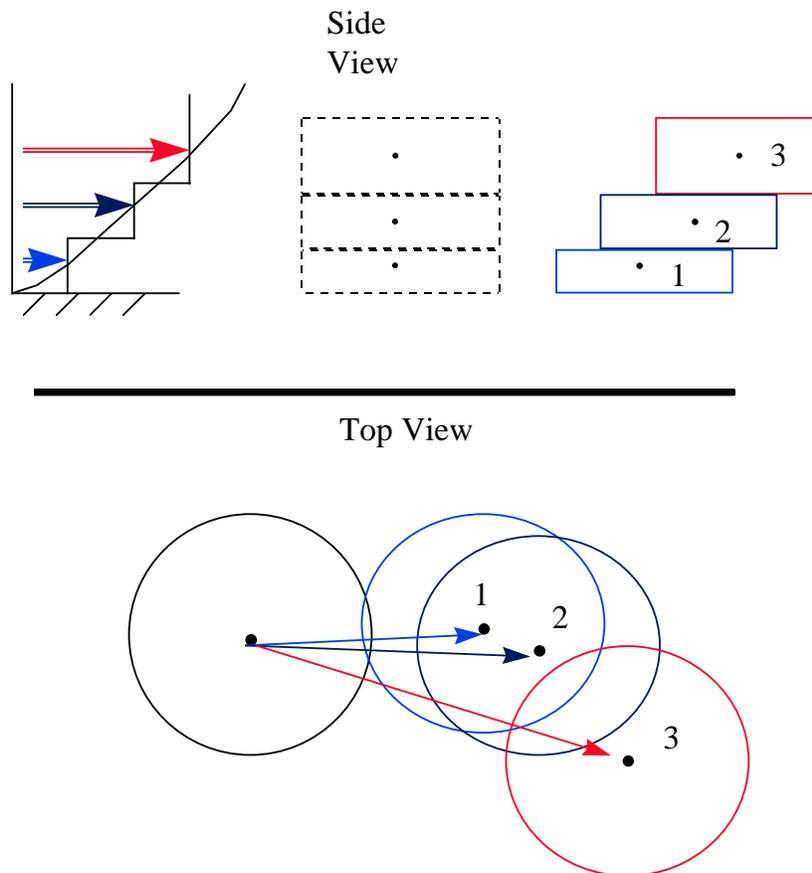
Figure 2-8.  Illustration of the puff splitting mechanism and the resultant effects on puff transport.

compared to the maximum mixing height experienced by the puff.  Furthermore, the current mixing height should not be negligible.  If it were negligible, the bulk flow across the depth of the puff should provide an adequate characterization of the transport.

Puff splitting is configured by a number of variables specified in the CALPUFF control file.  It is readily enabled or disabled by the MSPLIT option variable in Input Group 2.  Once enabled, the frequency with which a puff is split is controlled by the variables NSPLIT, IRESPLIT, ZISPLIT, and ROLDMAX in Input Group 12.

Whenever a puff is split, NSPLIT specifies the number of puffs that result from the split.  The original, well-mixed puff of thickness H is sliced NSPLIT-1 times.  The first slice is made at H/2; the second is made at H/4; the third at H/8, etc., so that the thinnest "new" puff is at the bottom of the original puff, and only it is in contact with the ground.  Each of the other new puffs reaches the surface only after a rising mixing heights exceeds its lower edge.

A puff may be split repeatedly, but several conditions must be met:

> 1)      The puff must be in contact with the ground.
> 2)      The puff's "split flag" must be on.
> 3)      The previous mixing height must exceed a minimum allowed value.
> 4)      The ratio of current mixing height to maximum past mixing height for this puff must be smaller than a maximum allowed value.

Condition (1) is always applied.  Condition (2) is controlled by IRESPLIT (the re-split flag).  It identifies the time(s) during each day when all puffs become eligible for splitting, provided all other conditions are met.  The minimum value for condition (3) is provided by ZISPLIT, and the maximum value for condition (4) is provided by ROLDMAX.

## 2.2.5    The P.D.F. Option for the Convective Boundary Layer

The puff and slug equations in Section 2.1 use a Gaussian distribution to characterize the vertical distribution of puff material within the CBL.  Image sources placed above the mixing lid and below the ground trap the mass within the layer, and as the puff grows, it soon fills the layer and the resulting vertical distribution becomes uniform.  Within this framework, the primary effect of the convective motions in the mixed layer is to cause a rapid growth in the vertical size of a puff.  Depending on the CALPUFF dispersion option selected, this growth rate is either parameterized by the stability class, scaled by measured turbulence intensity, or scaled by a turbulence intensity computed from the surface layer parameters.

In the last decade, modeling techniques that recognize the asymmetry of the vertical dispersion process in the CBL have matured. These techniques explicitly account for the differences between the distribution and strength of updrafts and downdrafts in the layer, as they relate to the ensemble-mean concentration distribution. One such technique that is simple yet effective is the "p.d.f." approach that relates the probability density function of the vertical position of puff mass in the layer to the skewed probability density function of vertical velocity. Using the superposition of two Gaussian distributions to characterize the skewed p.d.f of the vertical velocity, the p.d.f. model produces a "dual plume" formulation that maps the evolution of one plume that is initially carried towards the ground in a (mean) downdraft, and a second plume that initially rises towards the top of the mixed layer in a (mean) updraft. Subsequent "reflections" from both the ground and the lid are simulated using image sources. Because each of these plumes has its own mean vertical velocity and rate of spread, the resulting vertical distribution of mass is skewed in much the same way as the observed distributions. The initial downdraft plume is called the direct source because it travels directly from an elevated source (accounting for the plume rise velocity) to the ground, while the initial updraft plume is called the indirect source because it reaches the ground only after traversing the full depth of the mixed layer.

Weil et al. (1997) have extended the p.d.f. CBL formulation to include a simple way of simulating the tendency of highly buoyant plumes to "loft" at the top of the mixed layer, remaining there for some time before the convective eddies are able to overcome the buoyancy and mix their mass to the surface. This formulation forms the basis of the CBL component of AERMOD, and has been adapted for use in CALPUFF. In the following sections, we present their formulation for key components that are used in CALPUFF and describe how these are implemented.

2.2.5.1 P.D.F. Parameters for Vertical Velocity

Weil et al. (1997) approximate the p.d.f. for vertical velocity in the CBL, $p_w$, as the superposition of two Gaussian distributions:

$$p_w = \frac{\lambda_1}{\sqrt{2\pi}\sigma_{w1}} \exp(-\frac{(w-\overline{w_1})^2}{2\sigma_{w1}^2}) + \frac{\lambda_2}{\sqrt{2\pi}\sigma_{w2}} \exp(-\frac{(w-\overline{w_2})^2}{2\sigma_{w2}^2}) \qquad (2\text{-}80)$$

where the weights given to the two, $\lambda_1$ and $\lambda_2$, sum to unity. The $\overline{w_j}$ and $\sigma_{wj}$ ($j$ = 1, 2) are the mean vertical velocity and standard deviation for each distribution, and are assumed to be proportional to $\sigma_w$. The subscripts 1 and 2 denote the updraft and down draft distributions, respectively. Defining a parameter $R = \sigma_{w1} / \overline{w_1} = -\sigma_{w2} / \overline{w_2}$, Weil (1990) found the solution for $\overline{w_1}$ and $\overline{w_2}$ to be

$$\frac{\overline{w_1}}{\sigma_w} = \frac{\gamma_1 S}{2} + \frac{1}{2}\sqrt{(\gamma_1^2 S^2 + \frac{4}{\gamma_2})}$$

$$\frac{\overline{w_1}}{\sigma_w} = \frac{\gamma_1 S}{2} - \frac{1}{2}\sqrt{(\gamma_1^2 S^2 + \frac{4}{\gamma_2})}$$

(2-81)

where S is the skewness, and

$$\gamma_1 = \frac{1+R^2}{1+3R^2} \qquad \gamma_2 = 1+R^2 \tag{2-82}$$

$$\lambda_1 = \frac{\overline{w_2}}{\overline{w_2} - \overline{w_1}} \qquad \lambda_2 = -\frac{\overline{w_1}}{\overline{w_2} - \overline{w_1}} \tag{2-83}$$

Although Weil et al. (1997) find that $R = 1$ yields fair-to-good agreement between the modeled and measured laboratory concentration fields, they choose $R = 2$ for field observations so that in the limit of a neutral boundary layer ($w_* = 0$) and an assumed $S = 0$, the p.d.f. approximates a Gaussian p.d.f.

In the upper 90% of the CBL, the vertical velocity variance $\sigma_w^2$ can be assumed to be uniform (Weil, 1988) as can the skewness (Wyngaard, 1988). Weil et al. (1997) use the form

$$\sigma_w^2 = 1.2u_*^2 + 0.31w_*^2, \tag{2-84}$$

where the 1.2 corresponds to Hicks' (1985) neutral limit ($w_* = 0$) and the 0.31 is consistent with Weil and Brower's (1984) convective limit ($u_* = 0$) or $\sigma_w/w_* = 0.56$. In the convective limit, they take $S$ to be 0.6 which is the vertically-averaged value from the Minnesota experiments (Wyngaard, 1988), and the corresponding $\overline{w^3} = 0.6\sigma_w^3 = 0.105w_*^3$. For arbitrary $u_*$ and $w_*$, they write the skewness as

$$S = 0.105 \frac{w_*^3}{\sigma_w^3} \tag{2-85}$$

so that as $w_* \rightarrow 0$, $S \rightarrow 0$ and for $w_*/u_* \gg 1$, $S = 0.6$.

## 2.2.5.2 Direct Source Treatment

The p.d.f. $p_z$ of the particle height $z_p$ can be found from $p_w$ provided that the $z_p$ is a monotonic function of $w$ :

$$p_z = p_w[w(z_p;x)] \; |\frac{dw}{dz_p}| \tag{2-86}$$

Weil et al. (1997) find the relationship between $z_p$ and $w$ by superposing the plume rise $\Delta h$ above the top of the stack, $h_s$ , and the vertical displacement due to $w$:

$$z_p = h_s + \Delta h + \frac{wx}{U}, \tag{2-87}$$

or

$$w = (z_p - h_s - \Delta h)\frac{U}{x} \tag{2-88}$$

With this and $p_w$ , they find the crosswind-integrated concentration field to be

$$C_d^y(x,z) = \frac{Q}{\sqrt{2\pi}U} \; [\frac{\lambda_1}{\sigma_{z1}} \; \exp(-\frac{(z-\psi_1)^2}{2\sigma_{z1}^2}) + \frac{\lambda_2}{\sigma_{z2}} \; \exp(-\frac{(z-\psi_2)^2}{2\sigma_{z2}^2})], \tag{2-89}$$

where

$$\psi_j = h_s + \Delta h + \frac{\overline{w_j}x}{U} \qquad \text{with } j = 1 \text{ or } 2, \tag{2-90}$$

and the corresponding $\sigma_{zj}$ scale with the $\sigma_{wj}$.

Introducing an image source at $z = -h_s$, and additional image sources at $z = 2z_i + h_s$, $-2z_i - h_s$, ....,

$$
\begin{aligned}
C_d^y(x,z) = \frac{Q}{\sqrt{2\pi}U} \; [\frac{\lambda_1}{\sigma_{z1}} \sum_{n=0}^{N} [\exp(-\frac{(z-2nz_i-\psi_1)^2}{2\sigma_{z1}^2}) + \exp(-\frac{(z+2nz_i+\psi_1)^2}{2\sigma_{z1}^2})] \\
+ \frac{\lambda_2}{\sigma_{z2}} \sum_{n=0}^{N} [\exp(-\frac{(z-2nz_i-\psi_2)^2}{2\sigma_{z2}^2}) + \exp(-\frac{(z+2nz_i+\psi_2)^2}{2\sigma_{z2}^2})] \; ]
\end{aligned}
\tag{2-91}
$$

where $N$ is the number of image sources.  Because the image-source terms add at intervals of $2z_i$, with the same sign as the $\psi_j$, the updraft plume (j=1) has little impact once it "passes" above the lid ($\psi_1 > 0$) while the downdraft plume (j=2) repeatedly produces a full impact at height z  ($\psi_2 < 0$).  This is the mathematical representation of the reflecting plume trajectory of the direct source.

2.2.5.3  Indirect or Modified-Image Source Treatment

The indirect source provides for the plume material that "escapes" through the top of the layer in the preceding representation, but does not physically penetrate the inversion.  It is developed separately to address the case of a lofting plume.  Weil et al. (1997) have developed a treatment that: 1) provides for a continuous variation of $C^y$ with the dimensionless buoyance flux, $f_*$, and other variables, and 2) simplifies computationally the analysis given in an earlier model, which used a distributed source with $x$ at the CBL top to satisfy the zero-flux condition (Hanna et al., 1986).

They introduce an "effective" additional plume rise $\Delta h_i$ to simulate the tendency of the buoyancy to keep the plume aloft.  With this change, reflecting both the plume rise and the vertical velocity at the lid produces

$$z_p = 2z_i - h_s - \Delta h - \frac{wx}{U} + \Delta h_i \tag{2-92}$$

so that

$$w = -(z_p - 2z_i + h_s + \Delta h_r)\frac{U}{x} \tag{2-93}$$

where

$$\Delta h_r = \Delta h - \Delta h_i; \tag{2-94}$$

Including image sources at  $z = -2z_i + h_s,\ 4z_i - h_s,\ -4z_i + h_s,\ ...$ to account for the zero flux at $z = 0, z_i$, the crosswind-integrated concentration field for the indirect source is

$$
\begin{aligned}
C_r^y(x,z) = \frac{Q}{\sqrt{2\pi}U}\ [ &\frac{\lambda_1}{\sigma_{z1}} \sum_{n=1}^{N} [\exp(-\frac{(z-2nz_i+\psi_1)^2}{2\sigma_{z1}^2}) + \exp(-\frac{(z+2nz_i-\psi_1)^2}{2\sigma_{z1}^2})] \\
+ &\frac{\lambda_2}{\sigma_{z2}} \sum_{n=1}^{N} [\exp(-\frac{(z-2nz_i+\psi_2)^2}{2\sigma_{z2}^2}) + \exp(-\frac{(z+2nz_i-\psi_2)^2}{2\sigma_{z2}^2})]\ ]
\end{aligned}
\tag{2-95}
$$

where

$$\psi_j = h_s + \Delta h_r + \frac{\overline{w_j}x}{U} \qquad \text{with} \quad j = 1 \text{ or } 2 \qquad (2\text{-}96)$$

This time $2nz_I$ and $\Psi_j$ are of opposite sign, so that the downdraft portion of this expression has little impact at a height z in the layer once $\Psi_2$ is sufficiently negative, whereas the updraft portion repeatedly crosses the level z.

Weil et al. (1997) develop the "effective" plume rise $\Delta h_i$ from a simple energy argument governing the descent of buoyant plume elements from the CBL top that are carried to the surface by downdrafts. For an element with an initial height $z_p = z_i$, initial vertical velocity $-w$, and no further entrainment of ambient air, the element's vertical velocity and trajectory are given by

$$\begin{aligned} w_p &= -w + g't \\ z_p &= z_i - wt + \frac{g't^2}{2}, \end{aligned} \qquad (2\text{-}97)$$

where $g' = g\,\Delta\rho/\rho_a$, $\Delta\rho = \rho_a - \rho$, and $\rho$ is the plume density when an element begins its downward displacement. When it reaches the ground, $w_p = 0$ and $z_p = 0$, so that the time required for this displacement to occur is $t = w/g'$. They use the corresponding $w$ for the displacement as the basic criterion governing the onset of the plume parcel displacement from the CBL top, but modify it by the constant $\alpha$ :

$$w = \sqrt{\frac{2g'z_i}{\alpha}} \qquad (2\text{-}98)$$

where $\alpha$ is estimated to be about 1.4.

For a plume originating at the CBL top, the trajectory for the plume elements carried by downdrafts is

$$z_p = z_i + \Delta h_i - \frac{wx}{U} \qquad (2\text{-}99)$$

This trajectory intersects the height $z = z_i$ when $\Delta h_i = wx/U$, so that

$$\Delta h_i = \sqrt{\frac{g'z_i}{\alpha}} \; \frac{x}{U}. \qquad (2\text{-}100)$$

For a plume trapped in the CBL, the local buoyancy flux $F$ is conserved and given by

$$F = F_b = U r_y r_z \frac{g\Delta\rho}{\rho_a}$$

(2-101)

so

$$\Delta h_i = \sqrt{\frac{2F_b z_i}{\alpha U r_y r_z}} \frac{x}{U}.$$

(2-102)

The half-widths, $r_y$ and $r_z$, of the plume cross section are obtained from a modified version of an entrainment model (Weil, 1989) for plumes lofting at the CBL top:

$$r_y r_z = r_i^2 + \frac{a_e \alpha_y^{\frac{3}{2}}}{4} \frac{w_*^2 x^2}{U^2},$$

(2-103)

where $r_i = \beta_2 (z_i - h_s)$ is the plume radius when the plume reaches the CBL top, $\beta_2 = 0.4$, $\alpha_y = 2.3$, and $a_e$ is a dimensionless entrainment parameter, which they empirically estimate to be 0.1.

2.2.5.4  CALPUFF Implementation

Weil et al. (1997) describe many other elements of their model for buoyant plumes in the CBL, but those presented above constitute the portion that has been implemented in CALPUFF.  We have adopted their CBL parameterizations for obtaining the mean updraft and downdraft properties, and also their novel simulation of the lofting plume by means of the effective rise of the indirect source.  However, the CALPUFF algorithms for treating partial penetration and subsequent entrainment into the mixed layer as the layer grows remain unchanged.

The resulting two-path model is implemented by explicitly computing the height of each path at each receptor (or wherever the distribution is evaluated), accounting for reflections from the ground and the mixing lid.  Image sources for the resulting puff height are introduced as before to bound the distribution within the layer.  The $\sigma_{zj}$ (j=1,2) are scaled by the ratio of the corresponding $\sigma_{wj}$, since ambient puff growth in the vertical is proportional to the turbulence velocity.  That is, we scale the ambient $\sigma_z$ for the receptor position computed using the existing CALPUFF routines by $\sigma_{wj}/\sigma_w$ and then add the buoyancy-induced component as before:

$$\sigma_z^2 = \sigma_{za}^2 \left(\frac{\sigma_{wj}^2}{\sigma_w^2}\right) + \sigma_{bid}^2$$

(2-104)

The buoyancy enhancement is computed for the rise that would have been experienced by the puff in the absence of any mean updraft or downdraft displacements.

Figure 2-9 shows the paths computed using the new algorithm for two CBL's of identical height and $u_*$, but differing Monin-Obukhov length, and $w_*$. A buoyant plume is placed at the middle of the mixed layer, and the mean direct and indirect paths are plotted, ignoring plume rise. The two solid lines show the paths for $w_*=1.3$ m/s, and the dashed lines show the paths for stronger convection, $w_*=2.4$ m/s. The direct path for the stronger convection reaches the ground sooner, as does the indirect path, because the mean updraft and downdraft velocities are larger. Furthermore, the puff remains at the top of the layer for a shorter period because the convection is better able to overcome the residual buoyancy of the puff.

2.2.6    Vertical Puff Stretching (Horizontal Convergence)

When a full three-dimensional wind field is used to provide the environment in which puffs are transported and sampled, puffs may enter regions of horizontal convergence (vertical divergence). If the transport algorithms only recognize the horizontal winds, such regions will tend to collect puffs and this can lead to unphysically large concentrations as the concentration distributions of these puffs overlap and add together. If the transport algorithms recognize the vertical component of the wind as well as the horizontal, puffs will be lifted in such regions, perhaps by the vertical velocity at the center of the vertical distribution of mass in the puff, or by the average vertical velocity across the puff. This will reduce the degree of overlap as the vertical motion compensates to some extent for the convergence of puffs in the horizontal plane. But this treatment would confuse notions about the meaning of the horizontal and vertical distributions of mass in each puff, and lead to reversing the mathematical reflection process used to obtain the vertical distribution of mass near the ground. The resulting ground-level concentrations could be unduly sensitive to the details of the vertical transport assumptions made.

Rather than use the vertical velocity field to transport puffs, CALPUFF uses the mean vertical gradient of the vertical velocity across each puff (which is the mean vertical divergence across the puff) to stretch the vertical distribution of mass in the puff. The logic for this is best illustrated by considering a puff that is in contact with the ground. The vertical velocity at the ground (perpendicular to the ground beneath the puff) is zero, but that at the top of the puff may be greater than zero. Hence, the bottom of the puff is constrained, while the top is carried upward, thereby stretching the mass distribution. The details of this process are complex in real flows, and are highly simplified in the modeled fields. Therefore, the effect is implemented by simply increasing the puff $\sigma_z$ in proportion to the vertical divergence during each sampling step.

**PDF Bounce Paths**
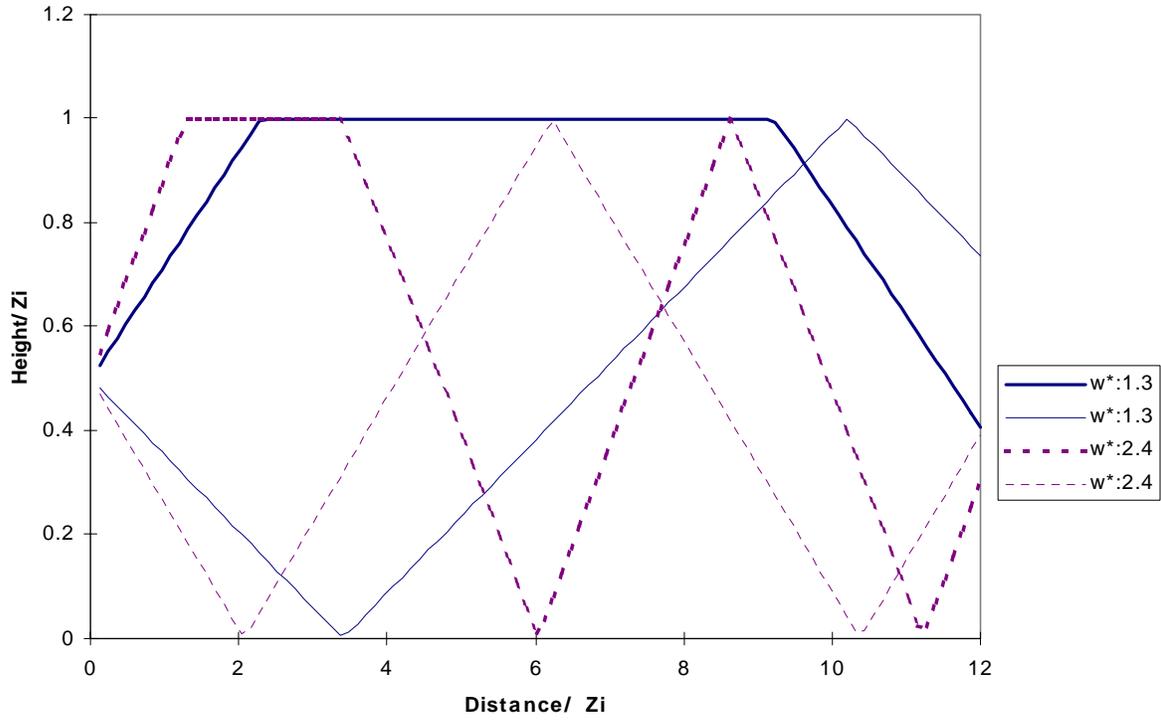


Figure 2-9.    Computed paths of the direct and indirect "sources" for two mixed layers of differing $w_*$.

CALMET provides the three-dimensional wind field for CALPUFF. Each face that separates the meteorological grid cells in the vertical has the vertical velocity, w, required to offset any convergence in the horizontal winds. Therefore, the difference in the vertical velocity between the top and bottom of a cell, divided by the thickness of the cell, is the mean divergence in the cell. For cell n:

$$\frac{dw}{dz}\Big|_n = \frac{w(z_{n+1}) - w(z_n)}{z_{n+1} - z_n} \qquad (2\text{-}105)$$

The mean divergence across the puff is obtained by assuming that the vertical divergence is a constant within each cell, equal to the mean in the cell, and integrating this divergence profile from the bottom of the puff, $z_b$, to the top, $z_t$. The $z_t$ and $z_b$ are defined to be the puff height plus/minus one $\sigma_z$, subject to the constraint of the ground and any mixing lid.

$$\frac{dw}{dz}\Big|_p = \frac{1}{z_t - z_b} \int_{z_b}^{z_t} \frac{dw}{dz}(z) \ dz \qquad (2\text{-}106)$$

This mean divergence is the fractional vertical stretching rate for the puff. Over one sampling step of duration $\Delta t$, the puff $\sigma_z$ is augmented as:

$$\sigma'_z = \sigma_z \ (1 + \Delta t \ \frac{dw}{dz}\Big|_p) \qquad (2\text{-}107)$$

As the vertical size of the puff grows, it extends over more vertical layers. By using the mean divergence across the puff, any changes in the divergence from one layer to the next are incorporated so that the effect of strong vertical divergence in one layer may be offset by convergence or much weaker divergence in other layers aloft.

## 2.3    Building Downwash

The dispersion and buoyant rise of plumes released from short stacks can be significantly modified by the presence of buildings or other obstacles to the flow. Hosker (1984) provides a description of the flow patterns in three regions near buildings. Figure 2-10 shows (1) a displacement zone upwind of the buildings, where the flow is influenced by the high pressure along the upwind building face, (2) a cavity zone characterized by recirculating flow, high turbulence intensity, and low mean wind speed, and (3) a turbulent wake region where the flow characteristics and turbulence intensity gradually approach the ambient values.

The parameterization of building downwash in CALPUFF is appropriate for use in the turbulent wake region and is based on the procedures used in the ISC3 model. ISC3 contains two building downwash

algorithms:

- Huber-Snyder model (Huber and Snyder, 1976; Huber, 1977).  In ISC3, this model is applied when the source height is greater than the building height ($H_b$) plus one-half $L_b$,  the lesser of the building height or projected width ($H_w$).  It applies either a full building wake effect or none at all, depending on the effective height of the emitted plume.

- Schulman-Scire model (Scire and Schulman, 1980; Schulman and Hanna, 1986).  This model applies a linear decay factor to the building-induced enhancement of the dispersion coefficients and accounts for the effect of downwash on plume rise. It is used in ISC3 for stacks lower in height than $H_b + 0.5 L_b$.

The main difference in the treatment of downwash between ISC3 and CALPUFF is that the height threshold determining which model is used is an input variable.  This option allows the user to apply one of the models for all stacks, which has the desirable effect of eliminating the discontinuity of the ISC3 approach at stack heights of $H_b + 0.5 L_b$.  Thus, in CALPUFF, the Huber-Snyder technique is used for stacks greater than $H_b + T_{bd} L_b$, where $T_{bd}$ has a default value of 0.5.  A negative value of $T_{bd}$ indicates the Huber-Snyder method is used for all stacks, and a value of 1.5 results in the Schulman-Scire method being always used.  If $T_{Tb}$ is set equal to 0.5 (its default value), the CALPUFF treatment will be equivalent to that in ISC3.

Both downwash methods use wind direction-specific building dimensions (i.e., $H_b$, $H_w$).  CALPUFF, like the short-term version of ISC3, uses 36 wind direction-specific values of the building dimensions, corresponding to wind vectors from 10° to 360° in increments of 10°.  The EPA Building Profile Input Program (BPIP) (EPA, 1993) can be used to develop the wind direction-specific building dimensions for CALPUFF and determine Good Engineering Practice (GEP) stack height associated with one or more buildings.

2.3.1    Huber-Snyder Downwash Procedure

If the stack height exceeds $H_b + T_{bd} L_b$, the Huber-Snyder algorithm is applied.  The first step is to compute the effective plume height, $H_e$, due to momentum rise at a downwind distance of two building heights.  If $H_e$ exceeds $H_b + 1.5 L_b$ (where $H_b$ and $L_b$ are the wind direction specific values), building downwash effects are assumed to be negligible.  Otherwise, building-induced enhancement of the plume dispersion coefficients is evaluated.  For stack heights, $H_s$, less than $1.2 H_b$, both $\sigma_y$ and $\sigma_z$ are enhanced.  Only $\sigma_z$ is enhanced for stack heights above $1.2 H_b$ (but below $H_b + 1.5 L_b$).
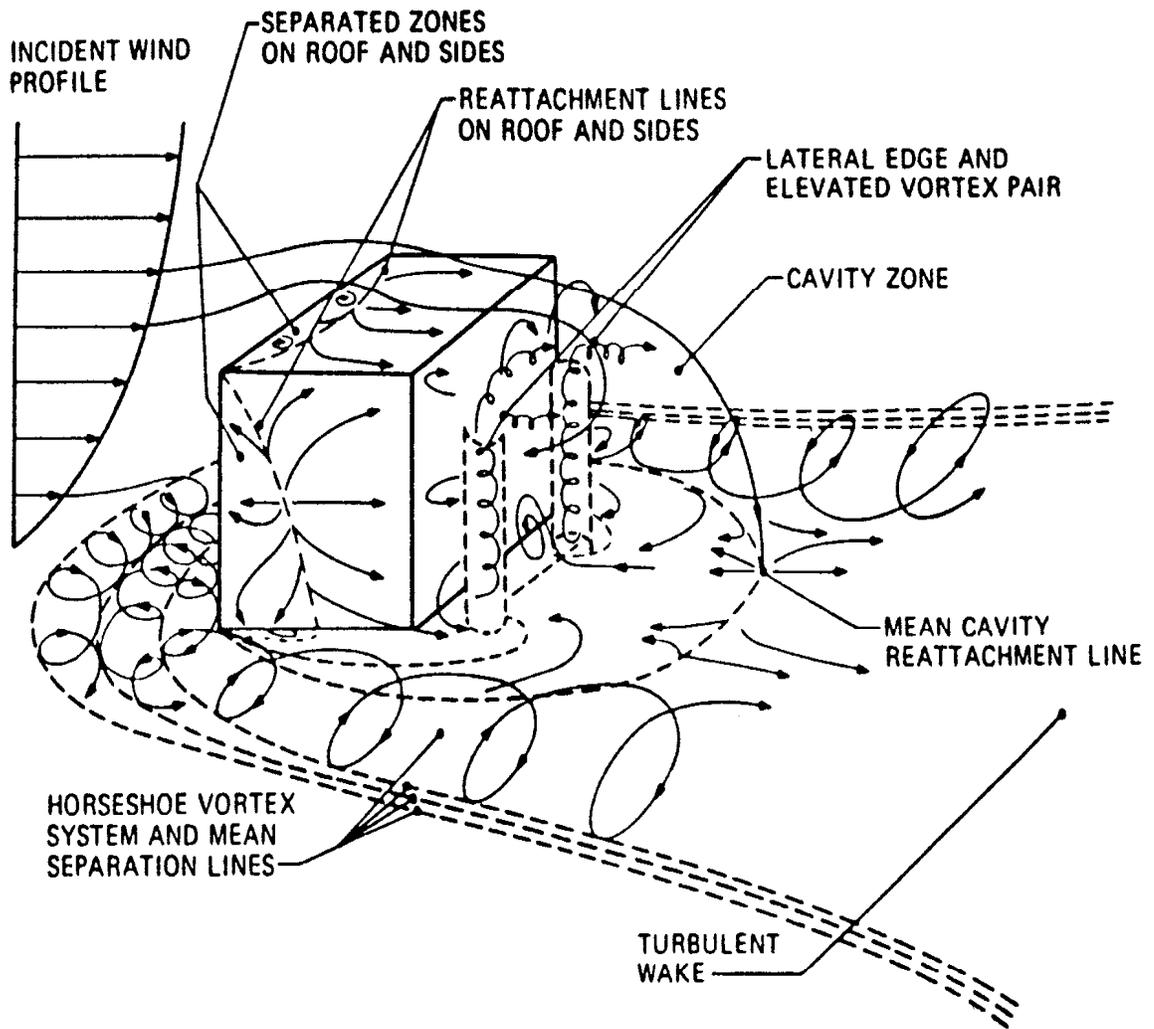
Figure 2-10.  Flow near a sharp-edged building in a deep boundary layer. (From Hosker, 1984)

A building is defined as a squat building if the projected building width, $H_w$, exceeds the building height (i.e., $H_w \geq H_b$ ). A tall building is defined as one for which $H_w < H_b$. Because both the controlling building height and projected width can vary with wind direction, the classification of a building as squat or tall can also vary by direction. For a squat building, the enhanced $\sigma_z$ is:

$$\sigma_z' = 0.7 \ H_b + 0.067 \left(x - 3H_b\right) \tag{2-108}$$

where x is the downwind distance (in meters).

For a tall building,

$$\sigma_z' = 0.7 \ H_w + 0.067 \left(x - 3H_w\right) \qquad 3H_w < x < 10H_w \tag{2-109}$$

If the ratio $H_s/H_b$ is less than or equal to 1.2, the horizontal dispersion coefficient, $\sigma_y$, is enhanced. For a squat building with a projected width to height ratio ($H_w/H_b$) less than 5, the equation for $\sigma_y$ is:

$$\sigma_y' = 0.35 \ H_w + 0.067 \left(x - 3H_b\right) \qquad 3H_b < x < 10H_b \tag{2-110}$$

For buildings with ($H_w/H_b$) greater than 5, two options are provided for $\sigma_y$.

$$\sigma_y' = 0.35 \ H_b + 0.067 \left(x - 3H_b\right) \qquad 3H_b < x < 10H_b \tag{2-111}$$

or,

$$\sigma_y' = 1.75 \ H_b + 0.067 \left(x - 3H_b\right) \qquad 3H_b < x < 10H_b \tag{2-112}$$

Eqn. (2-111) results in higher centerline concentrations than Eqn. (2-112), and is considered as an upper bound estimate of the impacts of the source. The ISC3 manual suggests that Eqn. (2-112) is most appropriate if the source is located within 2.5 $H_b$ of the end of the building. Eqn. (2-111) is a better estimate if the source is located near the center of the building. However, in practice, the more conservative Eqn. (2-111) is usually used for regulatory applications regardless of the position of the stack.

For a tall building, the equation for $\sigma_y$ is:

$$\sigma_y' = 0.35 \ H_w + 0.067 \left(x - 3H_w\right) \qquad 3H_w < x < 10H_w \tag{2-113}$$

## 2.3.2    Schulman-Scire Downwash Procedure

The main features of the Schulman-Scire algorithm are that the effects of building downwash on reducing plume rise are incorporated, and the enhancement of $\sigma_z$ is a gradual function of effective plume

height rather than a step function. As noted above, both schemes use wind direction specific building dimensions.

The plume rise equations incorporating building downwash effects are discussed in Section 2.4.4. Wind tunnel studies of buoyant emissions from sub-GEP height stacks have shown that plume rise is decreased during downwash conditions (e.g., Huber and Snyder, 1976). The increased mechanical turbulence in the building wake leads to enhanced plume dispersion (reflected in the enhanced dispersion coefficients), which causes a rapid dilution of the plume. This dilution reduces the rate of rise of the plume and results in lower plume heights. As discussed in Section 2.4.4, the initially high dilution rate is modeled by applying an initial "dilution radius" to the plume. The inclusion of downwash effects in the plume rise equations is a key part of the Schulman-Scire downwash method.

The second component of the model is the linear decay function which is applied to the enhancement of $\sigma_z$. The vertical dispersion coefficient is determined as:

$$\sigma_z^{//} = A \; \sigma_z^{/}$$  (2-114)

where $\sigma_z^{/}$ is determined from Eqns. (2-108) and (2-109), and

$$A = \begin{cases} 1 & H_e \leq H_b \\ \dfrac{H_b - H_e}{2L_b} + 1 & H_b < H_e \leq H_b + 2L_b \\ 0 & H_b + 2L_b < H_e \end{cases}$$  (2-115)

## 2.4    Plume Rise

The plume rise relationships in the CALPUFF model are generalized to apply to a variety of source types and plume characteristics. The following effects are included in the plume rise algorithm:

- ·     Plume buoyancy and momentum
- ·     Stable atmospheric stratification
- ·     Partial penetration of the plume into an elevated stable inversion layer
- ·     Building downwash and stack-tip downwash effects
- ·     Vertical wind shear
- ·     Area source plume rise
- ·     Line source plume rise

### 2.4.1    Basic Plume Rise Equations

The basic point source plume rise relationships are based on the Briggs (1975) equations.  The plume rise due to buoyancy and momentum during neutral or unstable conditions, $z_n$ is:

$$z_n = \left[ 3F_m x / \left( \beta_j^2 u_s^2 \right) + 3Fx^2 / \left( 2\beta_1^2 u_s^3 \right) \right]^{1/3} \tag{2-116}$$

where, $F_m$     is the momentum flux ($m^4/s^2$),
       $F$     is the buoyancy flux ($m^4/s^3$),
       $u_s$     is the stack height wind speed (m/s),
       $x$     is the downwind distance (m),
       $\beta_1$     is the neutral entrainment parameter ($\sim 0.6$),
       $\beta_j$     is the jet entrainment coefficient ($\beta_j = 1/3 + u_s/w$), and
       $w$     is the stack gas exit speed (m/s).

The distance to final plume rise, $x_f$, is:

$$x_f = \begin{cases} 3.5x^* & F > 0 \\ 4\,D\left( w + 3u_s \right)^2 / \left( u_s w \right) & F = 0 \end{cases} \tag{2-117}$$

where D is the stack diameter (m), and

$$x^* = \begin{cases} 14\ F^{5/8} & F \le 55 m^4/s^3 \\ 34\ F^{2/5} & F > 55\ m^4/s^3 \end{cases} \tag{2-118}$$

During stable conditions, the final plume rise, $z_{sf}$, is determined by:

$$z_{sf} = \left[ 3F_m / \left( \beta_j^2 u_s S^{1/2} \right) + 6F / \left( \beta_2^2 u_s S \right) \right]^{1/3} \tag{2-119}$$

where, $\beta_2$     is the stable entrainment parameter ($\sim 0.36$),
       $S$     is a stability parameter $[(g/T_a)(d\theta/dz)$,
       $g$     is the acceleration due to gravity  ($m/s^2$),
       $T_a$     is the ambient temperature (deg. K), and
       $d\theta/dz$     is the potential temperature lapse rate (deg. K/m).

Transitional plume rise during stable conditions is computed by Eqn. (2-116) up to the point at which $z_n = z_{sf}$.

For low wind speed and calm conditions during neutral or unstable conditions, a minimum wind speed of $u_s = 1$ m/s is imposed.  During stable conditions, the following equation (Briggs, 1975) is used to

compute the plume centerline rise for buoyant plumes:

$$z_{sf} = 4 \ F^{1/4} / S^{3/8}$$

(2-120)

Momentum rise during stable conditions is computed with a minimum wind speed of $u_s = 1$ m/s, but this is not allowed to exceed the momentum rise for neutral conditions.

## 2.4.2    Stack-tip Downwash

If the ratio of the stack gas exit speed to the ambient wind speed at the top of the stack is less than 1.5, the plume may be drawn into the lee of the stack.  Briggs (1973) suggests modifying the stack height to adjust for this stack-tip effect:

$$h_s^{/} = \begin{cases} h_s + 2D\left(w / u_s - 1.5\right) & w / u_s < 1.5 \\ h_s & w / u_s \geq 1.5 \end{cases}$$

(2-121)

where D is the stack diameter ans $h_s^{/}$ is the adjusted stack top height.

## 2.4.3    Partial Plume Penetration

Plumes from tall stacks may frequently interact with the capping inversion at the top of the mixed layer. A fraction of the plume mass may penetrate the inversion, and therefore be unavailable for immediate mixing to the ground.  Manins (1979) developed a procedure for estimating partial plume penetration into an elevated inversion using water tank experimental data.  This scheme is adopted for use in CALPUFF.

A penetration parameter, P, and the corresponding fraction, f, of the plume remaining below the inversion, is defined as:

$$P = \frac{F_b}{u_s \ b_i \ (h-h_s)^2}$$

(2-122)

$$f = \begin{cases} 1 & (P < 0.08) \\ \dfrac{0.08}{P} - P + 0.08 & (0.08 < P \leq 0.3) \\ 0 & (P > 0.3) \end{cases}$$

(2-123)

where $u_s$ is the stack height wind speed,

$F_b$ is the initial buoyancy of the stack emissions,

h is the height of the inversion

$h_s$ is the height of the stack

$b_i$ is the strength of the inversion ($b_i = g\Delta T_i/T_a$),

$\Delta T_i$ is the temperature jump across the inversion,

$T_a$ is the ambient air temperature, and

g is the acceleration due to gravity.

Thus, no penetration is predicted for P < 0.08, and nearly full penetration is suggested for P = 0.3 and above. Manins (1979) compared this scheme with the partial penetration methods of Briggs (1969) and Briggs (1975) using water tank data. He found that the Briggs (1969) model underestimates the amount of penetration into the inversion layer, while the Briggs (1975) method tends to overestimate it. Field data collected at the Gladstone power station in Queensland, Australia also supported these conclusions (Manins, 1984).

Knowing f from Eqn. (2-123), the effective final rise of plume material below ($z_{p1}$) and above ($z_{p2}$) the inversion are given by:

$$z_{p1} = \left( 1 - \frac{f}{3} \right) (h - h_s) \qquad (2\text{-}124)$$

$$z_{p2} = (2 - f)(h - h_s) \qquad (2\text{-}125)$$

The rise actually used for the mass below the inversion is estimated as the minimum of ($z_n$, $z_{p1}$) where $z_n$ estimated as the minimum of ($z_n$, $z_{p1}$) where $z_n$ is evaluated at $x = x_f$. Note that $z_n$, $z_{p1}$, and $z_{p2}$ are measured above the stack top height. Eqn. (2-125) is from Hanna and Chang (1991).

Eqns. (2-124) and (2-125) apply only for plumes which partially penetrate the inversion. If all of the plume penetrates the inversion (i.e., f=0), the plume rise $z_{p2}$ is computed following Briggs (1975). The final rise is the minimum of $z_n$ and $z_p$, where $z_p$ is a stable rise formula that depends on the inversion height above the stack, and the temperature stratification above the inversion height:

$$z_p = \left[ 1.8 \ (h - h_s)^3 + 18.25 \ F \ /(u_s S) \right]^{1/3} \qquad (2\text{-}126)$$

### 2.4.4 Building Downwash

Wind tunnel observations of plume dispersion and plume rise indicate that plume rise can be significantly reduced by building downwash. Huber and Snyder (1982) found that during downwash conditions,

plume rise was reduced by one-third below the value obtained in the absence of the building. In an analysis of plume rise observations, Rittmann (1982) found lower plume rise than predicted by the 2/3 law (a form of Eqn. 2-116) for smaller sources which are most likely to be affected by downwash. Several studies (e.g., Bowers and Anderson, 1981; Scire and Schulman, 1981; Thuillier, 1982) with the original version of the ISC building downwash algorithm, which did not account for the effects of building downwash on plume rise, showed that neglecting building downwash effects on plume rise can significantly underestimate peak concentrations during downwash conditions.

The increased mechanical turbulence in the building wake which leads to enhanced plume dispersion, causes a rapid dilution of the plume. This dilution reduces the rate of rise of the plume and leads to lower plume heights. One method of treating the initially high dilution rate is to assume an initial "dilution radius" for the plume (Scire and Schulman, 1980). This technique is incorporated in the Buoyant Line and Point Source (BLP) model (Schulman and Scire, 1980) and a modified version of the ISC model. It has been shown (Schulman and Hanna, 1986), to produce more realistic estimates of ground-level concentrations during building downwash conditions.

The plume rise of a downwashed plume with $\sigma_{yo} \le \sigma_{zo}$ during neutral-unstable conditions is given by:

$$z_d^3 + \left(3R_o z_d / \beta_1 + 3R_o^2 / \beta_1^2\right) z_d = 3F_m x / \left(\beta_j^2 u_s^2\right) + 3Fx^2 / \left(2\beta_1^2 u_s^3\right) \tag{2-127}$$

where $R_o$ is the dilution radius $[R_o = (2)^{1/2}\sigma_{zo}]$, and $\sigma_{yo}$, $\sigma_{zo}$ are the horizontal and vertical dispersion coefficients, respectively, at a downwind distance of $3H_b$ (see Section 2.3). The factor of $(2)^{\frac{1}{2}}$ in the $R_o$ equation converts the Gaussian dispersion coefficient into an effective top-hat distribution for the plume rise calculations.

Final stable plume rise is:

$$z_d^3 + \left(3R_o z_d / \beta_2 + 3R_o^2 / \beta_2^2\right) z_d = 3F_m / \left(\beta_j^2 u_s S^{1/2}\right) + 6F / \left(\beta_2^2 u_s S\right) \tag{2-128}$$

Transitional plume rise during stable conditions is computed with Eqn. (2-127) until the final plume height predicted by Eqn. (2-128) is obtained.

When horizontal mixing of the plume in the building wake causes $\sigma_{yo} > \sigma_{zo}$, it is necessary to account for the elongated shape of the plume. The plume can be represented as a finite line source. The plume rise for a line source of length $L_e$ during neutral-unstable conditions is:

$$z_d^3 + \left[3L_e / \left(\pi\beta_1\right)\right] z_d^2 + \left[3R_o z_d / \beta_1 + 6R_o L_e / \left(\pi\beta_1^2\right) + 3R_o^2 / \beta_1^2\right] z_d =$$
$$3F_m x / \left(\beta_j^2 u_s^2\right) + 3Fx^2 / \left(2\beta_1^2 u_s^3\right) \tag{2-129}$$

and, for final stable plume rise:

$$z_d^3 + \left[ 3L_e / \left(\pi\beta_2\right)\right]z_d^2 + \left[3R_o z_d / \beta_2 + 6R_o L_e / \left(\pi\beta_2^2\right) + 3R_o^2 / \beta_2^2\right]z_d =$$
$$3F_m / \left(\beta_j^2 u_s S^{1/2}\right) + 6F / \left(\beta_2^2 u_s S\right) \tag{2-130}$$

The effective line length, $L_e$, is $(2\pi)^{\frac{1}{2}}$ ($\sigma_{yo}$ - $\sigma_{zo}$) if $\sigma_{yo} > \sigma_{zo}$. Otherwise, $L_e = 0$, and Eqns. (2-129) and (2-130) reduce to Eqns. (2-127) and (2-128).

As described in Section 2.3, the enhanced dispersion coefficients, $\sigma_{zo}$ and $\sigma_{yo}$, vary with stack height, momentum rise, and building dimensions. The variation of $R_o$ with for several stack heights is illustrated in Figure 2-11. As $\sigma_{zo}$ and $\sigma_{yo}$ approach zero (i.e., building downwash effects become negligible), Eqns (2-119) to (2-120) approach the unmodified Briggs equations. The effect of $R_o$ and $L_e$ is always to lower the plume height, thereby tending to increase the predicted maximum ground-level concentration.

### 2.4.5   Vertical Wind Shear

The variation of wind speed up to stack height is usually accounted for in plume rise algorithms by the use of the stack height wind speed in the plume rise equations. Most formulations assume that the wind speed is constant above the stack top. This assumption is reasonable for mid-sized and tall stacks. However, the variation of wind speed above the stack top can have a significant effect on reducing the plume rise of buoyant releases from short stacks imbedded in the surface (shear) layer of the atmosphere (Scire and Schulman, 1980). Assuming the vertical wind speed profile above the stack can be approximated as $u(z) \simeq u_s(z/h_s)^p$, where $u_s$ is the wind speed at the stack top, $h_s$, and $u(z)$ is the wind speed at height z, the plume rise from a short stack can be represented during neutral and unstable conditions

as:
$$z_w = \left[\left[e^2 / (6 + 2p)\right] \left(F z_m^{3p}\right) / \left(\beta_1^2 u_m^3\right)\right]^{1/e} x^{2/e} \tag{2-131}$$

$$e = 3 + 3p \tag{2-132}$$

where p is the wind speed power law exponent.

During stable conditions, the final plume height is:

$$z_w = \left[\left[2 (3 + p)z_m^p F\right] / \left(\beta_2^2 u_m S\right)\right]^{1/(3+p)} \tag{2-133}$$

The wind shear exponent can be estimated from the atmospheric stability class or computed from the vertical wind data generated from the wind field model. It should be noted that Eqns. (2-131) and (2-133) both reduce to the Briggs buoyant plume rise equations when there is no wind shear above the stack top (i.e., p = 0).

I:\calpuff\uguide\nov99\sect2.wpd                                2-57

Figure 2-11.    Illustration of the initial dilution radius, $R_o$, as a function of stack height for a squat building (From Schulman and Scire, 1981).  Momentum plume rise is neglected in the figure.

The assumption of $u(z) \simeq u_s (z/h_s)^p$ is most valid for short stacks where the shear effect is expected to be the greatest. However, it breaks down for taller stacks. Therefore, Eqns. (2-131) and (2-133) are used to provide an upper limit of the plume height for short stacks, i.e., that the actual plume height be taken as the minimum of the predictions of the shear, downwash, and no-shear predictions, as appropriate.

2.4.6    Area Source Plume Rise

The treatment of plume rise from large buoyant area sources requires special considerations that include effects of vertical wind shear, large initial plume size, and potentially large density differences between the plume and ambient air.

The area source plume rise model in CALPUFF is formulated to calculate the rise of buoyant plumes resulting from forest fires, the burning of leaking oil, and other type of buoyant area sources. The model is designed to be general, with applicability to the following conditions:

    (a)    all types of ambient temperature stratifications;
    (b)    all types of wind stratifications;
    (c)    any size of finite emission source;
    (d)    includes the effects of plume radiative heat loss; and
    (e)    is free of the limitations of the Boussinesq approximation.

All these factors may be important in large forest fire plumes. Due to the complex mountainous terrain in many forested areas and the strong influence it has on meteorological conditions, complex temperature and wind patterns may exist. The ambient temperature stratification is usually more complicated than linear stratification which is normally assumed in most plume rise models. Wind shear is important because the forest fire plume starts at ground where there is a zone of large velocity gradients in the vertical. Therefore, it is necessary to allow for arbitrary profiles of winds and temperatures to be accounted for in the plume rise, including potential stability and wind reversals in the vertical. The initial fire size may be large, of the order of ten or more kilometers in radius. Since the plume temperature near the burning source is much higher than the ambient air temperature, up to 1600 °K, radiative heat loss will reduce the heat flux which is carried by the plume along its trajectory. This reduction of heat flux also reduces the buoyancy flux and thus eventually reduces the final plume rise. Also, since the initial temperature of the plume is high, and the initial density difference between the plume and ambient air is large, the application of Boussinesq approximation becomes questionable.

The source parameters of a forest fire are usually not constant. The life cycle of a forest fire includes an initial developing stage with large increases in heat generation and pollutant emission rates, followed by a stage of decreasing values. The magnitude of the variation in heat generation and emission rates may be two orders of magnitude over the course of burn. The resulting time dependency to the plume rise can

be calculated assuming that the plume motion is quasi-steady so that the input of source condition is time-dependent but the time-derivatives in the governing equations are neglected. This assumption is reasonable because the time scale for plume rise is much shorter than that of the fire life-span.

The derivation of the governing equations are similar to the one given by Weil (1988) except that the Boussinesq approximation has not been applied. The Boussinesq approximation simplifies the plume rise equations by assuming that the plume density is close enough to the ambient density that density variations, other than in the buoyancy term, can be neglected. The plume cross section is assumed to be circular with radius r. (Although the plume cross section, as it rises, appears to be dominated by a pair of counter-rotating line vortices, its effect on the plume rise trajectory can still be well quantified by integral models (Zhang, 1993)). All the physical quantities are assumed to be uniform within this cross section. The mass conservation law can be expressed in terms of entrainment hypothesis, which accounts for the entrainment of the ambient air flowing both parallel and cross the plume centerline (Hoult and Weil, 1972),

$$\frac{d}{ds}\left(\rho U_{sc} r^2\right) = 2 r \alpha \rho_a \left|U_{sc} - U_a \cos\varphi\right| + 2 r \beta \rho_a \left|U_a \sin\varphi\right| \tag{2-134}$$

where $\alpha = 0.11$ and $\beta = 0.6$ are the entrainment parameters corresponding to the differences of velocity components between the wind and the plume in directions parallel and normal to the plume centerline, respectively (Weil, 1988); $U_a$ (z) is the ambient horizontal wind speed, which can be an arbitrary function of height; and

$$U_{sc} = \sqrt{u^2 + w^2} \tag{2-135}$$

is the velocity of the plume cross section along its centerline, with two components u and w in the horizontal and vertical directions, $\rho$ and $\rho_a$ are the plume density and air density, respectively, s is the length of the plume centerline measured from the emission source, and $\varphi$ is the centerline inclination. See Figure 2-12 for a schematic view of the plume rise and various variables.
The momentum equation in the wind direction is

$$\frac{d}{ds}\left(\rho U_{sc} r^2 \left(u - U_a\right)\right) = -r^2 \rho w \frac{dU_a}{dz} \tag{2-136}$$

where the right hand side is related with the wind shear. The momentum equation in the vertical direction is a balance among inertial acceleration, entrained momentum, and buoyancy:

$$\frac{d}{ds}\left(\rho U_{sc} r^2 w\right) = g r^2 \left(\rho_a - \rho\right) \tag{2-137}$$

where g is the gravitational acceleration.
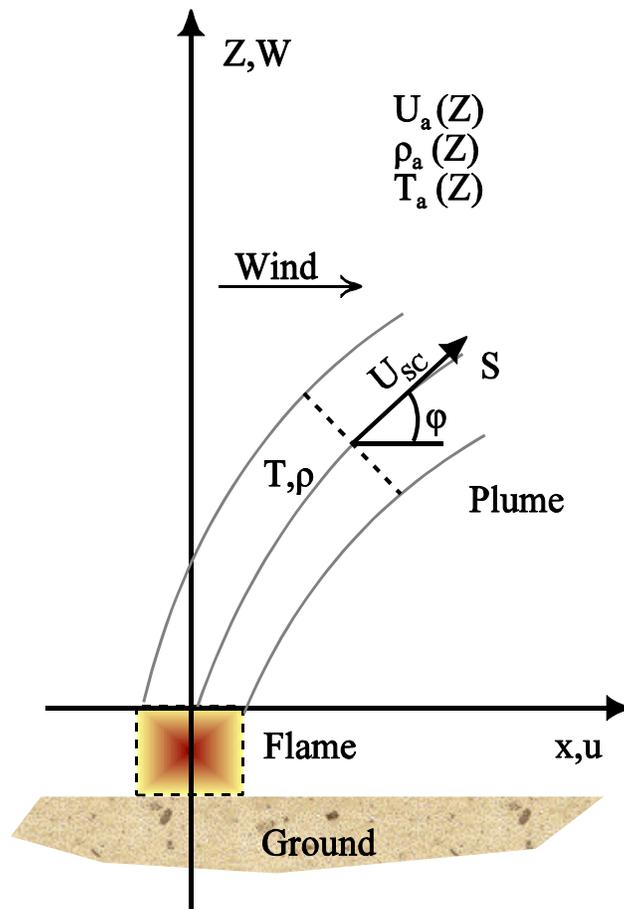
Figure 2-12.    Schematic and nomenclature for plume in a crosswind.

The energy equation can be written as

$$\frac{d}{ds}\left(\rho \, U_{sc} \, r^2 \, (T - T_a)\right) = \rho \, \frac{d\eta_a}{dz} \, w \, r^2 + \frac{Q}{c_p} \, r^2 \tag{2-138}$$

where

$$\frac{d \, \eta_a}{dz} = \frac{dT_a}{dz} + \frac{g}{c_p} \tag{2-139}$$

is the vertical lapse rate of the ambient potential temperature. The constant on the right hand side is

$$\frac{g}{c_p} = 9.76 \, x \, 10^{-3} \, °K \, /m \tag{2-140}$$

where $c_p$ is the specific heat of the ambient air.

The last term in Eqn. (2-138) corresponds to the radiative heat loss from the plume to the ambient air. This term is expected to be important only initially when the plume temperature is high. Q is the heat loss per unit volume of the plume. This last term can be estimated by

$$\frac{Q}{c_p} \, r^2 = -2 \, \varepsilon \, \sigma \, r \left(T^4 - T_a^4\right)/c_p = -R_p \, r\left(T^4 - T_a^4\right) \tag{2-141}$$

where $\sigma$ and $\varepsilon$ are the Stefan-Boltzmann constant and the emissivity respectively, and $R_p = \dfrac{2 \, \varepsilon \, \sigma}{c_p}$ is a

variable which characterizes the radiation properties.
If we choose,

$$c_p = 10^3 \, J / kg{\cdot}K, \sigma = 5.67 \, x \, 10^{-8} \, \frac{W}{m^2 K^4} \tag{2-142}$$

and let $\varepsilon = 0.8$, then $R_p = 9.1 \times 10^{-11}$ kg/m²K³s. The energy equation finally becomes

$$\frac{d}{ds}\left[\rho \, U_{sc} \, r^2 \, (T - T_a)\right] = -\left(\frac{dT_a}{dz} + \frac{g}{c_p}\right) \rho \, w \, r^2 - R_p \, r\left(T^4 - T_a^4\right) \tag{2-143}$$

It is expected that the radiative heat loss is large for high T and small r.

In deriving Eqns (2-136) and (2-138), it is assumed that the ambient wind is horizontal and the vertical gradients of ambient properties $\dfrac{dU_a}{dz}, \dfrac{dT_a}{dz}$ do not vary significantly across the plume cross section.

To close the equation set, two geometric relations are needed:

$$\frac{dz}{ds} = \frac{w}{U_{sc}} = \sin \varphi \tag{2-144}$$

$$\frac{dx}{ds} = \frac{u}{U_{sc}} = \cos \varphi \tag{2-145}$$

These equations can be solved subject to the following initial conditions and ambient meteorological conditions. Initial conditions are specified at the source location s = 0, where x = 0. The following information is needed as input: plume density, $\rho_o$; vertical velocity, $w_o$; plume radius, $r_o$; and temperature, $T_o$. The ambient conditions are specified in terms of horizontal wind profile, $U_a(z)$, and air temperature profile, $T_a(z)$. (In the case of a forest fire plume, the source parameters are to be provided by EPM and the meteorological conditions by the CALMET model.)

Most meteorological observations give the atmospheric stratification in the form of temperature distribution versus pressure. To obtain relations of air density versus height, and plume density versus height, it is assumed that the atmospheric pressure distribution can be approximated as that of an adiabatic atmosphere.

$$p = p_o \left[ 1 - \frac{\gamma - 1}{\gamma} \frac{gz}{RT_{ao}} \right]^{\frac{\gamma}{\gamma - 1}} \tag{2-146}$$

where $T_{ao}$ is the ground level air temperature. Based on (2-146), if the air temperature and plume temperature are $T_a$ and T respectively at height z, the corresponding densities can be obtained as

$$\rho_a = \frac{p(z)}{RT_a} \quad and \quad \rho = \frac{p(z)}{RT} \tag{2-147}$$

where R is the gas constant of the ambient air and the plume.
The equations described above are solved numerically using a second order, marching in s, Heun's predictor-corrector scheme:

$$\frac{dy}{ds} = f(s, y) \tag{2-148}$$

$$y* = y^n + f(s^n, y^n) \Delta s \tag{2-149}$$

$$ y^{n+1} = y^n + \frac{1}{2} \left[ f\!\left(s^n, y^n\right) + f\!\left(s*, y*\right) \right] \Delta s \qquad (2\text{-}150) $$

2.5    Overwater and Coastal Dispersion

There are important differences in the structure of the marine and continental boundary layers which can have significant effects on plume dispersion in the overwater and coastal environments. These differences arise for three basic reasons (LeMone, 1978):

- Water has a high heat capacity and is partially transparent to solar radiation, resulting in a relatively small diurnal temperature range (~ 0.5 deg. C).
- The sea surface is generally more uniform and less aerodynamically rough than typical land surfaces.
- There is a constant source of moisture in the marine boundary layer.

As a result of these differences, the sensible heat flux over the open water is typically more than an order of magnitude less than that over land.  The absence of a strong sensible heat flux to drive the marine mixed-layer and the small surface roughness result in relatively low mixing heights that offer the potential for significant plume trapping effects.  LeMone (1978) indicates that the typical marine mixing depth is only about 500 m.  Data from three offshore and coastal experiments reported by Hanna et al. (1985) (two of which were conducted in California) show many hours with mixing heights less than 100 m.

Another result is that the diurnal and annual variations of stability over water are unrelated to the typical overland behavior.  For example, North Sea observations of water and air temperatures reported by Nieuwstadt (1977) (Figure 2-13) show that temperature inversions typically persist most of the day in June, while unstable conditions occur all day in January.  During other times of the year, the overwater diurnal stability cycle is out of phase with the overland cycle (i.e., stable over water during the day and unstable at night).

The techniques used in the CALMET meteorological model for determining overwater mixing height, stability, and surface layer parameters are based on the air-sea temperature difference, wind speed, and the specific humidity (Scire et al., 1998).  These methods are applied by CALMET to the portions of the modeling domain over water.  At the land-sea interface, rapid changes in the dispersion characteristics may occur which can significantly affect the ground-level concentrations from coastal sources.  The puff model formulation is well-suited to accommodate these spatial changes in the coastal transition zone.
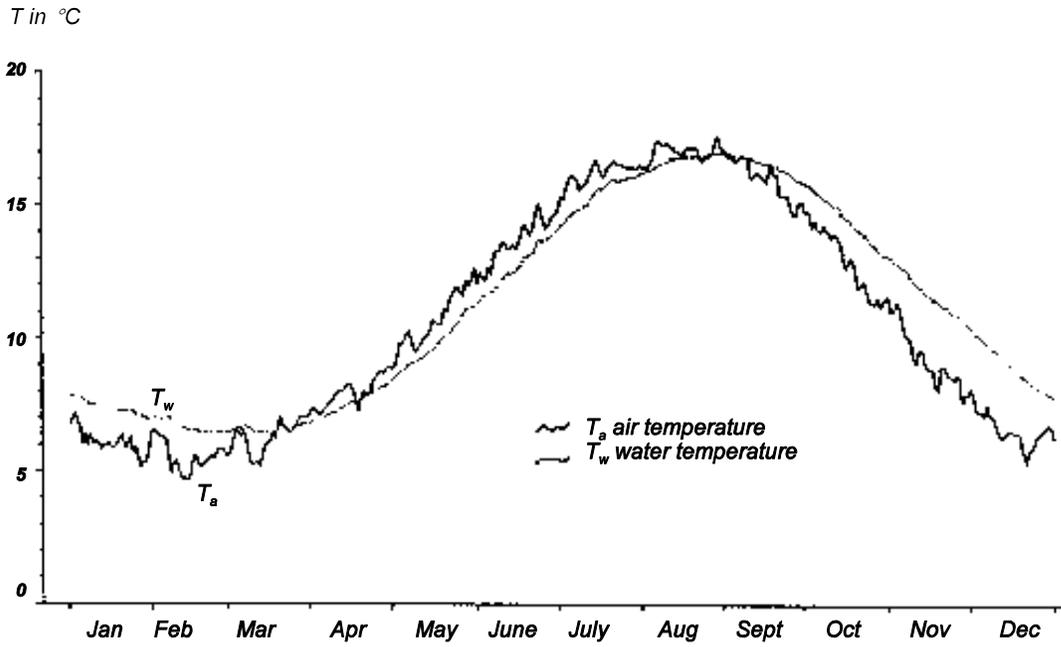
Figure 2-13. Daily average air and water temperatures measured in the North Sea (from Nieuwstadt,1977).
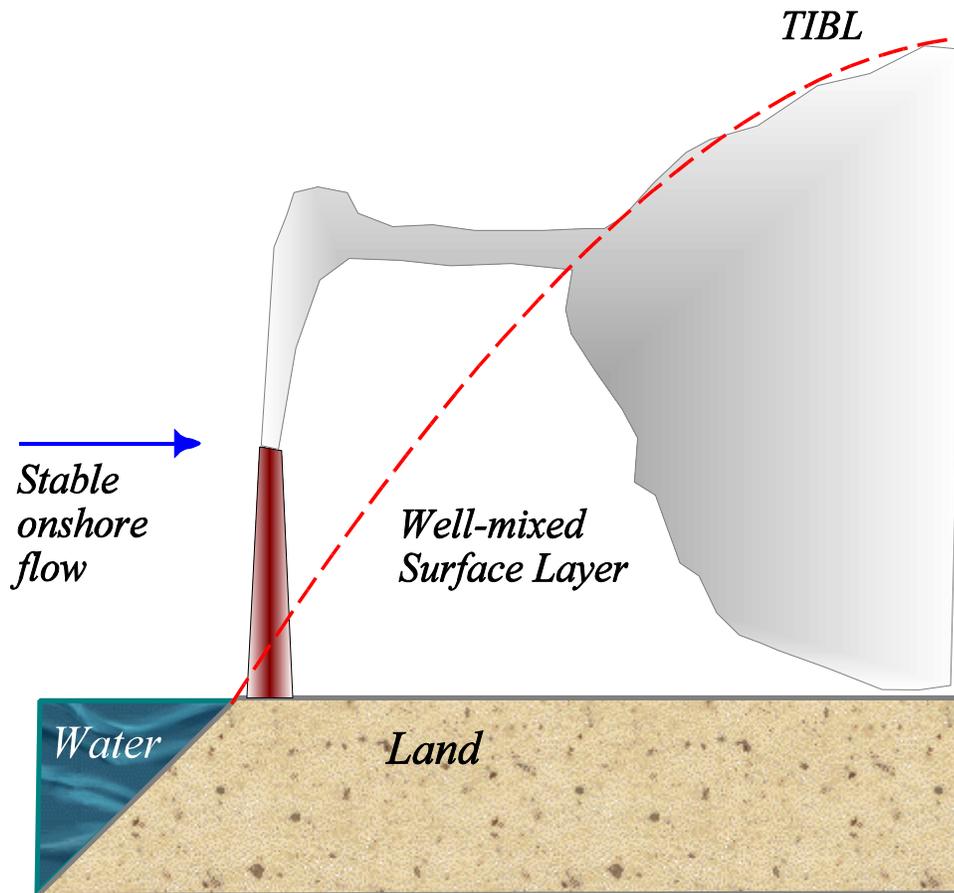
Figure 2-14.    Schematic illustration of a typical coastal fumigation condition (from Hanna et al., 1985).

A typical situation during stable onshore flow conditions is shown in Figure 2-14.  A narrow plume imbedded in the stable layer above the shallow marine surface layer is intercepted by a growing Thermal Internal Boundary Layer (TIBL) over land.  The growth of the TIBL is caused by the sensible heat flux associated with solar heating of the land surface.  The convection over land can rapidly bring the elevated pollutant to the ground, causing locally high ground-level concentrations.  Many coastal fumigation models assume immediate mixing of the pollutant intercepted by the TIBL to the ground (e.g., Lyons and Cole, 1973, Misra, 1980).  Deardorff and Willis (1982), based on laboratory experiments, suggest the importance of turbulent fluctuations in the TIBL height and indicate that the plume does not become well-mixed immediately.  In the Offshore and Coastal Dispersion (OCD) model, Hanna et al. (1985) use the minimum concentration predicted by a virtual source technique or that predicted by the Deardorff and Willis model to describe shoreline fumigation.

In CALPUFF, the land-sea interface is typically resolved on the scale of the computational grid.  The model computes turbulence and dispersion characteristics that are consistent with the land use properties of each cell in the grid, whether the cell is classified as water or land, for the gridded meteorological fields provided by CALMET.  The transition from marine to continental dispersion rates  occurs at the coastal boundary determined from these land use data.  Once a puff within a marine layer enters the mixed layer over land, the puff growth is changed from that appropriate for the marine layer to that appropriate for the overland boundary layer.

A sub-grid scale TIBL module (SGTIBL) is provided for cases in which the position of the coastal boundary within a grid cell and the growth of the TIBL must be modeled with greater spatial resolution.  SGTIBL accepts a piecewise linear representation of the coastline explicitly, and for onshore puff transport during convective conditions, it

- subdivides the sampling step into smaller sub-steps
- computes the change in the local TIBL height for each sub-step
- defines the appropriate dispersion properties for the puff

and then proceeds with the normal puff transport and sampling computations.  This sequence preserves the spatial relationships among the puff trajectory (determined by the source location and the CALMET wind field), the position of the coast, the rate of growth of the TIBL, and the receptor positions.  The boundary layer is characterized by the local grid cell properties if the step occurs within a cell that does not contain a coastline segment.  Otherwise, it uses the nearest land or water cell properties, depending on the relative location of the step and the coastline.  Therefore, the coastline must be consistent with the gridded land use data --- there must be at least one predominantly water cell and one predominantly land cell adjacent to any cell through which a coastline passes.  Once a puff crosses a coastline from water to land during conditions conducive to the formation of a TIBL, the current mixing height for the puff grows with distance along the trajectory of the puff.  The TIBL treatment for such a puff continues until the calculated TIBL height exceeds the mixed layer height for the local cell, or if the conditions for the

TIBL subside (e.g., the puff could move back out over the water, or it could be late in the day). Note that CALPUFF adopts the minimum sensible heat flux criterion of 5 W/m$^2$ used by the Shoreline Dispersion Model (SDM) (EPA, 1988) as a necessary condition for invoking SGTIBL.

The growth of the TIBL is based on the model presented by Garratt (1992). In the absence of subsidence, the conservation equations for the zero-order jump (or slab) model of the convective boundary layer (CBL) give

$$\frac{\partial h_T}{\partial x} = \frac{(1+2\beta) \; H_0(x)}{\gamma \; \rho c_p \; u \; h_T} \tag{2-151}$$

which, when integrated a distance s along sampling sub-step n for constant $H_0$, $\gamma$, and u gives

$$h_T(s) = \sqrt{\frac{2(1+2\beta) \; H_{0n}}{\gamma \; \rho c_p \; u_n} \; s \; + \; h_{T0}{}^2} \tag{2-152}$$

where

$\quad$ $h_T$ $\qquad$ is the TIBL height (m)

$\quad$ $h_{T0}$ $\qquad$ is the TIBL height at the start of the sub-step (m)

$\quad$ $H_0$ $\qquad$ is the surface sensible heat flux (W/m$^2$) over land

$\quad$ $\gamma$ $\qquad$ is the (constant) potential temperature gradient (K/m) above the mixed layer

$\quad$ $\rho$ $\qquad$ is the density of the air at the surface (kg/m$^3$)

$\quad$ $c_p$ $\qquad$ is the specific heat at constant pressure (J/kg/K)

$\quad$ u $\qquad$ is the mean wind speed within the TIBL (m/s)

$\quad$ $\beta$ $\qquad$ is the ratio of the downward heat flux at the TIBL height to the upward heat flux at the surface, $\approx$ 0.2 for the CBL over land

$\quad$ n $\qquad$ subscript indicates that a constant value is used for step n.

The $\beta$ parameter is introduced by a closure assumption used in the CBL model, that the entrainment flux at the top of the layer is a constant fraction of the surface flux. A value of zero indicates that there is no entrainment at the top of the layer, and so the mixed layer height grows solely due to the heat input at the surface, which warms the mixed layer. With no entrainment at the top of the layer, the potential temperature at the top is equal to that of the mixed layer. The complementary limit of $\beta = \infty$ indicates that the surface layer grows by mechanical entrainment at the top of the layer alone (no heat flux at the surface), which produces a mechanically mixed layer whose potential temperature is the average temperature of the original potential temperature profile over the depth of the layer. The potential temperature jump at the top of layer of thickness h is $\gamma h/2$. The CBL typically grows due to both the heat flux at the surface, and due to an entrainment flux across the top of the layer, thereby resulting in a temperature jump at the top. Garratt reports that $\beta = 0.2$ is supported by the bulk of experimental data for the daytime CBL over land. Note that SDM uses the TIBL height equation of Weisman (1976), which is equivalent to Eqn. (2-152) with $\beta = 0$.

2.6     Complex Terrain

The effect of terrain on ground-level concentrations is simulated in CALPUFF in three ways:

1.      Adjustment of the wind field to large-scale terrain features (CALMET);
2.      Explicit simulation of puff-terrain interaction for distinct features too small to influence the large-scale wind field;
3.      "Simplified" treatment for puff-terrain interaction with both large and small-scale features.

This allows CALPUFF to respond to the presence of terrain on two scales. Options are available in CALMET for invoking either a diagnostic or prognostic wind field model to simulate the response of the large-scale flow to the presence of terrain. The effect of terrain that extends over a scale large enough to be resolved by the grid used in CALMET will be manifest in the boundary conditions for the flow field. A puff embedded in this flow will either rise with the flow along the surface of the terrain, or it will be steered by the flow along the terrain, depending on the degree of stratification. Smaller-scale terrain features encountered by a puff in this flow can then be simulated explicitly by a separate subroutine, CTSG (Complex Terrain algorithm for Sub-Grid-scale features), that embodies the methods used in the Complex Terrain Dispersion Model (CTDM). Concentration estimates on any terrain features not treated by CTSG (this is an option in CALPUFF) include simpler adjustments to the effective height of the puff above the ground, and/or to the size of the puff in the vertical. Three options are provided for this type of adjustment, including the original "ISC" treatment, the plume path coefficient treatment, and a new treatment that draws on CTSG concepts, without requiring the terrain description procedures of CTSG. Section 2.6.1 provides a complete description of the CTSG module and Section 2.6.2 describes the alternative terrain adjustment procedures.

2.6.1    Complex Terrain Algorithm for Sub-grid Scale Features (CTSG)

CTSG accepts the flow field produced by the flow model (both the wind and temperature structure) in the vicinity of a terrain feature as the incident flow toward that feature. It then proceeds to simulate changes in the flow and in the rate of dispersion that are induced by that terrain feature. At the core of CTSG is the modeling approach adopted in CTDM, the complex terrain model developed in EPA's Complex Terrain Model Development program. Our goal in designing CTSG is to produce a puff algorithm that contains those elements of the CTDM approach that have the greatest impact on ground-level concentrations.

Figure 2-15 illustrates the intended role of CTSG in the CALPUFF system. In the upper panel of the figure, cross-section of steep terrain rising with distance inland from a coast is depicted. The vertical dashed lines show the boundaries of a grid used by the wind-field model. The idealized terrain consists of a nearly uniform slope over much of the grid-square, plus a secondary feature right at the coast.

At night, one might imagine a puff of material traveling down this slope in a drainage flow toward the secondary feature. The interaction of the puff with this secondary feature would be simulated by CTSG.

In the lower panel, the puff is shown as it is "seen" in the modeling system. The wind model provides the transport speed and direction for the puff, and concentrations are computed at receptors beneath the puff as if the terrain were flat. However, the secondary feature is now represented as an obstacle to the flow, and CTSG produces concentrations at receptors on this feature using methods developed for CTDM.

2.6.1.1 Modeling Regions

A central feature of CTDM adopted for use in CTSG is the dividing-streamline concept. The flow is taken to be composed of two layers. In the upper layer, the approach flow has sufficient energy to transport a fluid parcel up and over the hill against a stable potential density gradient. In the lower layer, the flow is constrained to travel around the hill. This concept was suggested by theoretical arguments of Drazin (1961) and Sheppard (1956) and was demonstrated through laboratory experiments by Riley et al. (1976), Brighton (1978), Hunt and Snyder (1980), Snyder (1980), and Snyder and Hunt (1984). $H_d$, the dividing-streamline height (m), is obtained from profiles of wind speed (m/s) and temperature (as the Brunt-Vaisala frequency, N (1/s)). $H_d$ is computed for each hill by locating the lowest height at which the kinetic energy of the approach flow just balances the potential energy attained in elevating a fluid parcel from this height to the top of the hill.

The statement that defines this balance is:

$$.5 \; u^2 \left( H_d \right) = \int_{H_d}^{H} N^2(z) \left[ H - z \right] dz \qquad (2\text{-}153)$$

where $u(H_d)$ is the wind speed at $z = H_d$, H is the elevation of the top of the hill, and N(z) is the Brunt-Vaisala frequency at height z. In practice, the value of $H_d$ is obtained by rewriting the integral on the right-hand side (RHS) of Eqn. (2-153) as a sum over layers of constant N. For layer n,

$$RHS_n = RHS_{n+1} + \int_{z_n}^{z_{n+1}} N_n^2 \left( H - z \right) dz = N_1^2 \left( H - z_{mn} \right) \left( z_{n+1} - z_n \right) \qquad (2\text{-}154)$$

where $z_{mn}$ denotes the mean height of the layer, 0.5 $(z_{n+1} + z_n)$. The layer that contains $H_d$ is found by comparing the LHS of Eqn. (2-153) at each measurement height n with the corresponding $RHS_n$, starting with the layer that contains the top of the hill. If $LHS_n$ exceeds $RHS_n$, then $H_d$ must lie below $z_n$, and so the process is repeated until the lowest layer is found in which the LHS becomes less than the RHS (in the layer above, the LHS is greater than the RHS). This then identifies the layer that contains $H_d$. $H_d$ is then computed within this layer by assuming that the wind speed follows a linear profile. Denote this as layer j, where the elevations at the top and bottom of the layer are $z_{n+1}$ and $z_j$, respectively.

# CTSG TERRAIN MODULE

Cell Boundary

Puff

Terrain

CTSG Feature

Mean Cell
Elevation
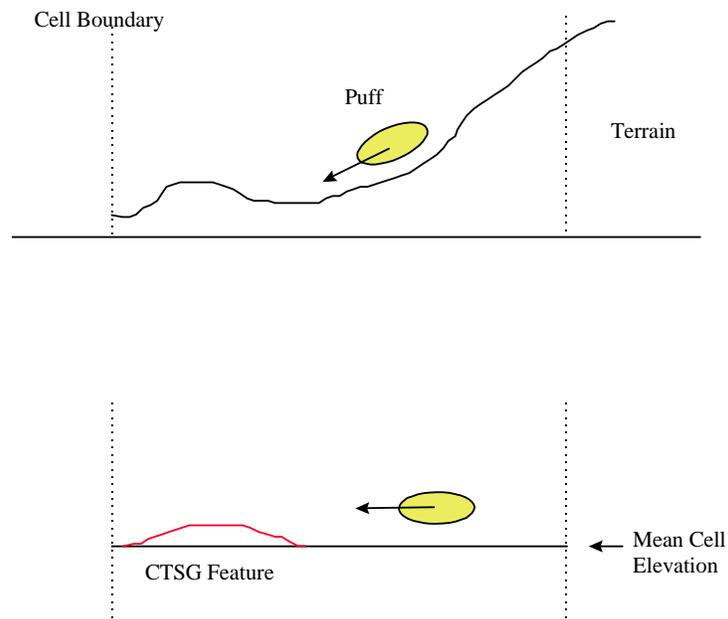
Figure 2-15.    Depiction of the intended use of CTSG.  The lower panel illustrates the portion of the
terrain present in the upper panel that can be simulated by CTSG, and it illustrates the
relationship between the gridded terrain, the modeled winds, and the CTSG terrain
feature.

Denote u(z) in the layer as

$$u(z) = a_j + b_j\, z \tag{2-155}$$

then Eqn. (2-153) becomes

$$\frac{1}{2}\left( a_j \,+\, b_j\, H_d \right)^2 \,=\, N_j^2 \left( H \,-\, 0.5 \left[\, z_{j+1} \,+\, H_d \,\right] \right) \left( z_{j+1} \,-\, H_d \right) \,+\, RHS_{j+1} \tag{2-156}$$

where the last term, $RHS_{j+1}$, denotes the value of the RHS from $z_{j+1}$ to the top of the hill. Eqn. (2-156) is quadratic in $H_d$, and is readily solved for $H_d$ .

Once $H_d$ is computed for a hill, the stratification length scale for the flow above $H_d$ is computed as $u_m/N_m$ where $u_m$ and $N_m$ are average values between $H_d$ and the first model-layer above the top of the hill. This length scale characterizes the degree of stratification of the flow above $H_d$. Note that $N_n$ is computed from the temperature difference across the layer.

Puff material above $H_d$, the dividing-streamline height, experiences an altered rate of diffusion in the deformed flow field over the hill. It is this change in the effective dispersion that leads to increased ground-level concentrations (GLC's) observed over hills when $H_d$ is zero. When $H_d$ is not zero, only that portion of the puff that lies above $H_d$ as the puff encounters the hill travels over the hill. The puff is modeled as if it were sheared off at $H_d$ so that material nearer the center of the puff may reach the surface without further dilution. The theory of diffusion of narrow plumes embedded in a deforming flow field (Hunt and Mulhearn, 1973) provides the basis for estimating GLC values in the upper layer (subroutine UPPER).

Puff material below $H_d$ is deflected around the hill, being embedded in a horizontal two-dimensional flow. The stagnation streamline in this flow forms the boundary of the hill and therefore separates portions of the puff which travel around one side or the other. The center of the puff is able to impinge on the hillside only if the puff is centered on the stagnation streamline, and lies below $H_d$. Concentration estimates from subroutine LOWER are based on the analysis of Hunt et al. (1979) which indicates that the GLC near the impingement point is essentially that obtained by sampling the puff (in the absence of the hill) along the stagnation streamline at the elevation of the receptor. As the puff encounters the hill, the lateral distribution of material in the puff is separated along the stagnation streamline, and each segment is allowed to travel around the hill with complete reflection at the plane z=0 as well as y=$Y_d$ (stagnation streamline), i.e., the hillside. Figure 2-16 illustrates how the puff material is treated in CTSG. For the sake of illustration, the outline of a continuous series of puffs is portrayed as a plume and the height of the center of the plume exceeds $H_d$.

Three regions are identified in the figure. Boundaries between these three regions are defined differently in the upper and lower layers, as discussed later. For illustration, we will consider the boundaries

identical, as drawn in Figure 2-16. The distinction between the upper flow and the lower flow as described above is strictly applied in region 2. Prior to this, in region 1, the portion of the puff above $H_d$ has not reached the hill (at $z = H_d$) and so the vertical structure remains continuous. Concentrations are estimated as if receptors in this region were positioned on poles. Receptors below $H_d$ in region 1 are placed on poles to simulate an impingement calculation. The pole height is equal to the height of the receptor above the base of the hill, and the lateral position of the pole is shifted to the location of the stagnation streamline. In essence, the flow below $H_d$ in region 1 is turned much as it is in region 2, but no reflection from the side of the hill is included. Receptors may also be located above $H_d$ in region 1.

Figure 2-17 depicts a situation in which departures in shape between the actual terrain feature and the simplified hill used in CTSG cause ground-level receptors to be placed above $H_d$ in region 1. In this case receptor 2 is also modeled as a receptor-on-a-pole, but the height of this pole is set to $H_d$, and its lateral position is the same as that of the receptor. This approach assumes that flow above $H_d$ is deflected in the vertical, but not in the lateral direction. No alterations are made to the dispersion rates. Differences in the way receptors in region 1 are treated can be summarized as follows: the flow above $H_d$ is considered to be terrain-following in the vertical, with no horizontal deflection, and the flow below $H_d$ is considered to be terrain-following in the horizontal, with no vertical deflection. Note that the stagnation streamline defines the boundary that shifts the flow left or right in the horizontal. Using $H_d$ in this way enforces a clear and sometimes abrupt distinction in the way concentrations may be obtained at nearby receptors. This can lead to discontinuities in concentrations determined at receptors that straddle $H_d$ just upwind of the hill, when the puff is located "far" from the stagnation streamline of the flow below $H_d$, yet travels toward the hill in the layer above $H_d$. Subroutine PUFFC performs these calculations in region 1. Details of the model for regions 2 and 3 are provided in the following subsections.

The CTSG algorithm may be invoked whenever concentration estimates are needed at receptors that are located on terrain elements that are not resolved by the grid in the flow-field model. It specifies the relationship between a single puff and all receptors on a single terrain feature for the current averaging/transport time-period. Consequently, CTSG is called for each puff/terrain-element pair during each time-step. Some reduction in execution time is gained by screening out puff/terrain-element pairs for combinations of puff size and position, relative to those of the terrain feature, that exhibit minimal terrain influence. These combinations are then modeled as if the terrain were absent.

2.6.1.2  Description of Terrain Features

CTSG uses simple analytical obstacle shapes to represent sub-grid scale terrain features. Below $H_d$, CTSG uses an elliptical cylinder to represent the hill. The axes and orientation of this ellipse represent the overall scale and orientation of the terrain feature at the minimum of the elevation of the puff, or $H_d$. Above $H_d$, CTSG uses a Gaussian shape to represent the hill. The height of the Gaussian hill is equal to the difference in height from the peak of the hill to $H_d$. The horizontal length scales and orientation of the hill are chosen so that the lateral extent of the Gaussian hill at one half its height is representative of
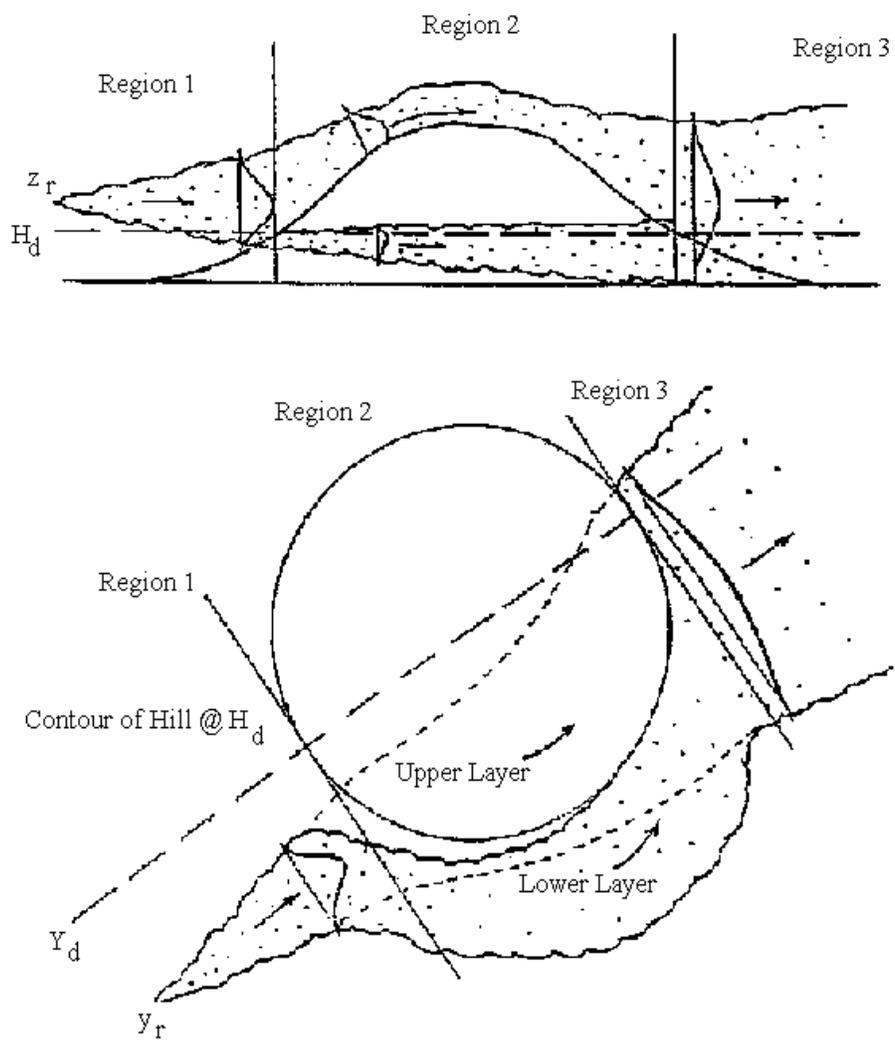
Figure 2-16.    Illustration of modeling regions and partitioning of the flow above and below the dividing-streamline height, $H_d$.

## Actual Receptor Heights



**Actual Hill Shape**

1

2

Modeled Hill Shape

$H_d$
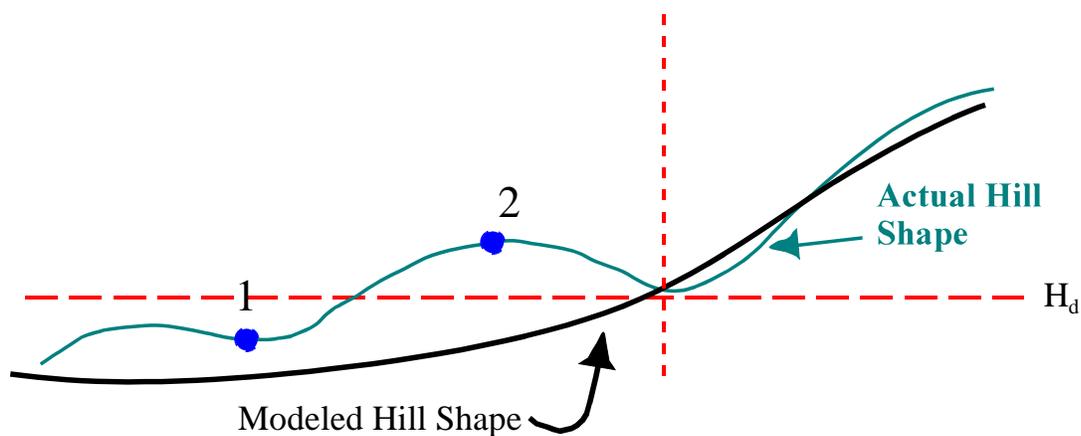
## Modeled Receptor Heights



Region 1

Region 2

1

2

$H_d$
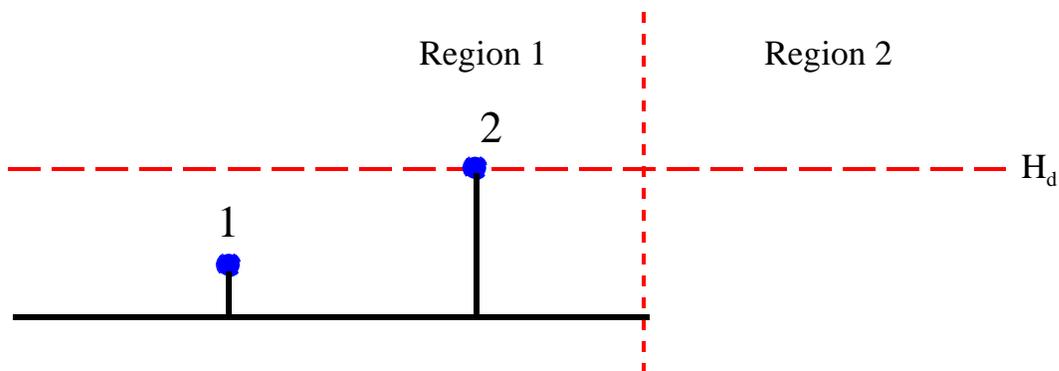
Figure 2-17.     Treatment of height of receptors located upwind of the impingement point (Region 1).

the scale of the terrain feature half way between $H_d$ and the top of the hill.  When the major axis of the hill lies along the x-axis of the coordinate system, these shapes are defined by :

$$ellipse: \quad 1 = \left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 \qquad (2\text{-}157)$$

$$Gaussian: \quad h = H \, e^{-(x/L_x)^2} \, e^{-(y/L_y)^2} \qquad (2\text{-}158)$$

where (a,b) are the semi-axis lengths of the horizontal cross-section of the elliptical cylinder below $H_d$, and $(L_x, L_y)$ are the Gaussian length scales along the two axes of the hill above $H_d$.  For each puff, hill, and value of $H_d$, the model selects a particular elliptic cylinder and Gaussian-shaped hill.

To do this, the user must describe each terrain feature as an inverse polynomial hill (Figure 2-18).  For each axis, the shape that must be fit to the height-profile of the terrain feature has the functional form:

$$ht = relief \left[ \frac{1 - (|x| / axmax)^{expo}}{1 + (|x| / scale)^{expo}} \right] \qquad (2\text{-}159)$$

where "ht" is the elevation of a point on the hill above the grid-plane, "$|x|$" is the unsigned distance from the center of the hill to the inverse polynomial profile at the elevation "ht", "axmax" is the value of "$|x|$" at which "ht" equals zero (the base of the hill), "relief" is the height of the hill above the grid-plane, "scale" is the length scale of the polynomial function which is half the span of the function at one half the peak of the function, and "expo" is the power (exponent) of the function.

Given this description of the hill, CTSG solves for "x" at specific elevations "ht" along each axis of the hill to obtain the semi-axes for the elliptic cylinder and the Gaussian hill:

$$axis \; (ht) = scale \left[ \frac{1 - ht / relief}{ht / relief + (scale / axmax)^{expo}} \right]^{1/expo} \qquad (2\text{-}160)$$

Below $H_d$, the height used to obtain the axes of the elliptic cylinder is the minimum of $H_d$ and the puff height.  Above $H_d$, the length scales are obtained halfway between $H_d$ and the top of the hill, and the corresponding length scales for the Gaussian hill are formed by multiplying these scales by 1.20.  The factor 1.20 is obtained by demanding that the Gaussian hill and the polynomial hill function have the same span at an elevation halfway between $H_d$ and the top of the hill (Figure 2-19).
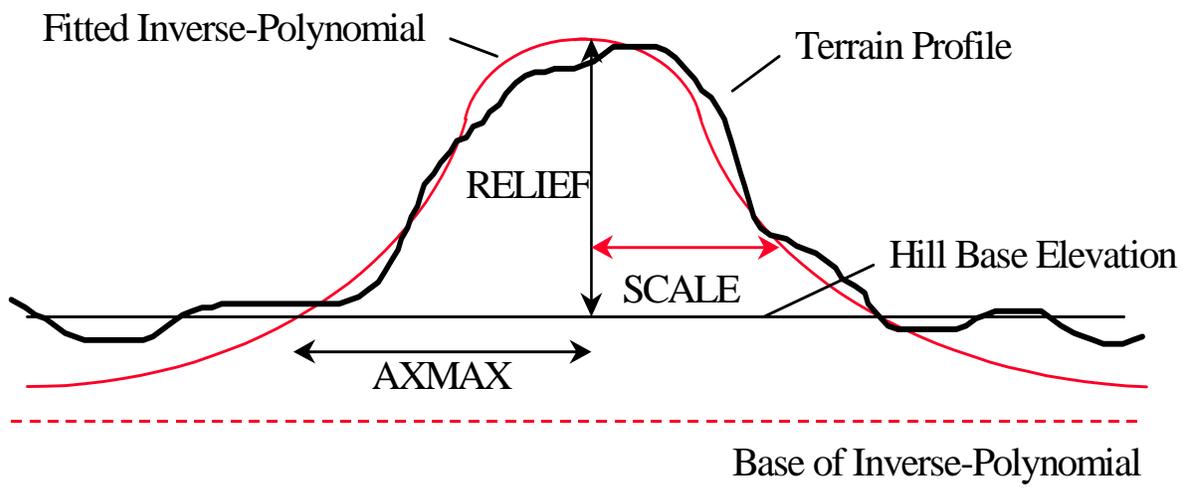
Figure 2-18.    Profile of a terrain feature along one of its two axes.  A best-fit inverse pool polynomial function describes this profile to CTSG.

CROSS-SECTION ALONG ONE AXIS

**Gaussian Shape Matches
At These Points**

HT-Hd

Hd

Puff Height

Axis
(2D Cylinder)
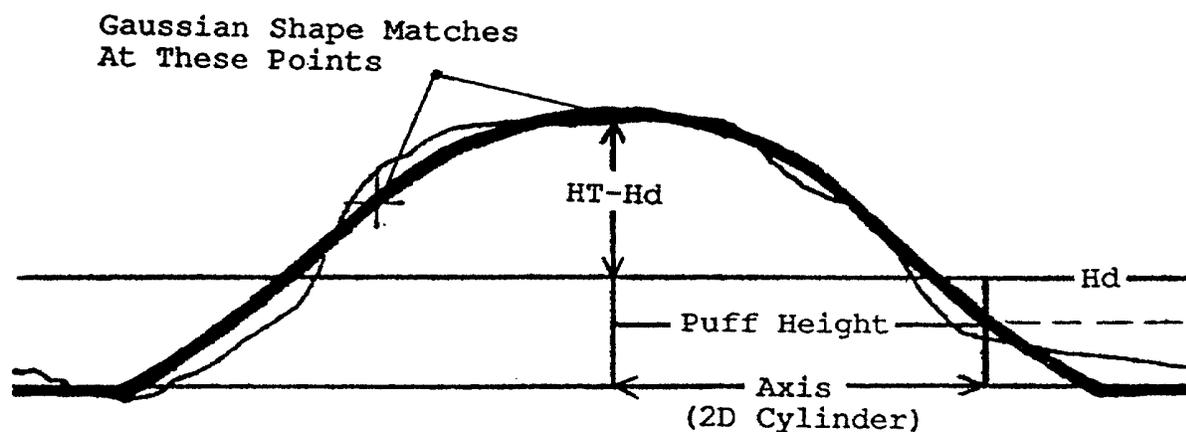
Figure 2-19.    Use of hill profile function within CTSG.  The model extracts the length scales for a
                Gaussian profile above $H_d$, and an elliptical cylinder below $H_d$.

Alternatively, the user may elect to use a terrain feature description file that is identical to the one used in CTDMPLUS. The file, named "TERRAIN" (as in CTDMPLUS), provides the model with a series of parameters that define ellipses and polynomial hill profiles which have been fit to the terrain feature at a series of $H_d$'s. With this option, CALPUFF uses the interpolation functions of CTDMPLUS to obtain the ellipse and Gaussian hill information appropriate to a specific value of $H_d$. An example of the format of this file can be found in Section 4.11. Anyone wishing to use this option should be familiar with the contents of the CTDMPLUS users guide (Perry et al., 1989).

2.6.1.3  Upper Layer

An estimate of the concentration (g/m$^3$) at a receptor at the surface of a hill in region 2, due to a <u>plume</u> whose initial position is ($z_p$,$y_p$), is given by

$$C\left(t_R, y_R, 0 \; ; \; t_o\right) = qF_zF_y / \left[2\pi u \sigma_{ze} \sigma_{ye}\right]$$

(2-161)

where $t_R$ is the travel-time (s) from the source to the receptor, $t_o$ is the travel-time along the plume centerline from the source to the upwind base of the hill (if $H_d$ is non-zero, $t_o$ is the time to the point where the flow first encounters the hill at an elevation equal to the lesser of $z_p$ and $H_d$), $y_R$ is the cross-wind location (m) of the receptor, q is the mass flux (g/s), $F_z$ and $F_y$ are the vertical and horizontal distribution functions, u is the mean wind speed (m/s) at the elevation of the center of the plume, and $\sigma_{ze}$ and $\sigma_{ye}$ are the effective dispersion parameters (m) given by

$$\sigma_{ze}^2 = \sigma_{zo}^2 + \left(\sigma_{z*} / T_z\right)^2 \qquad \sigma_{ye}^2 = \sigma_{yo} + \left(\sigma_{y*} / T_y\right)^2$$

(2-162)

The subscript o denotes a value obtained at $t = t_o$ and the subscript * denotes

$$\sigma_{x*}^2 = \sigma_x^2\left(t_R\right) - \sigma_x^2\left(t_o\right) \qquad \left(for \; x = y \; or \; z\right)$$

(2-163)

$T_z$ and $T_y$ are factors that contain the effects of the distortion of the flow over the hill on the rates of vertical and lateral diffusion.

In the case of a puff, the sampling function allows us to rewrite the concentration estimate for a receptor on the surface (Equation 2-161) as

$$GLC = \frac{Q}{t_2 - t_1} \frac{F_y\left(t_R\right) F_z\left(t_R\right)}{4 \pi u \sigma_{ze} \sigma_{ye}} \left\{erf\left(\frac{t_2 - t_R}{\sqrt{2} \; \sigma_{ye} / u}\right) - erf\left(\frac{t_1 - t_R}{\sqrt{2} \; \sigma_{ye} / u}\right)\right\}$$

(2-164)

for the period $t_1$ to $t_2$ where Q is now the total mass of material (g) in the puff.

The distribution functions are given by

$$F_y = \exp\left(-.5\left(y_{Re} - y_p\right)^2 / \sigma_{ye}^2\right)$$

(2-165)

$$F_z = \exp\left(-.5\left(z_p - H_d\right)^2 / \sigma_{ze}^2\right) erfc\left(\sigma_z *\left[H_d - z_p\right]/\left[2T_z\ \sigma_{ze}\ \sigma_{zo}\right]\right)$$
$$+ \exp\left(-.5\left(z_p + H_d\right)^2 / \sigma_{ze}^2\right) erfc\left(\sigma_z *\left[H_d + z_p\right]/\left[2T_z\ \sigma_{ze}\ \sigma_{zo}\right]\right) \qquad (2\text{-}166)$$

$F_y$ contains information on the deflection in the trajectory over the hill as well as information on changes in the diffusivity. The effective lateral position of the receptor relative to the centerline of the plume is altered by the deformation in streamlines over the hill, and the effective rate of growth of the plume is altered as well. Hence, an effective receptor location ($y_{Re}$) and an effective lateral plume size ($\sigma_{ye}$) are used to compute the horizontal distribution function. $F_z$ also contains the change in diffusivity in the effective vertical plume size, $\sigma_{ze}$ , and it includes complete reflection from the surface of the hill (marked by $H_d$) for only that material which lay above $H_d$ at $t = t_o$. "Cutting" the puff at $z = H_d$ and allowing reflection from this surface gives rise to the combination of exponential and error function products in Eqn. (2-166). A full discussion of the development of these equations is contained in Strimaitis et al. (1988).

These expressions do not include the effect of an elevated inversion on the vertical distribution of the puff. When a mixing lid is present, the $F_z$ function contains many more terms to simulate multiple reflections. The derivation of $F_z$ with a mixing lid is an extension to the formulation found in CTDMPLUS, because the lid is not treated for the stable boundary layer, and it is explicitly included in the PDF representation of dispersion in the mixed layer. It is required in the puff implementation because puffs with a Gaussian distribution of mass in the vertical can be released below either a mechanical or convective mixing lid, a may remain Gaussian in the vertical (not well-mixed) during subsequent sampling steps.

For a mixing lid of height $z_L$, the vertical distribution function in a puff just upwind of the hill is given by

$$F_{zo} = \exp\left(-\left(z_p - z\right)^2 / 2\sigma_{zo}^2\right) + \exp\left(-\left(z_p + z\right)^2 / 2\sigma_{zo}^2\right)$$
$$+ \sum_{i}^{\infty}\left\{\exp\left(-\left(2iz_L - z_p - z\right)^2 / 2\sigma_{zo}^2\right) + \exp\left(-\left(2iz_L - z_p + z\right)^2 / 2\sigma_{zo}^2\right)\right\}$$
$$+ \sum_{i}^{\infty}\left\{\exp\left(-\left(2iz_L + z_p - z\right)^2 / 2\sigma_{zo}^2\right) + \exp\left(-\left(2iz_L + z_p + z\right)^2 / 2\sigma_{zo}^2\right)\right\} \qquad (2\text{-}167)$$

Over the hill, the vertical distribution function (evaluated for a receptor at the surface of the hill, $H_d$) due to a point source located at a height "z" just upwind of the hill is given by

$$F_{zh} = 2 \left\{ \exp \left( - (z - H_d)^2 / 2(\sigma_{z*} / T_z)^2 \right) \right.$$

$$+ \sum_i^\infty \exp \left( - [2i(z_L - H_d) - (z - H_d)]^2 / 2(\sigma_{z*} / T_z)^2 \right)$$

$$\left. + \sum_i^\infty \exp \left( - [2i(z_L - H_d) + (z - H_d)]^2 / 2(\sigma_{z*} / T_z)^2 \right) \right\} \qquad \text{(2-168)}$$

Therefore, the total influence of the vertical distribution of puff material just upwind of the hill on the concentration at a receptor on the surface of the hill is obtained by integrating the product of these two distributions from $z = H_d$ to $z = z_L$. The resulting $F_z$ is given by

$$F_z = 0.5 \left\{ \sum_{i=1}^\infty \sum_{j=1}^\infty A_j \, B\left(E_j, E_{oi}^+\right) + \sum_{i=2}^\infty \sum_{j=1}^\infty A_j \, B\left(E_j, E_{oi}^-\right) \right\} \qquad \text{(2-169)}$$

where

$$A_j = MIN(2, j) \qquad \text{(2-170)}$$

$$E_J = 2(j - 1)(z_L - H_d) \qquad \text{(2-171)}$$

$$E_{oi}^+ = 2 z_L (i - 1) + z_p \qquad E_{oi}^- = 2 z_L (i - 1) - z_p \qquad \text{(2-172)}$$

and

$$B(E, E_o) = \exp\left(-(E - E_o + H_d)^2 / 2\sigma_{ze}^2\right) \left\{ erf\left(K\left(\sigma_{ze}^2(z_L - H_d) - D1\right)\right) + erf(K \, D1) \right\}$$

$$+ \exp\left(-(E + E_o - H_d)^2 / 2\sigma_{ze}^2\right) \left\{ erf\left(K\left(\sigma_{ze}^2(z_L - H_d) - D2\right)\right) + erf(K \, D2) \right\}$$

$$+ \exp\left(-(E + E_o + H_d)^2 / 2\sigma_{ze}^2\right) \left\{ erf\left(K\left(\sigma_{ze}^2(z_L - H_d) + D3\right)\right) - erf(K \, D3) \right\}$$

$$+ \exp\left(-(E - E_o - H_d)^2 / 2\sigma_{ze}^2\right) \left\{ erf\left(K\left(\sigma_{ze}^2(z_L - H_d)] + D4\right)\right) - erf(K \, D4) \right\} \qquad \text{(2-173)}$$

where

$$K = T_z / \left(\sqrt{2} \, \sigma_{ze} \, \sigma_{zo} \, \sigma_{z*}\right) \qquad \text{(2-174)}$$

$$D1 = \sigma_{z*}^2 (E_o - H_d) / T_z^2 + \sigma_{zo}^2 E \qquad \text{(2-175)}$$

$$D2 = \sigma_{z*}^2 \left(E_o - H_d\right)/T_z^2 - \sigma_{zo}^2 \, E \qquad (2\text{-}176)$$

$$D3 = \sigma_{z*}^2 \left(E_o + H_d\right)/T_z^2 - \sigma_{zo}^2 \, E \qquad (2\text{-}177)$$

$$D4 = \sigma_{z*}^2 \left(E_o + H_d\right)/T_z^2 + \sigma_{zo}^2 \, E \qquad (2\text{-}178)$$

Each term in the sum in Eqn. (2-169) is a product of the exponential function and error functions as in Eqn. (2-166), representing the multiple reflections at $H_d$ and $z_L$. Clearly, not all of the terms in the sum are needed. The inner sum over index j represents reflections between $H_d$ and $z_L$ once the puff moves over the hill, whereas the outer sum over index I represents reflections between 0 and $z_L$ before the puff reaches the hill. The algorithm that evaluates these sums continues to include greater values of the index until the fractional change in $F_z$ is reduced to less than 1%. The distribution of material in the vertical becomes well-mixed when $\sigma_z$ reaches 1.6 $z_L$. At this point, $F_z$ in Eqn. (2-169) reduces to

$$F_z = \sqrt{2\pi} \, \sigma_z/z_L \qquad (2\text{-}179)$$

These equations take on a more familiar form when $H_d$ is zero and when $z_L$ is infinite. In that limit D1 = D4, D2 = D3, and inspection of the exponential factors reveals that the indices (i,j) must be equal to obtain non-zero terms. Further inspection of the error functions shows that the only non-zero term is that for I = j = 1, so that

$$F_z\left(H_d{=}0, z_L{=}\infty\right) = 2 \, \exp\!\left(-z_p^2/2\sigma_{ze}^2\right) \qquad (2\text{-}180)$$

which is the form commonly used for flat terrain.

Evaluation of the $F_z$ and $F_y$ distribution functions requires the use of a flow model that provides streamlines for stratified flow over a hill. The effective lateral receptor location, $y_{Re}$, and the effective puff dimensions, $\sigma_{ze}$ and $\sigma_{ye}$, depend on the properties of the flow. These properties are provided by the flow algorithm contained in CTDMPLUS. This algorithm incorporates an approximate solution to the linearized equation of motion for steady-state Boussinesq flow over a Gaussian-shaped hill. It is formulated as a "backwards-looking" solution in which the deflection of a streamline that passes through a given point over a hill is provided. Hence, the algorithm answers the question: "Where did the streamline that passes through the point (x,y,z) come from?" rather than the question: "Where does the streamline that passes through the point (x,y,z) in the flow upwind of a hill go as the flow is deflected by the presence of the hill?" As such, the relationship between the lateral position of the center of the puff in the absence of terrain deflections ($y_p$), and the "original" lateral position ($y_{Re}$) of the streamline that passes through the receptor is directly obtained from the flow algorithm because the receptor position on

the hill $(x_R, y_R, z_R)$ is known.  The description of the algorithm is contained in the CTDMPLUS user's guide (Perry et al. 1989), as modified by Strimaitis and Yamartino (1992).

Evaluation of $\sigma_{ze}$ and $\sigma_{ye}$ is more complicated.  As indicated in Eqn. (2-162), these effective puff dimensions require the quantities $\sigma_{z*}/T_z$ and $\sigma_{y*}/T_y$, which depend on the rate of puff growth in the absence of the hill and on the amount of distortion to the flow induced by the hill.  These are estimated on the basis of the theory for a narrow plume embedded in a flow with axisymmetric strain developed by Hunt and Mulhearn (1973).  Their results show that the spread of material in a straining flow is approximately equal to

$$\sigma_{zd}^2(t) \;=\; \frac{1}{S_z^2(t)} \int\limits_{o}^{t} S_z^2(t') \, 2K_z(t') \, dt' \tag{2-181}$$

$$\sigma_{yd}^2(t) \;=\; \frac{1}{S_y^2(t)} \int\limits_{o}^{t} S_y^2(t') \, 2K_y(t') \, dt' \tag{2-182}$$

where $K_z$ and $K_y$ are the diffusivities, $S_z$ and $S_y$ are functions of the strain in the flow, and $\sigma_{yd}$ and $\sigma_{zd}$ describe the size of a deformed plume.  Because we assume that the strain is negligible away from the hill, Eqns. (2-181) and (2-182) can be rewritten as

$$\sigma_z^2(t) \;=\; \frac{1}{S_z^2(t)} \left[ \sigma_{zo}^2 \;+\; \int\limits_{t_o}^{t} S_z^2(t') \, 2K_z(t') \, dt' \right] \tag{2-183}$$

$$\sigma_y^2(t) \;=\; \frac{1}{S_y^2(t)} \left[ \sigma_{yo}^2 \;+\; \int\limits_{t_o}^{t} S_y^2(t') \, 2K_y(t') \, dt' \right] \tag{2-184}$$

The expressions in brackets are equivalent to the quantities $\sigma_{ze}^2$ and $\sigma_{ye}^2$ defined by Eqn. (2-162), so that

$$\frac{\sigma_{z*}^2}{T_z^2} \;=\; \frac{\sigma_z^2(t) \;-\; \sigma_{zo}^2}{T_z^2} = \int\limits_{t_o}^{t} S_z^2(t') \, 2K_z(t') \, dt' \tag{2-185}$$

$$\frac{\sigma_{y*}^2}{T_y^2} = \frac{\sigma_y^2(t) - \sigma_{yo}^2}{T_y^2} = \int_{t_o}^{t} S_y^2(t') \, 2K_y(t') \, dt' \tag{2-186}$$

The strain functions are given by

$$S_z(t) = \exp(1 - Th(t)) \qquad S_y(t) = \exp(1 - Tl(t)) \tag{2-187}$$

where Th and Tl are deformation factors. Th is the ratio of streamline spacing in the vertical in the deformed flow to that in the undistorted flow. Tl is the corresponding ratio for streamline spacing in the lateral direction (normal to the flow). The inverse of the product of these two factors at any point in the flow equals the speed up factor, Tu. These factors are computed from the flow model contained in CTDMPLUS. The integrals in Eqns. (2-185) and (2-186) are evaluated numerically along the trajectory of the center of the puff. Vertical and lateral diffusivities (m$^2$/s) in the absence of the terrain are found from the dispersion coefficients as

$$2K(t) = d\sigma^2 / dt \tag{2-188}$$

where $\sigma$ denotes either $\sigma_y$ or $\sigma_z$. The effect of the terrain on the diffusivity is assumed to be restricted to the change in the vertical turbulence over the hill. We write the dispersion coefficient as the product of the turbulence and a function of time (in the absence of terrain). Over the hill, the vertical turbulence velocity is assumed to increase with wind speed as in the "inner layer" theory, and the lateral turbulence velocity is assumed constant as in the "rapid distortion" theory (e.g., see Britter et al. (1981) for a discussion of these theories). These assumptions tend to accentuate the effect of the hill in the diffusion calculation. Substituting Eqns. (2-187) and (2-188) and augmenting the vertical turbulence intensity by the speed-up factor Tu, the integrands of Eqn2. (2-185) and (2-186) become

$$S_z^2 \, 2K_z = \exp 2(1 - Th) \, Tu^2 \, \frac{d\sigma_z^2}{dt} \tag{2-189}$$

$$S_y^2 \, 2K_y = \exp 2(1 - Tl) \, \frac{d\sigma_y^2}{dt} \tag{2-190}$$

Due to the computations required to obtain Th, Tl, and Tu, these factors are evaluated at no more than 25 points along the streamline that passes through the center of the puff. Linear interpolation between these points is then used in the numerical integration required to evaluate Eqns. (2-185) and (2-186) for each receptor. The range of points is centered at the midpoint of the intersections of the puff trajectory (without deflection) and the ellipse that marks the boundary of the portion of the hill below $H_d$, and cover a distance equal to one and one-half times the distance between points of intersection of the line $y = 0$

(the centerplane of the flow over the hill) and the ellipse. If the undeflected trajectory of the puff does not intersect the ellipse, then the distortion factors are set to unity and the hill has no effect on $\sigma_z$ and $\sigma_y$. Note that the hill also has no effect on $\sigma_z$ or $\sigma_y$ when the growth rate of the puff is virtually zero. This is not to say that the hill has no effect on concentrations, however, because the flow distortion over the hill results in $y_{Re} \neq y_R$, and the dividing-streamline height still allows puff material at $z = H_d$ to contact the surface of the hill.

2.6.1.4  Lower Layer

The equation for estimating the concentration (g/m$^3$) at a receptor at the surface of a hill in region 2, due to a <u>plume</u> whose initial position is $(z_r, y_r)$, is given by

$$C\left(t_r, Y_d, z_R, t_o\right) = q \, F_z \, F_y / \left[2 \, \pi \, u \, \sigma_z \, \sigma_y\right] \tag{2-191}$$

where $Y_d$ is the cross-wind location (m) of the lateral dividing-streamline which coincides with the side of the hill, $z_R$ is the elevation of the receptor on the surface of the hill, $F_z$ and $F_y$ are the vertical and horizontal distribution functions, u is the mean wind speed (m/s) at the elevation of the center of the plume, and $\sigma_z$ and $\sigma_y$ are the dispersion parameters (m) at $t_R$. Note that unlike Eqn. (2-161) for the upper layer, changes to the rate of diffusion that are induced by the hill in the lower layer are considered small.

In the case of a puff, the sampling function allows us to rewrite the concentration estimate for a receptor on the surface (Eqn. (2-191)) as

$$GLC = \frac{Q}{t_2 - t_1} \; \frac{F_y(t_R) \, F_z(t_R)}{4\pi \, u \, \sigma_z \, \sigma_y} \left\{ erf\left\{\frac{t_2 - t_R}{\sqrt{2}\sigma_y/u}\right\} - erf\left(\frac{t_1 - t_R}{\sqrt{2}\sigma_y/u}\right) \right\} \tag{2-192}$$

The distribution functions are given by

$$F_y = \exp\left(-(Y_d - y_p)^2 / 2\sigma_y^2\right) \left[1 \pm erf\left((Y_d - y_p) \, \sigma_{y*} / \left(\sqrt{2} \, \sigma_{yo} \, \sigma_y\right)\right)\right] \tag{2-193}$$

$$F_z = 0.5 \, \exp\left(-(z_p - z_R)^2 / 2\sigma_z^2\right) \left[erf\left((b1 - b2 - b3)K\right) + erf\left((b1 + b2 + b3)K\right)\right]$$
$$+ 0.5 \, \exp\left(-(z_p + z_R)^2 / 2\sigma_z^2\right) \left[erf\left((b1 - b2 + b3)K\right) + erf\left((b1 + b2 - b3)]K\right)\right] \tag{2-194}$$

where

$$K = \frac{1}{\sqrt{2} \, \sigma_z \, \sigma_{zo} \, \sigma_{z*}} \qquad b1 = H_d \, \sigma_z^2 \tag{2-195}$$

$$b2 = z_R \, \sigma_{zo}^2 \qquad b3 = z_p \, \sigma_{z*}^2$$

The notation is the same as that in section 2.6.1.3. The only new quantity introduced in these equations is $Y_d$, the lateral position of the stagnation streamline upwind of any flow distortion. As in CTDMPLUS, it is found by solving for the two-dimensional streamline pattern about an ellipse.

$F_y$ contains information about the amount of material on each side of the hill and about how the puff is sampled in the lateral direction. The lateral offset is the distance from the centerline to $Y_d$, reflecting the notion that all receptors lie along the side of a hill, coincident with the lateral dividing-streamline position. Furthermore, material may be split on either side, and complete reflection of material is allowed along this surface, giving rise to the form of the product of the exponential and error functions in Eqn. (2-193). Note that the sign of the error function (taking the sign of its argument into account) is positive when both the receptor and the trajectory of the center of the puff lie on the same side of $Y_d$. If all of the material were to reside on one side of $Y_d$ at $t_o$, then $F_y$ would equal either 2 or 0, depending on whether the receptor were on the same side or on the other side of $Y_d$ as the puff.

$F_z$ contains information about the amount of material below $H_d$ at $t_o$, and about how this material is sampled in the vertical. The form is a product of an exponential function and error functions in which the sampling height $z_R$ is most evident in the exponential function, and the effects of splitting the plume at $H_d$ are contained in the error functions. A full discussion of the development of these equations is contained in Strimaitis et al. (1988).

These expressions do not include the effect of an elevated inversion on the vertical distribution of the puff. When a mixing lid is present, the $F_z$ function contains many more terms to simulate multiple reflections and the result is similar to that discussed in 2.6.1.3:

$$F_Z = 0.5 \left\{ \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} B\left(E_j^+, E_{oi}^+\right) + \sum_{i=1}^{\infty} \sum_{j=2}^{\infty} B\left(E_j^-, E_{oi}^+\right) \right.$$
$$\left. + \sum_{i=2}^{\infty} \sum_{j=1}^{\infty} B\left(E_j^+, E_{oi}^-\right) + \sum_{i=2}^{\infty} \sum_{j=2}^{\infty} B\left(E_j^-, E_{oi}^-\right) \right\}$$

(2-196)

where

$$E_j^+ = 2(j-1)z_L + z_R$$
$$E_j^- = 2(j-1)z_L - z_R$$
$$E_{oi}^+ = 2(i-1)z_L + z_p$$
$$E_{oi}^- = 2(i-1)z_L - z_p$$

(2-197)

and

$$B\left(E,E_o\right) = \exp\left(- \left(E_o - E\right)^2 / 2\sigma_z^2\right) \{ \; erf\left( K \left(b1 - b2 - b3\right) \right) \; + \; erf\left( K \left(b1 + b2 + b3\right)\right) \}$$
$$+ \; \exp\left(- \left(E_o + E\right)^2 / 2\sigma_z^2\right) \{ \; erf\left( K \left(b1 + b2 - b3\right) \right) \; + \; erf\left( K \left(b1 - b2 + b3\right)\right) \} \qquad (2\text{-}198)$$

where

$$K \; = \; \frac{1}{\sqrt{2} \; \sigma_z \; \sigma_{zo} \; \sigma_{z*}} \qquad\qquad b1 \; = \; H_d \; \sigma_z^2$$

$$b2 \; = \; E \; \sigma_{zo}^2 \qquad\qquad\qquad b3 \; = \; E_o \; \sigma_{z*}^2 \qquad (2\text{-}199)$$

The form of the "B-function" is identical to $F_z$ (Eqn. (2-194)) for the case of no limit to vertical mixing. Differences arise in the use of $(E, E_o)$ rather than $(z_R, z_p)$, so that the presence of the mixing lid is manifest in Eqn. (2-197).

The outer sum over the index i accounts for reflections between the mixing lid and the surface before the puff reaches the hill. The inner sum over the index j accounts for reflections that may occur as material diffuses above $H_d$ when the puff passes the hill. The inner summation will generally produce non-zero terms only for j = 1, unless a mixing height only slightly greater than $H_d$ is found. This circumstance may not occur at all, given the definition of $H_d$ and $z_L$. In evaluating the sums, terms are included for greater values of each index until the fractional change in $F_z$ is reduced to less than 1%. The distribution of material in the vertical becomes well-mixed when $\sigma_z$ reaches 1.6 $z_L$. At this point, $F_z$ in Eqn. (2-192) reduces to

$$F_z \; = \; \sqrt{2\pi} \; \sigma_z / z_L \qquad (2\text{-}200)$$

2.6.1.5  Operational Characteristics

The best way to illustrate the behavior of CTSG is to present concentrations obtained for a specific application, and to compare these with what would have been obtained if the terrain feature had been ignored. We take this approach in this section by simulating ground-level concentration patterns at receptors on a hill for the situation in which a single puff moves across the hill along a curved trajectory.

The hill chosen for this exercise is twice as long as it is wide, with its major dimension oriented north-south. The relief height of the hill is set to 100 m, and its dimensions at its base are 2264 m by 1132 m.

The polynomial function describing its shape is characterized by the following parameters:

|  |  |
|---|---|
| relief (m) | 100 |
| expo (1,2) | 2, 2 |
| scale (1,2) (m) | 800, 400 |
| axmax (1,2) (m) | 1132, 566 |
| xc, yc (m) | 0, 0 |
| thetah (deg) | 0 |
| zgrid (m) | 25 |

Note that (xc,yc) are the coordinates of the center of the hill, thetah is the angle (CW) from north to the major axis of the hill, and zgrid is the elevation of the grid-plane above sea level.

The incident flow for this hill consists of a height-profile in which wind speeds are constant at 1.5 m/s, and the temperature gradient is constant with a Brunt-Vaisala frequency of 0.0167 s$^{-1}$. For the 100 m tall hill, this profile produces a dividing-streamline height of 10.18 m. The mixing height is set at 2000 m.

For this demonstration, the following formulas were used to specify the dispersion parameters:

$$\sigma_z = \sqrt{\sigma_{zi}^2 + \left(i_z t\, f_z\right)^2} \tag{2-201}$$

$$f_z = 1/\left(1 + .945(t/100)^{.806}\right) \tag{2-202}$$

where $\sigma_{zi}$ = 5 m and $i_z$ = 0.1; and

$$\sigma_y = \sqrt{\sigma_{yi}^2 + \left(i_y t\, f_y\right)^2} \tag{2-203}$$

$$f_y = 1/\left(1 + .9\sqrt{t/1200}\right) \tag{2-204}$$

where $\sigma_{yi}$ = 50 m and $i_y$ = 0.25. These equations result in a puff size that produces significant concentrations on the ground in the absence of the hill, since the puff height is set at 45 m (MSL), or 20 m above the local grid elevation. Hence, the center of the puff is approximately 10 m above $H_d$ for this demonstration.

The puff initially lies to the southwest of the hill. Its movement is tracked in timesteps of 5 minutes, so that it takes several timesteps to move across the hill. The wind direction shifts by 10 degrees each time-step, from an initial direction of 270 degrees. The puff contains 600 g of material.

The 1-hour average "foot-print" of concentrations produced by the movement of this puff is shown in Figure 2-20. The left panel illustrates simulated concentrations in the absence of the hill, and the right

panel illustrates concentrations simulated by CTSG when terrain is present. The base of the hill function is outlined as an ellipse in each of these panels. Major features of CTSG are immediately apparent in these concentration patterns. Peak concentrations over the crest of the hill are larger by almost a factor of two, and puff material below $H_d$ travels around the hill on either side. Note that some detail in the contours arises from discrete receptor locations. Even though 325 receptors were used (one at each intersection of the 100 m tic-marks), there is not enough coverage to produce smooth contours everywhere.

The "foot-prints" of the puff during each of the time-steps in which the puff was over the hill are shown in Figures 2-21 (a-c) corresponding to time-steps 4 through 6. These figures illustrate how CTSG partitions the puff during each step according to the relative position of the center of the puff, the dividing streamline height ($H_d$), and the position of the stagnation streamline. It is important to note that this partition does not increase the number of puffs in the model. Although the distribution becomes fragmented in the mathematics, all information remains referenced to a circular puff of a prescribed size. When a variable such as the flow direction changes between steps as it does in this example, the concentrations are obtained as if the current properties of the flow existed for all time, and the puff is partitioned according to those properties.

Hence, the stagnation streamline in this demonstration differs from one step to another, and so the separation distance between the trajectory of the center of the puff and the stagnation streamline also differs from one step to another.

## 2.6.2 "Simple" Terrain Adjustments

Terrain adjustments other than those provided by the wind field model and the CTSG subroutine are needed in CALPUFF. The wind field transports a puff along the surface of the terrain, but never causes its height above the surface to change. Hence, puffs in the flow may be channeled or deflected by the terrain, but they do not "impinge" or otherwise strongly interact with the terrain without a simple terrain treatment. General applications typically involve terrain variations on many spatial scales which are impractical to address with CTSG.

Three simple terrain adjustment methods are offered in CALPUFF. Two are incorporated in existing plume models: the original ISC terrain adjustment, and the plume path coefficient adjustment (e.g., the half-height or partial height adjustments found in plume models such as COMPLEX I, RTDM, and ISC3 which now incorporates COMPLEX I). The third is a new treatment that is consistent with the concepts about the effects of strain in the flow on puff growth that lie behind the CTSG treatment, but employs sufficient simplifications that it is readily applied to the gridded terrain fields already available to CALPUFF. We review the ISC and the plume path coefficient adjustments in Sections 2.6.2.1 and 2.6.2.2, and we present the strain-based treatment in Section 2.6.2.3.

1-HOUR AVERAGE (g/m3) - FLAT        1-HOUR AVERAGE (g/m3) - CTSG
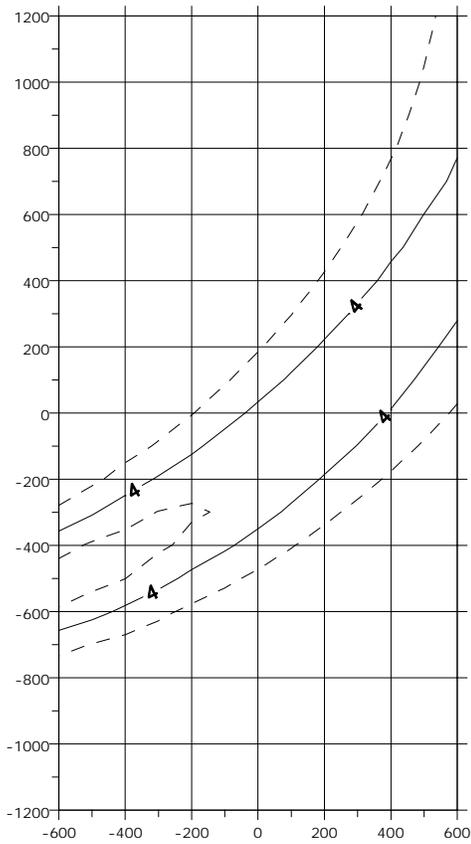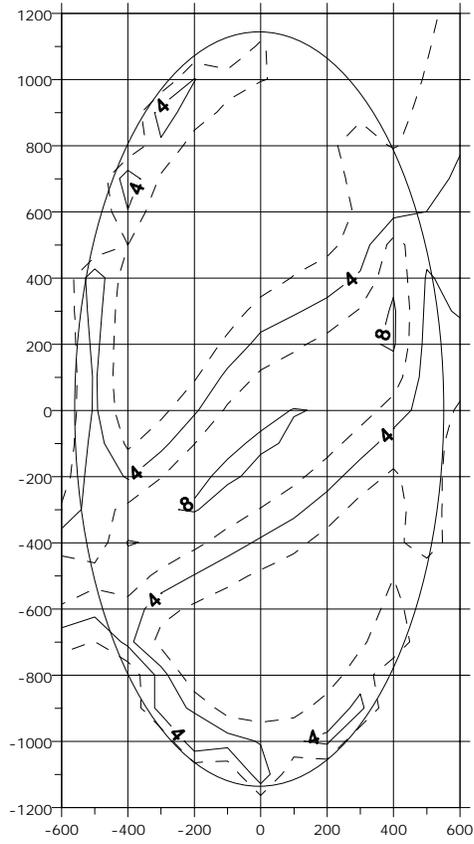


Figure 2-20.    Concentrations (g/m³) produced by CTSG (both with and without the hill), averaged over
a period of one hour.  The single puff that was simulated traveled over the hill in
approximately 25 minutes during the hour.

PUFF STEP 4          PUFF STEP 4
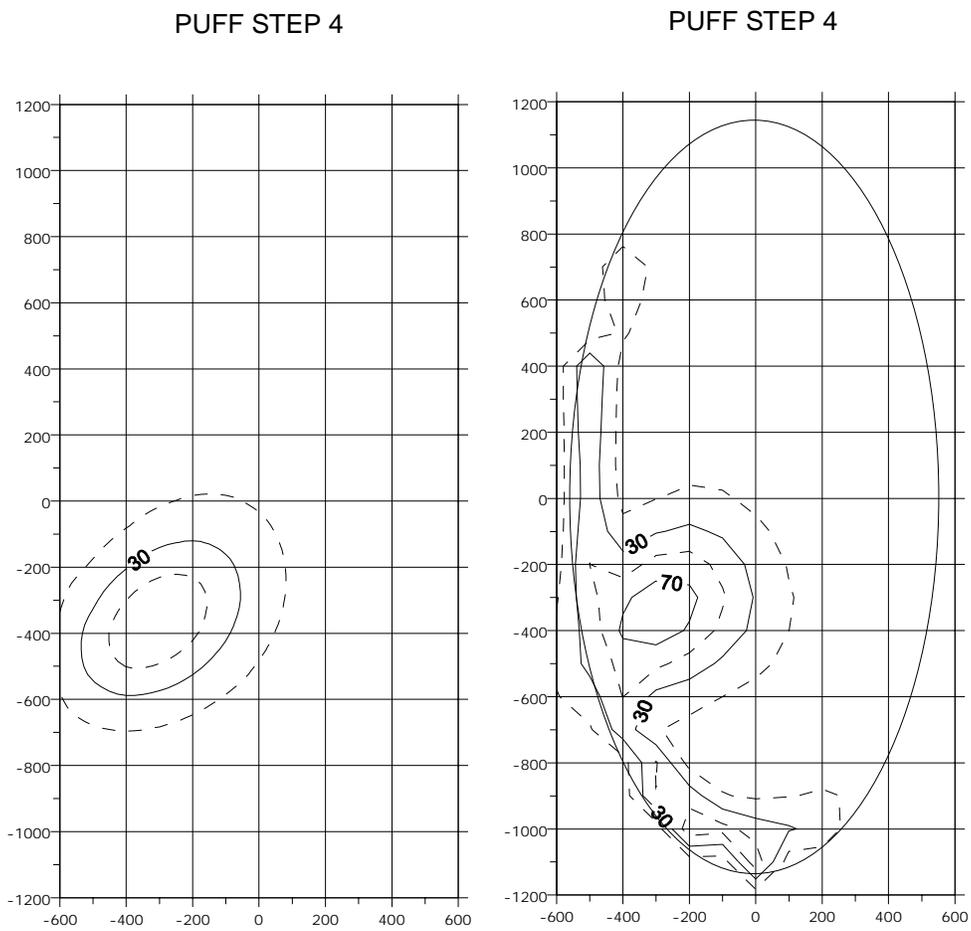


Figure 2-21a.    Concentrations (g/m$^3$) produced by CTSG (both with and without the hill) during 5-minute time-step number 4.  (Contour interval = 20 g/m$^3$; grid units = m).
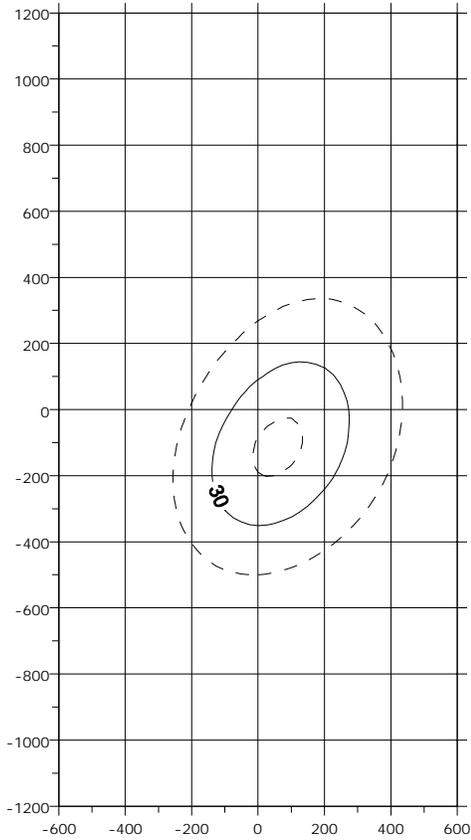
PUFF STEP 5                           PUFF STEP 5
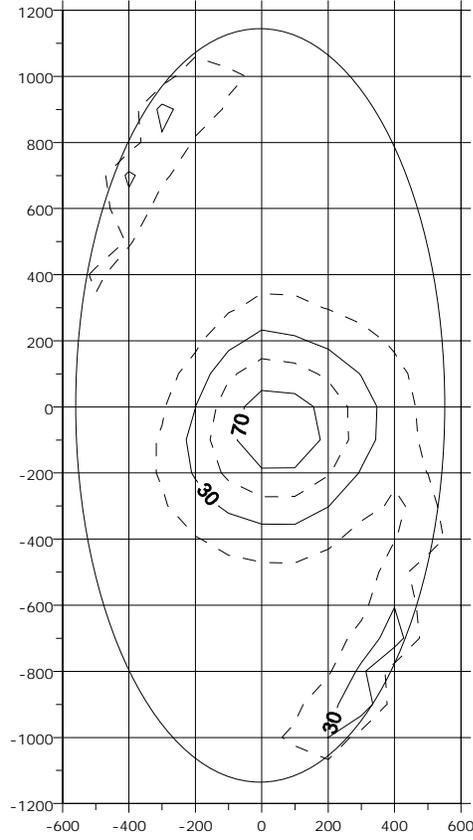


Figure 2-21b.    Concentrations (g/m$^3$) produced by CTSG (both with and without the hill) during
5-minute time-step number 5.  (Contour interval = 20 g/m$^3$; grid units = m).

PUFF STEP 6                    PUFF STEP 6
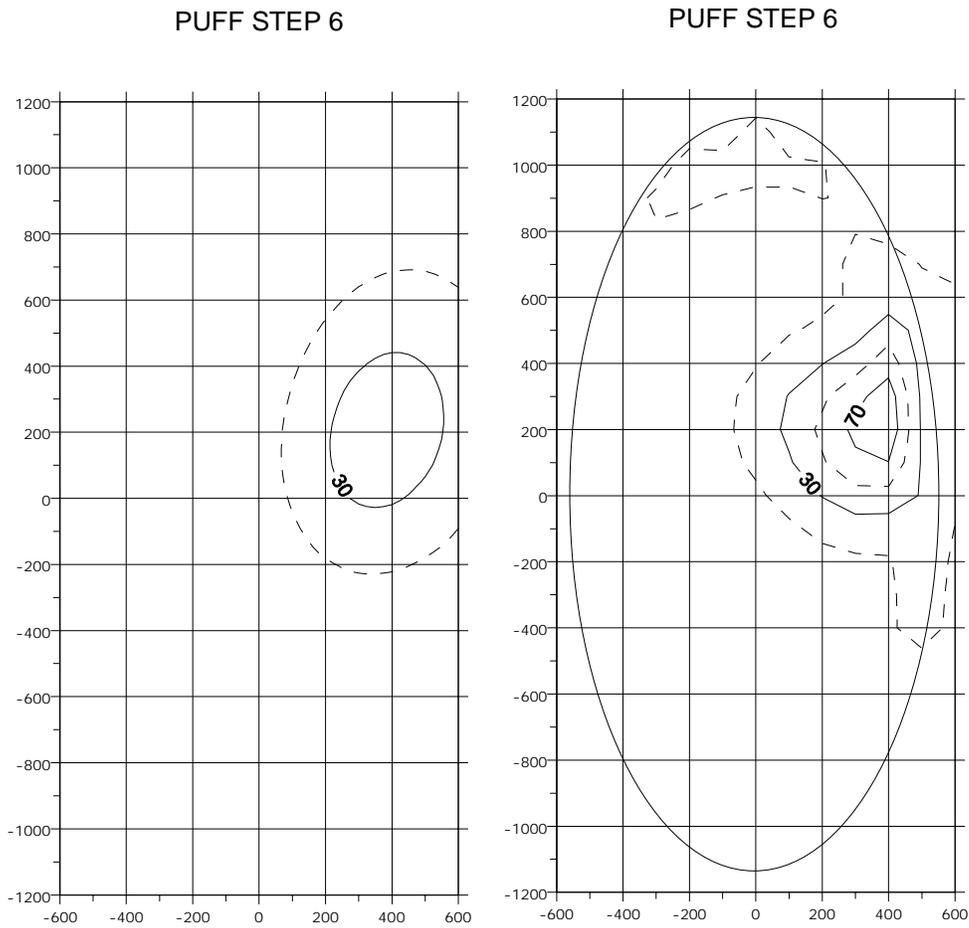
Figure 2-21c.    Concentrations (g/m$^3$) produced by CTSG (both with and without the hill) during
5-minute time-step number 6.  (Contour interval = 20 g/m$^3$; grid units = m).

2.6.2.1  ISC Terrain Treatment

The original ISC model is not intended for use in situations in which receptors are placed on terrain that exceeds the height of the "stack".  Any receptors that are found above this height are lowered to a height that is 0.005 m below the height of the stack.  This is done hourly for each source in the simulation, and is therefore source-specific.  The mixing height is not adjusted for the presence of any terrain feature, and the result of any downwash calculations does not modify the stack height used to determine the height of the receptor.  Once the receptor height is determined, the vertical distribution factor contains the difference in elevation between the centerline of the plume and the receptor.  In effect, the centerline of the plume is <u>lowered</u> by an amount equal to the modified elevation of the receptor above the base of the stack.

Figure 2-22 portrays this adjustment.  The terrain shown in the upper part of the figure is "chopped" at the stack-height elevation, and the plume subsequently travels over the chopped terrain  profile without any further adjustments.  Note that receptors "located" on the upper surface of this feature are treated as if the plume were released at ground-level (before plume rise).  For these receptors, the dotted line in the figure now represents the reflecting surface for the vertical distribution of plume material.

2.6.2.2  Plume Path Coefficient Treatment

In the plume path coefficient treatment, the height of the plume at a receptor depends on the height of the plume over level terrain (which is taken to be the height of the plume above the elevation at the base of the stack from which the plume was released), the receptor height (above the base of the stack), and a plume path coefficient (which depends on the stability class).  Values for the plume path coefficient are typically $C=0.35$ for stable (classes E and F), and $C=0.5$ for the rest (classes A, B, C, and D).  The "half-height" correction model is equivalent to $C=0.5$.

Let $H_s$ be the elevation of the base of the stack above sea level, and $H_r$ be the elevation of the receptor above sea level.  Furthermore, let $H_{po}$ be the height of the plume at the source (after any plume rise), and $H_p$ be the height of the plume at the receptor.  If the elevation of the receptor exceeds the elevation of the centerline of the plume at the source,

$$H_p \; = \; H_{po} \; C \tag{2-205}$$

If the elevation of the receptor lies below the centerline of the plume at the source,

$$H_p \; = \; H_{po} \; - \; (H_r \; - \; H_s) \; (1 \; - \; C) \tag{2-206}$$

Note that $H_r \geq H_s$ is not a restriction in the above equation.  If the terrain elevation drops below stack-base elevation along the puff trajectory, the puff height above receptors below stack-base will appear to increase. The mixing height is not altered unless the effective puff height becomes greater than the

mixing height, in which case the mixing height is reset to unlimited mixing for the current concentration calculation.

When C = 0.0, the full difference between the stack-base elevation and the receptor elevation is subtracted from the puff height. This gives the appearance of keeping the plume level, and is therefore known as the level-plume treatment. A schematic representation of the plume path coefficient treatment is illustrated in Figure 2-23 which depicts the situation for C = 0.5.

2.6.2.3 CALPUFF Strain-based Approach to Terrain Adjustment

The method of adjusting properties of a puff to simulate the effects of dispersion over terrain should include the following attributes:

(1)     Adjustment should be analytic functions of readily-available physical properties of the flow, dispersion, and terrain.
(2)     Problems associated with "reflections" should be minimized.
(3)     Adjustments should be based on local properties of the terrain, so that heights relative to particular "stack-base" elevations or "base-plume" elevations are not required.
(4)     Adjustments should be related to concepts used in the CTSG (CTDM) routine.
(5)     Puffs from different sources that happen to coincide at some point should be treated alike as they interact with subsequent terrain features.

In the method outlined below, the properties of a puff are adjusted on the basis of the local strain to the flow imparted by the underlying terrain, using a simplification of the theory on which CTSG is based. Essentially, the effective spread of the puff in the vertical may be altered by the terrain, thereby increasing ground-level concentrations in the region where the height of the puff is approximately equal to $\sigma_z$. In addition to modifying properties of the puff, the vertical sampling point may also be changed to simulate impingement processes. Both of these treatments are described below.

Impingement Calculation

For very stable conditions (Froude number less than 1), we assume that the wind field model will force much of the flow to be parallel to contours of the terrain elevation, so that puffs will directly encounter relatively minor terrain. While minor, this terrain may itself generate a local dividing streamline height ($H_d$) below which the flow remains largely two-dimensional. If this terrain slopes upward along the puff trajectory, a portion of the flow beneath the puff may be diverted laterally, thereby allowing the flow containing the puff to more closely approach the surface. The resulting change in puff height above ground is modeled explicitly in CALPUFF if the puff has not already reached the surface. That is, "clear" air beneath the puff (and below $H_d$) is allowed to be diverted, but air containing significant portions of puff material is not.
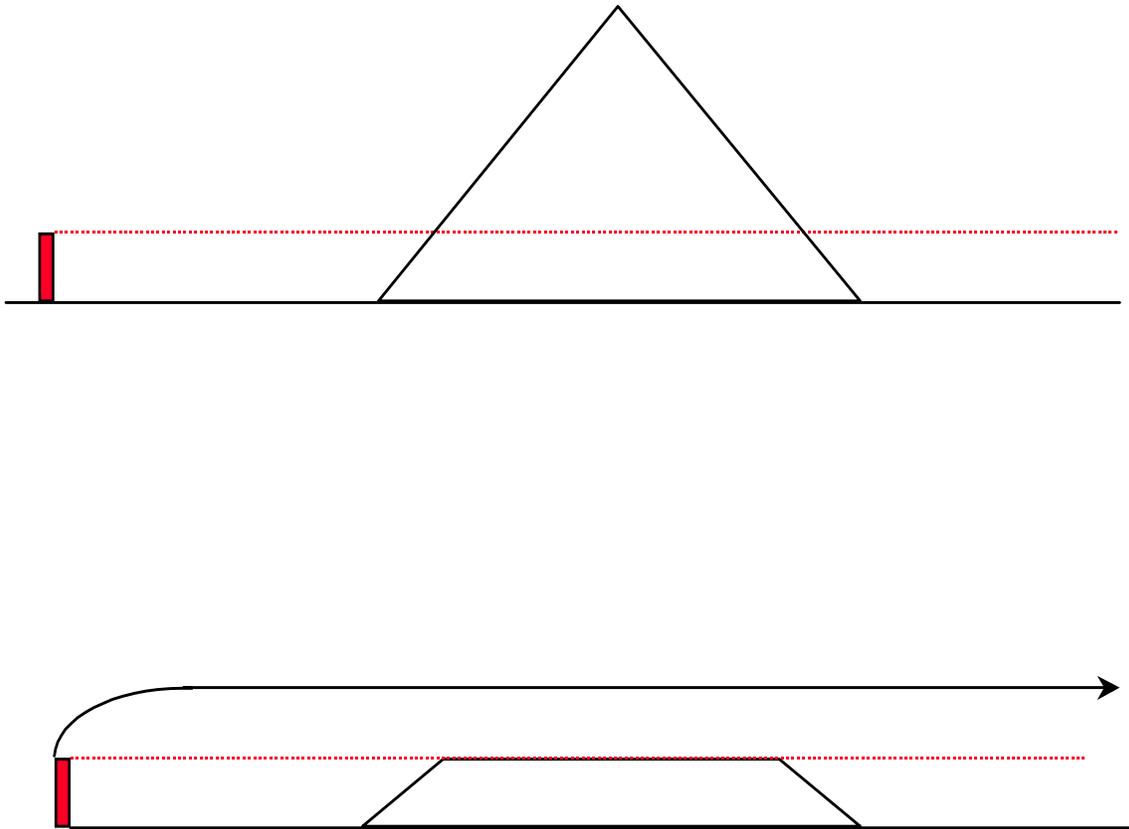
Figure 2-22.    ISC terrain adjustment method.  The plume is modeled as if the terrain above the stack were removed.
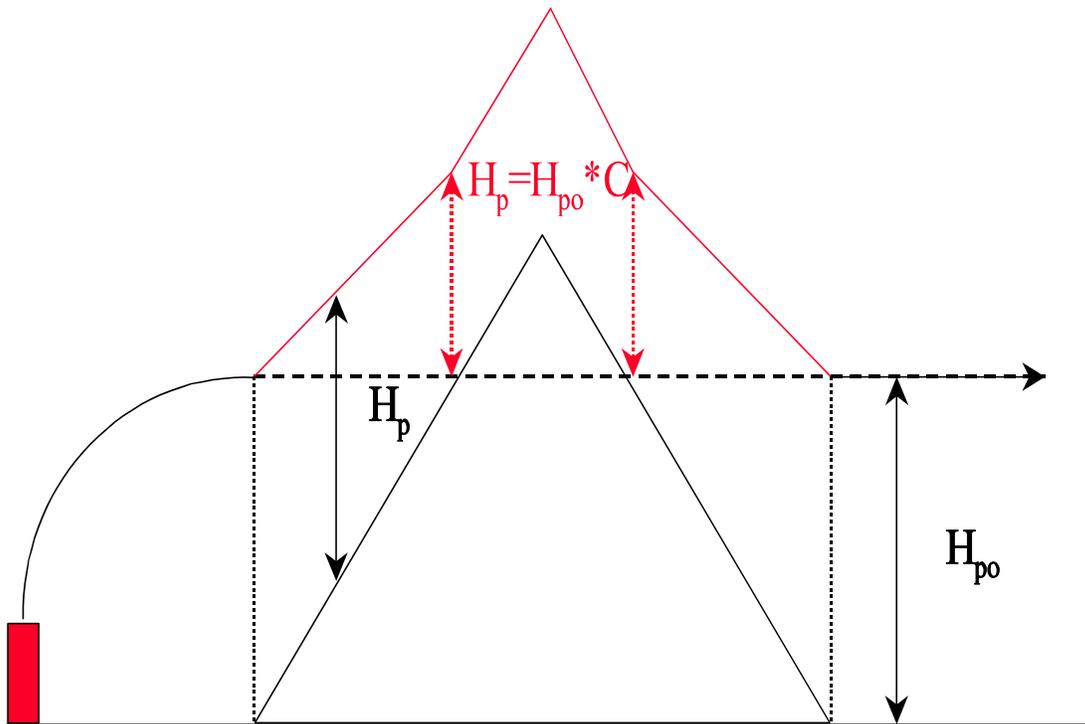
Figure 2-23.    Plume path coefficient adjustment method. (C = 0.5)

This adjustment is illustrated in Figure 2-24, for the case in which the local $H_d$ actually exceeds the puff height. As the flow carries the puff across the page in the upslope direction, the puff remains level until its height above the ground is reduced to a "critical" fraction ($R_c$) of the puff $\sigma_z$. At that point no further adjustment is made to its height above ground, and it becomes terrain-following. Had $H_d$ been smaller than the puff height, and intersected the slope before the $R_c$ criterion was satisfied, the puff would have become terrain-following sooner, and would not have approached as near the surface. The value used for $R_c$ is 1.8. By this measure, a puff is said to materially reach the surface when the ground-level concentration first equals about 40% of the freestream peak concentration, and the elevated centerline concentration increases by 0.15%.

The lateral distribution of the puff remains <u>level</u> below $H_d$, and this is simulated by placing receptors on "flagpoles" whose heights are marked relative to the elevation of the terrain beneath the center of the puff. This allows the "edges" of a puff to brush against the side-walls of a valley or channel, producing "impingement" concentrations. If a receptor lies on terrain that is above the elevation of the terrain beneath the puff, but below $H_d$, the receptor is placed on a pole. The height of the pole is the difference in elevation between the receptor and the puff location, and so the receptor samples the puff distribution above the "surface".

If the pole height happens to be equal to the puff height above ground, the concentration obtained will be an "impingement" concentration. If the pole height happens to exceed the top of the puff, the concentration observed will be negligible, and the puff material will appear to be confined within a valley below this receptor.

Figure 2-25 depicts this treatment. The puff is traveling into the plane of the figure, and its size is denoted by the extent of the ellipse with axes equal to $\sigma_y$, $\sigma_z$. The elevation of the terrain under the puff is denoted by the horizontal dashed line, and the actual terrain is denoted in the cross-section by the jagged solid lines. A receptor is marked by the star. When the Froude number is small and $H_d$ is large, the receptor is placed on a "flagpole" as illustrated, so that it intercepts concentrations <u>within</u> the puff. When the Froude number is large and $H_d$ is zero, this receptor would be placed at the elevation of terrain beneath the center of the puff, so the centerplane of the puff would appear to be terrain-following.

Implementation of this scheme requires a method for estimating $H_d$. First, a "hilltop" elevation (in MSL) is assigned to each cell in the modeling grid, using the terrain data array provided in the CALMET data file. This elevation represents the peak elevation upslope from the cell. If a local peak is resolved, the slope will eventually flatten, and reverse sign. This signals the top of the hill for this segment of the terrain. Next, using the hilltop elevation for the cell in which a receptor is located ($E_t$), the elevation $E_d$ (m MSL) of the dividing-streamline is computed as

$$E_d = E_t - u/N \tag{2-207}$$

# REDUCTION IN PUFF HEIGHT

Dividing Steamline Height

Flow

Puff Height:   H

$H/\sigma_z = R_c$
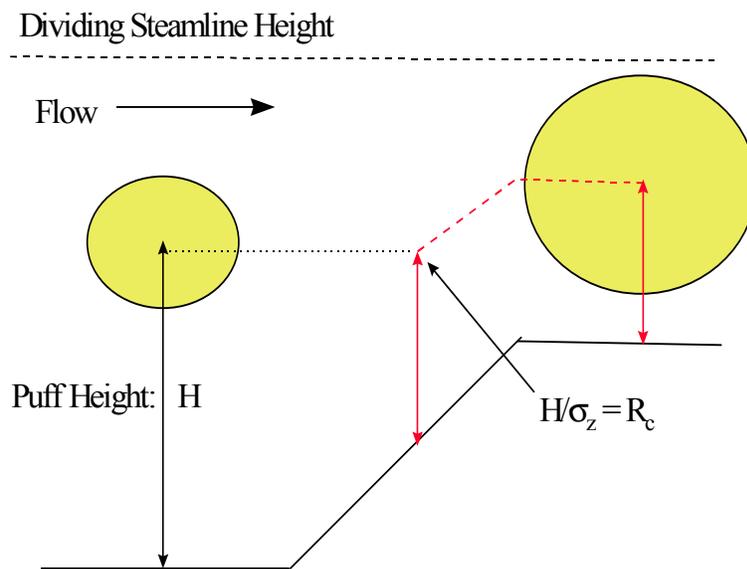
Figure 2-24.   Schematic illustration of the reduction in puff height for upslope flow during stably stratified conditions.

# SIDEWALL INTERACTION

## (Flow is Into Page)
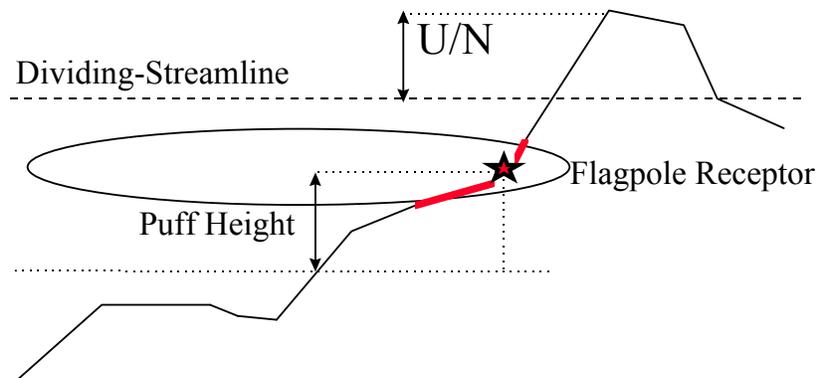


Figure 2-25.  Depiction of treatment of puff interaction with a "side-wall" for strongly stratified (stable) conditions.  The flow is into the page.

where the wind speed u and the Brunt-Vaisala frequency N are bulk properties of the flow from the bottom to the top of the puff being modeled. The height of the dividing-streamline above the "surface" for this puff and this receptor is:

$$H_d = \text{MAX}( \ 0.0 \ , \ E_d - E_p \ ) \tag{2-208}$$

where $E_p$ is the elevation (m MSL) of the terrain beneath the puff. Similarly, the height of the receptor above the "surface" for this puff is:

$$z_r = \text{MAX}( \ 0.0 \ , \ E_r - E_p \ ) \tag{2-209}$$

where $E_r$ is the elevation (m MSL) of the terrain at the receptor.

Now, the pole height ($z_{rp}$) can be specified as:

$$
\begin{array}{llll}
\text{for} & H_d = 0.0 & , & z_{rp} = 0.0 \\
\text{for} & H_d > z_r & , & z_{rp} = z_r \\
\text{for} & H_d \le z_r & , & z_{rp} = H_d
\end{array}
\tag{2-210}
$$

The first case results in a "flat terrain" calculation, and the second results in a full impingement, or no deflection, calculation. The third is an intermediate case in that any puff material that lies above $H_d$ is allowed to rise along the terrain slope. Receptors above $H_d$ only see concentrations in the puff at $H_d$, because these are the ones that contact the surface. In practice, we only expect impingement concentrations to arise in valley situations for very stably-stratified flow. These will primarily be seen along the side-walls, at elevations approximately equal to puff height, when the puffs remain in a flow confined to the valley.

A consideration related to the treatment of receptors along the side-walls of a valley is the effect of the sidewalls on the growth of the lateral puff distribution. With strong, stable stratification, the mean flow within a valley is along the axis of the valley. Lateral motions superimposed on the mean are limited by the cross-valley dimension. Therefore, the time-averaged $\sigma_y$ under these conditions should not become much larger than the valley width. This effect is introduced in CALPUFF by stopping the growth of $\sigma_y$ once it reaches the limiting value:

$$\sigma_{yc} = 0.4 \ W_v \tag{2-211}$$

where $W_v$ is the valley width at the current position of the center of the puff. Valley widths are computed for each cell in the field of gridded terrain, at a range of heights above ground. The limiting width for a particular puff is then interpolated to the height of the center of the puff above ground. The value 0.4 is obtained by matching the area within the Gaussian profile for the lateral puff distribution with the top-hat distribution of width $W_v$, subject to the constraint that the peak concentration of each are equal. Because this limiting $\sigma_{yc}$ changes as the puff moves along a valley, there will be times when it may be substantially

less than the current $\sigma_y$ for the puff. When this happens, the lateral puff growth is zero, and $\sigma_y$ remains at its initial value during the step.

Strain Calculation

In the absence of a dividing-streamline, the LIFT component of CTDMPLUS essentially computes an effective $\sigma_y$ and $\sigma_z$ from which terrain-altered concentrations are obtained using the "standard" Gaussian plume equation. The effective $\sigma_y$ and $\sigma_z$ are given in the notation of CTSG by Eqns. (2-183) and (2-184). For the "simplified" approach described below, we will focus solely on changes induced on the vertical spread of the puff. Following the implementation for $\sigma_z$ in CTSG, we define a strain factor $T_z = \eta / z_f$, where $\eta$ is the spacing between streamlines in the strained flow, and $z_f$ is the spacing between the same streamlines in the unstrained flow over "flat" terrain. The notion of an <u>effective</u> size of the cloud is introduced to allow concentrations to be calculated in the flat-terrain frame of reference. It is assumed that the primary effect of strain in the flow is to alter the rate of exchange of material across streamlines in the flow. Hence, the ratio of $\sigma_z / \eta$ in the straining flow can be larger than the corresponding ratio $\sigma_{zf} / z_f$. Therefore, the effective size of the cloud in the flat-terrain frame of reference ($\sigma_{ze}$) is defined by:

$$\frac{z_f}{\sigma_{ze}} = \frac{\eta}{\sigma_z} \qquad (2\text{-}212)$$

or

$$\sigma_{ze}^2 = \frac{1}{T_z^2} \sigma_z^2 \qquad (2\text{-}213)$$

As in CTSG, the effect of strain on $\sigma_z$ can be estimated as

$$\sigma_z^2(t) = \frac{1}{S_z^2(t)} \int_o^t 2K(t') \, S_z^2(t') \, dt' \qquad (2\text{-}214)$$

The integral is evaluated over the life of a cloud, thereby incorporating the history of all of the strain experienced by the cloud. The strain function $S_z$ depends on the local value of the strain factor, $T_z$:

$$S_z(t) = e^{\left(1 - T_z(t)\right)} \qquad (2\text{-}215)$$

For weak strain, we note that the strain function is approximately

$$S_z(t) = 1 / T_z(t) \qquad (2\text{-}216)$$

In CALPUFF, the integral in Eqn. (2-181) is evaluated incrementally, as the puff is advected in timesteps of $\Delta t$.

Therefore, we recast the integral to evaluate the effect of the strain on the growth in $\sigma_z$ from time t to time $t + \Delta t$:

$$\sigma_z^2(t + st) = \frac{S^2(t)\sigma_z^2(t) + \int_0^{\Delta t} 2K(t + t')\ S^2(T + t')\ dt'}{S^2(t + \Delta t)} \tag{2-217}$$

Over a short timestep, Eqn. (2-217) can be approximated by replacing $2K(t + t')$ with its mean value during the timestep:

$$2\ \overline{K}\ (t,\Delta t) = \frac{\sigma_{ze}^2\ (t,\ t + \Delta t) - \sigma_{ze}^2\ (t)}{\Delta t} \tag{2-218}$$

Here, we introduce the notation $\sigma_{ze}\ (t,\ t+\Delta t)$ to denote the value of the effective $\sigma_z$ estimated at time $(t + \Delta t)$ on the basis of its value at time $(t)$. That is, if we use a dispersion curve for $\sigma_z$, we find the current value $\sigma_{ze}(t)$, and we estimate the value at $(t + \Delta t)$ by moving $\Delta t$ along the curve, assuming no <u>further</u> terrain effects. This defines the diffusivity in the <u>ambient</u> flow.

Furthermore, we assume that the strain factor $T_z$ varies <u>linearly</u> over the timestep, so that

$$T_z\big(t + t'\big) = T_z(t) + \frac{dT_z}{dt}\ t' \tag{2-219}$$

and Eqn. (2-217) becomes

$$\sigma_z^2\ \big(t + \Delta t\big) = \frac{S^2(t)\ \sigma_z^2(t) + 2\overline{K}\ (t,\Delta t) \int_o^{\Delta t} e^{\ 2\left(1 - T_z(t) - \frac{dT_z}{dt}t'\right)}\ dt'}{S^2(t + \Delta t)} \tag{2-220}$$

Evaluating the integral in Eqn. (2-220),

$$S^2(t + \Delta t)\sigma_z^2\ \big(t + \Delta t\big) = S^2(t)\sigma_z^2(t) + 2\overline{K}\ (t,\Delta t)S^2(t)\left[\frac{1 - e^{-2\Delta t\ dT_z/dt}}{2\ dT_z/dt}\right] \tag{2-221}$$

This result is interpreted further by <u>associating</u> $S^2(t)\ \sigma_z^2(t)$ with $\sigma_{ze}^2(t)$, on the basis of Eqn. (2-213) and the approximate relationship in Eqn. (2-216). Therefore,

$$\sigma_{ze}^2(t + \Delta t) = \sigma_{ze}^2(t) + S^2(t)\Big[\sigma_{ze}^2(t,\ t + \Delta t) - \sigma_{ze}^2(t)\Big]\left[\frac{1 - e^{-2\Delta t\,dT_z/dt}}{2\Delta t\ dT_z/dt}\right] \tag{2-222}$$

provides the growth in the effective vertical spread during one timestep, under the influence of a straining flow field.

Implementation of Eqn. (2-222) requires a model for the strain $T_z(t)$ in the flow field. In CTSG, we have a description of the length scales and position of a terrain feature, and a flow model within CTSG provides information about the strain in the flow over the feature. Here, we use a surrogate to obtain the strain--we infer the scale of a two-dimensional terrain feature (lying across the flow) from the <u>slope</u> of the underlying surface along the flow (Figure 2-26). The slope $|\alpha|$ of the terrain is identified with a surrogate hill of height $h_o$, and half-length L, so that

$$|\alpha| \equiv \frac{h_o}{2L} \tag{2-223}$$

The flow model used in CTSG provides the following equation for the deflection of a streamline ($\delta$) over a two-dimensional ridge in stratified flow:

$$\delta(x,\eta) = h(x) \, e^{-\eta/L} \left( \cos \ell\eta - \frac{x}{L} \sin \ell\eta \right) \tag{2-224}$$

where the hill height function has the form

$$h(x) = \frac{h_o}{1 + \left(\dfrac{x}{L}\right)^2} \tag{2-225}$$

The stratification factor is $\ell = N/u$, x is directed downwind, with origin at the center of the "hill", and $\eta$ is the height of the streamline above the surface at the position x.

Because we wish to associate a strain with the local slope along the puff trajectory and not a complete hill feature, we must assign representative values of $T_z$ and $dT_z/dt$ from somewhere over our surrogate hill. The location chosen to evaluate $T_z$ and $dT_z/dt$ is the point at which $dT_z/dx$ is an extreme value. The strain factor is defined by the local streamline height divided by the streamline height far upwind (Figure 2-27):

$$T_z(x) = \frac{\eta(x)}{\eta_\infty} = \frac{\eta(x)}{h(x) + \eta(x) - \delta(x,\eta)} \tag{2-226}$$

The strain factor at (x/L) is given by

$$T_z^{-1}(x/L) = 1 + \frac{2|\alpha|}{\eta/L \left(1 + (x/L)^2\right)} \left[ 1 - e^{-\eta/L} \left( \cos \ell\eta - \frac{x}{L} \sin \ell\eta \right) \right] \tag{2-227}$$
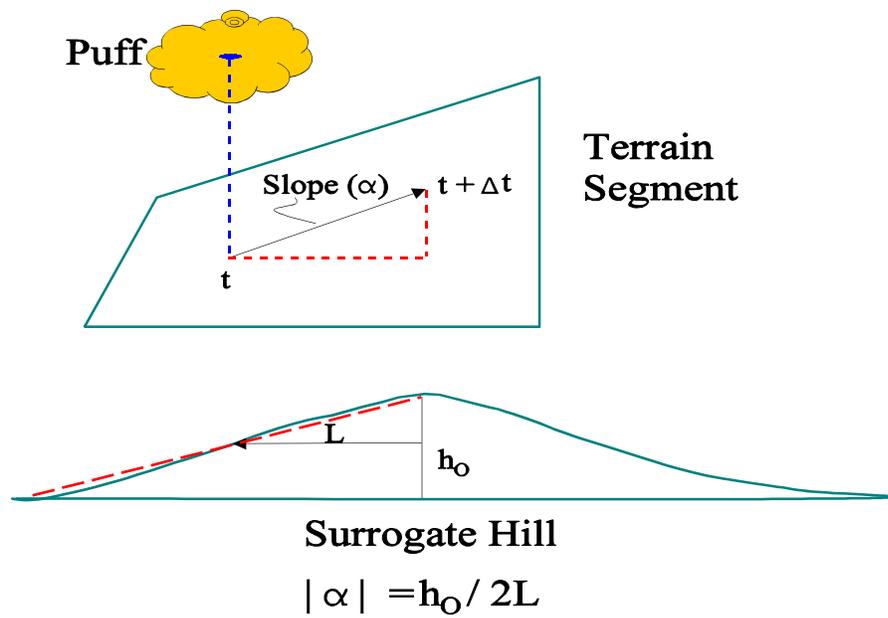
Figure 2-26.    Identification of a surrogate 2-D hill of the same overall slope ($\alpha$) as the terrain directly beneath the puff.
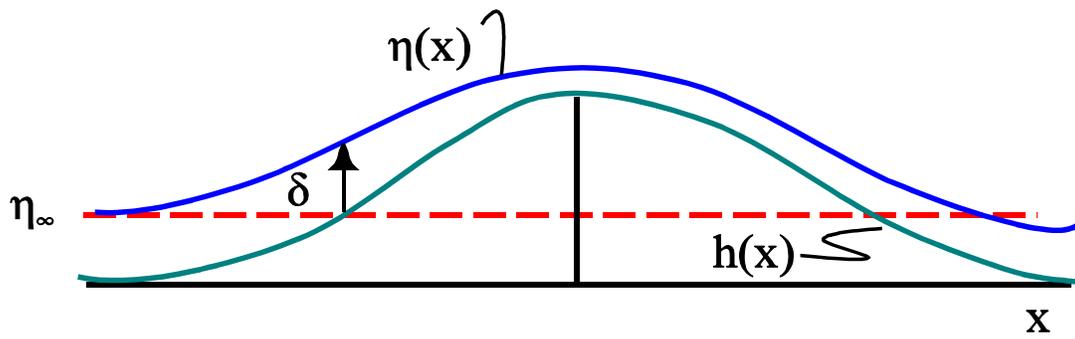
Figure 2-27.    Depiction of streamline height ($\eta$), streamline deflection ($\delta$), and strain factor ($T_z$) nomenclature.

and the change in $T_z$ with distance at $(x/L)$ is

$$\frac{dT_z}{dx}(x/L) = \frac{-2\ |\alpha|\ T_z^2}{\eta\ \left(1\ +\ (x/L)^2\right)}\left[-2(x/L)\ +\ e^{-\eta/L}\left(2(x/L)\ \cos\ \ell\eta\ +\ \left(1\ -\ (x/L)^2\right)\sin\ \ell\eta\right)\right] \qquad (2\text{-}228)$$

The streamline height $\eta$, relative to the length scales of the surrogate hill, remains to be assigned. We set $\eta$ equal to the height of the puff, because the strain over the scale of the puff will determine its modified growth. The scale of the hill, however, is as yet not determined, because so far, we have only used the slope of the terrain. To fix this scale, we process the gridded terrain field to obtain the local relief for each grid cell. This is done for each orientation (N/S, NE/SW, E/W, and SE/NW) about each cell, so that the hill height, $h_o$, in Eqn. (2-223) can be assigned for the direction in which the puff travels. The relief for a particular cell and orientation is obtained by following the incremental elevation change in both directions along the orientation, and comparing this with the first change (at the cell). Interpreting each change in elevation as a slope, $\alpha_i$, and denoting the slope at the cell as $\alpha_o$, we accumulate the changes in elevation until the following condition is satisfied:

$$\frac{\alpha_i}{\alpha_o}\ -\ 1\ |\ >\ \beta \qquad (2\text{-}229)$$

where we take $\beta = 1$. With this choice of $\beta$, the terrain elevation changes are accumulated in each direction until the slope either doubles, or until it changes sign. In this way, <u>local</u> features define the hill height for each cell (and orientation), which is appropriate for defining the "strength" of the interaction between the terrain and the puff during each step. If $\eta/h_o$ is large (say > 10), the puff is well above the terrain, and the effect of the terrain on the flow at puff height is "small". If $\eta/h_o$ is small (say < 0.1), the puff moves in a flow that is substantially altered by the terrain. In both of these limits, the slope of the terrain along the puff trajectory may be the same, so that it is $\eta/h_o$ that differentiates the strength of the terrain effect.

In summary, this simplified implementation of the principles embodied in CTSG involve the following steps:

1)      The slope $|\alpha|$ of the terrain beneath the puff, taken along the transport direction, and the local relief provide the information used to estimate the influence of the terrain on the growth of the puff on the vertical during one timestep.

2)      A surrogate, two-dimensional hill of the same overall slope is used to represent the scale of the terrain.

3)      The strain factor $T_z$ is found from the streamline deflection equation used in CTSG, for the surrogate hill.

4)      Both $T_z$ and its derivative $dT_z/dt$ are evaluated at the location on the surrogate hill at which $dT_z/dt$ is an extreme value (upwind face of hill if the terrain slope is positive,

downwind face if slope is negative).

5) The strain factor is assumed to be a linear function over the timestep, and $\sigma_{ze}$ is computed from $T_z$, $dT_z/dt$, and the ambient rate of growth (the diffusivity).

This formulation conforms to all five attributes stated at the beginning of this subsection. However, several assignments have been made without the benefit of an evaluation study. Because of this, this terrain adjustment procedure should be used with caution at this time.

## 2.7 Dry Deposition

Many complex processes are involved in the transfer and deposition of pollutants at the surface. Sehmel (1980) compiled a list (Table 2-9) of some of the most important factors that are known to influence dry deposition rates. The variables listed include the properties of the depositing material (e.g., particle size, shape, and density; gas diffusivity, solubility, and reactivity), the characteristics of the surface (e.g., surface roughness, vegetation type, amount, and physiological state), and atmospheric variables (e.g., stability, turbulence intensity). Hicks (1982) noted the important differences controlling the deposition of large particles (e.g., gravitational settling, inertial impaction) and those controlling gases (e.g., turbulence, molecular diffusion). Deposition of small particles is complicated by the fact that they may be influenced by the processes affecting both gases and large particles.

A commonly used measure of deposition is the deposition velocity, $v_d$, defined as:

$$v_d = F / \chi_s \tag{2-230}$$

where, $v_d$     is the deposition velocity (m/s),

     $F$     is the pollutant deposition flux ($g/m^2/s$), and

     $\chi_s$     is the pollutant concentration ($g/m^3$).

Due to the number and variability of the factors influencing dry deposition rates, reported deposition velocities exhibit considerable variability. For example, $SO_2$ deposition velocity measurements summarized by Sehmel (1980) range over two orders of magnitude (Figure 2-28). Particle deposition velocities (Slinn et al., 1978) show an even greater variability (Figure 2-29). Although it is not practical to include in the deposition model the effects of all of the variables listed in Table 2-9, it is possible, based on the atmospheric, surface, and pollutant properties to parameterize many of the most important effects. The CALPUFF deposition module provides three options reflecting different levels of detail in the treatment of dry deposition.

·     Full treatment of spatially and temporally varying gas/particle deposition rates predicted by a resistance deposition model.

Table 2-9

Factors Influencing Dry Deposition Rates

| Micrometeorological Variables | Depositing Material | Surface Variables |
|---|---|---|
| Aerodynamic roughness | _Particles_ | Accommodation |
| | | |
| - Mass transfer | | - Exudates |
| (a) Particles | Agglomeration | - Trichome |
| (b) Gases | Diameter | - Pubescence |
| - Heat | Density | - Wax |
| - Momentum | Diffusion | Biotic surfaces |
| - Atmospheric stability | - Brownian | Canopy growth: |
| Diffusion, effect of: | - Eddy equal to | - Dormant |
| - Canopy | (a) Particle | - Expanding |
| - Diurnal variation | (b) Momentum | Senescent |
| - Fetch | © Heat | Canopy Structure: |
| Flow separation: | Effect of canopy on | - Areal density |
| - Above canopy | Diffusiophoresis | - Bark |
| - Below canopy | Electrostatic effects | - Bole |
| Friction velocity | - Attraction | - Leaves |
| Inversion layer | - Repulsion | - Porosity |
| Pollutant concentration | Gravitation settling | - Reproductive structure |
| Relative humidity | Hygroscopicity | - Soils |
| Seasonal variation | Impaction | - Stem |
| Solar radiation | Interception | - Type |
| Surface heating | Momentum | Electrostatic properties |
| Temperature | Physical properties | Leaf-vegetation: |
| Terrain | Resuspension | - Boundary layer |
| - Uniform | Shape | - Change at high winds |
| - Nonuniform | Size | - Flutter |
| Turbulence | Solubility | - Stomatal resistance |
| Wind velocity | Thermophoresis | Non-biotic surfaces |
| Zero-plane | | pH effects on: |
| displacements | | - Reaction |
| - Mass transfer | _Gases_ | - Solubility |
| (a) Particles | | Pollutant |
| (b) Gases | Chemical activity | penetration and |
| - Heat | Diffusion: | distribution in |
| - Momentum | - Brownian | canopy |
| | - Eddy | Prior deposition loading |
| | Partial pressure in | Water |
| | equilibrium   with surface | |
| | Solubility | |

From: Sehmel (1980)
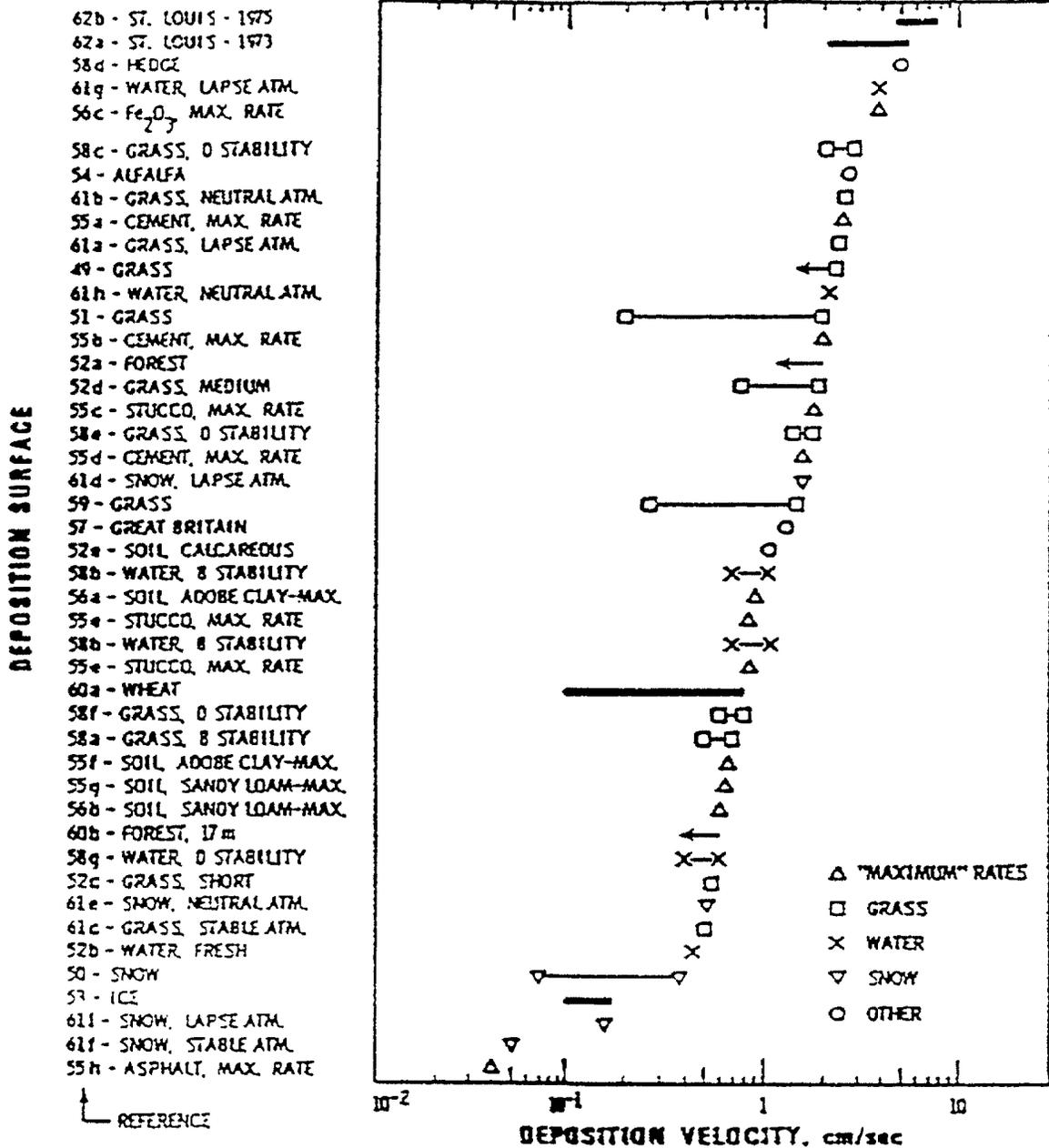
Figure 2-28. Summary of observed SO₂ deposition velocities (from Sehmel (1980)).
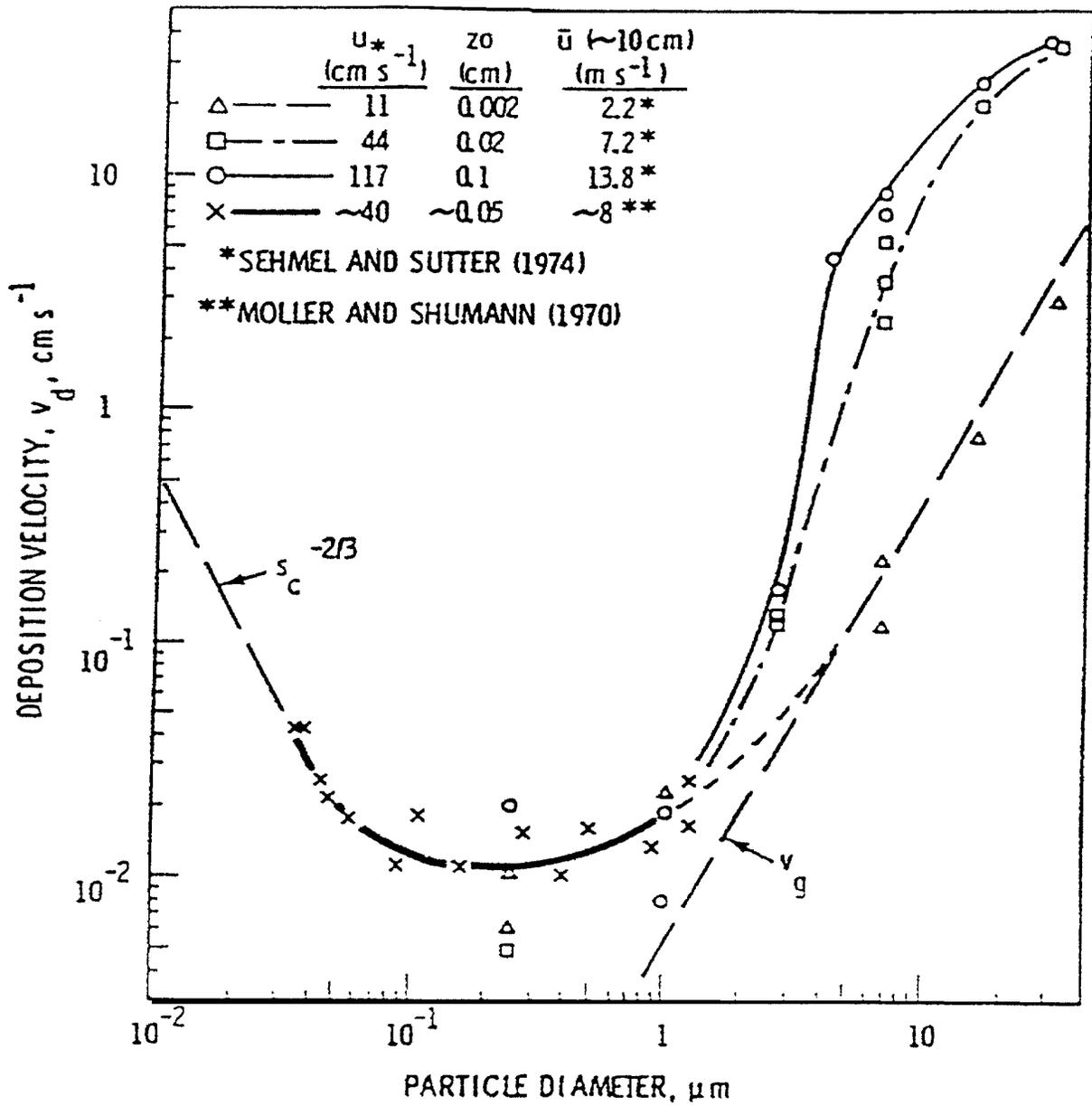
Figure 2-29.    Observed deposition velocities as a function of particle size for 1.5 g/cm density particles.  Measured by Sehmel and Sutter (1974) and Moller and Schumann (1970). Figure from Slinn et al. (1978).

· User-specified 24-hour cycles of deposition velocities for each pollutant. This option allows a "typical" time dependence of deposition to be incorporated, but does not include any spatial dependencies.

· No dry deposition. A switch is incorporated into the model to bypass all the dry deposition calculations. This option will provide for faster model execution for screening runs or pollutants not experiencing significant deposition.

The user specifies a flag in the control file for each pollutant which determines if dry deposition is treated and the specific method used to compute the deposition velocities (see Input Group 2, Section 4.1).

If the resistance deposition model is used, the user must input values for several parameters describing the characteristics of the pollutant (e.g., solubility, reactivity, diffusivity for gases, the size distribution for particles; see Input Group 7 and 8) which are used in the computation of the resistances. In addition, several reference parameters and a flag indicating the state of unirrigated vegetation (i.e., stressed, unstressed, or inactive) are required (see Input Group 9). If any pollutant is flagged as using "user-specified" deposition velocities, the user must prepare a data file with a 24-hour diurnal cycle of deposition velocities for each flagged species (see Section 4.7).

2.7.1    Vertical Structure and Mass Depletion

The CALPUFF dry deposition model is based on an approach which expresses the deposition velocity as the inverse of a sum of "resistances" plus, for particles, gravitational settling terms. The resistances represent the opposition to transport of the pollutant through the atmosphere to the surface. Slinn et al. (1978) describe a multi-layer resistance model for dry deposition. As illustrated in Figure 2-30, the atmosphere can be divided into four layers for purposes of computing dry deposition rates. For gases, an additional (vegetation) layer is included.

(A) Layer Aloft. The top layer is the region above the current mixing height. It contains pollutant material either injected directly from tall stacks, or dispersed upward during previous turbulent activity. Due to the low rate of turbulent mixing in this layer, its pollutant is essentially cut off from the surface. Therefore, this material is not subject to dry deposition until it becomes entrained into the mixed-layer.

(B) Mixed-Layer. The top of the mixed-layer defines the depth of the turbulent boundary layer. Layer B extends down to a reference height within the atmospheric surface layer. Pollutant mixing is dominated by turbulent processes. During convective conditions, pollutants in this layer quickly become uniformly mixed in the vertical. The resistance to pollutant transfer during these conditions is very small compared to the resistances in layers C, D, and E. However, during stable conditions, the mixed-layer resistance may be substantial (Wesely and Hicks, 1977). The treatment

| LAYER | RESISTANCE | | TYPICAL DEPTH (M) | HEIGHT (M) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| (A) Layer Aloft | $C_u$ | *1 | $10^4$ | |
| | | | | h |
| (B) Atmospheric Boundary Layer (Mixed-Layer) | $C_m$ | *2 | $10^2$-$10^3$ | |
| | | | | $z_s$ |
| (C) Surface-Layer (Constant-Flux Layer) | $C_s$ | $r_a$ | $10^1$-$10^2$ | |
| | | | | $z_d$ |
| (D) Deposition Layer (Quasi-Laminar Layer) | $C_d$ $C_o$ | $r_d$ | $v/u*$ | |
| | | | | 0 |
| (E) Vegetation Layer | $C_m$ | $r_c$ | | |

*1    Material in the top layer is not available for deposition at the surface until entrained into the mixed-layer.

*2    Overall mixed-layer resistance included in Equation (2-236).

Figure 2-30.    Multi-layer structure used in the dry deposition resistance model (adapted from Slinn et al., 1978).

of the mixed-layer resistance is based on the overall boundary layer diffusivity parameterized in terms of micrometeorological scaling variables.

(C) Surface Layer.  The surface layer is a shallow layer ($\sim 10$ m) next to the ground that rapidly adjusts to changes in surface conditions.  Because vertical fluxes are nearly constant, this layer is also called the constant-flux layer.  The atmospheric resistance, $r_a$, is used to parameterize the rate of pollutant transfer in Layer C.

(D) Deposition Layer.  Over very smooth surfaces, a thin non-turbulent layer (the deposition layer) develops just above the surface.  For typically rough surfaces, this layer is constantly changing and is likely to be intermittently turbulent.  For this reason, Hicks (1982) calls this layer the "quasi-laminar" layer.  The primary transfer mechanisms across the laminar deposition layer are molecular diffusion for gases, and Brownian diffusion and inertial impaction for particles.  However, surface roughness elements (e.g., leaf hairs) can sometimes penetrate the deposition layer, providing an alternate route for the pollutant transfer (Hicks, 1982).  Under conditions of low atmospheric resistance, the deposition layer resistance, $r_d$, can be the dominant resistance controlling the rate of deposition for particles and some soluble, high molecular weight gases.

(E) Vegetation Layer.  Vegetation is a major sink for many soluble or reactive gaseous pollutants.  After passing through the stomata, soluble pollutants dissolve in the moist mesophyll cells in the interior of the leaves.  Reactive pollutants may also interact with the exterior (cuticle) of the leaves.  Due to the response of the stomata to external factors such as moisture stress, temperature, and solar radiation, the resistance in the vegetation layer (i.e., the canopy resistance, $r_c$) can show significant diurnal and seasonal variability.  An alternate pathway that is potentially important in sparsely vegetated areas or overwater is deposition directly to the ground/water surface.  Although not involving vegetation, it is convenient to include the ground/water surface resistance as a component of $r_c$ because, like the vegetation resistances, it is a resistance in a layer below the laminar deposition layer.

In the CALPUFF model, the fraction of the pollutant mass above and below the current mixed layer is tracked.  At any point in time, only pollutant material below the mixing height can be deposited at the surface.  However, each time step as the mixing height changes, pollutant mass is transferred between Layers A and B.  Typically, in the morning, as the boundary layer grows in response to solar heating of the land surface, material in the top layer is entrained into the mixed-layer and becomes available for dry deposition at the surface.  In the evening, convective activity ceases, and material above the shallow nocturnal boundary layer height is isolated until the next diurnal cycle.

Once puffs have become uniformly mixed through the boundary layer, a surface depletion method (Scire et al., 1984b) can be used to account for the mixed-layer (Layer B) resistance.  The pollutant flux, F, at the reference height within the surface layer can be written as:

$$F = D_{bl} \left(\chi_m - \chi_s\right)/\left(h - z_s\right) = v_d\chi_s \qquad (2\text{-}231)$$

where, $\chi_m$      is the pollutant concentration ($g/m^3$) within the mixed-layer,

$\chi_s$      is the pollutant concentration ($g/m^3$) at the top of the surface layer,

h      is the mixed-layer height (m),

$z_s$      is the surface layer height (m), and

$D_{bl}$      is an overall boundary layer eddy diffusivity ($m^2/s$).

The boundary layer eddy diffusivities during stable conditions (Brost and Wyngaard, 1978) can be expressed as:

$$D_{bl} = k_1 u_* h \qquad (2\text{-}232)$$

and during neutral or unstable conditions as:

$$D_{bl} = Maximum \left[k_1 u_* h, \; k_2 w_* h\right] \qquad (2\text{-}233)$$

where $k_1$ and $k_2$ are constants with default values of 0.01 and 0.1, respectively.

The term $v_d\chi_s$ can be written as $v_d'\chi_m$, where $v_d'$ is an effective deposition velocity taking into account boundary layer mass transfer. From Eqn. (2-231), $v_d'$ is:

$$v_d' = D_{bl} v_d / \left[D_{bl} + v_d\left(h - z_s\right)\right] \qquad (2\text{-}234)$$

When turbulent mixing within Layer B is rapid compared to the rate of deposition at the surface, the atmosphere quickly replaces material that is deposited. During these conditions, $D_{bl}$ is large, and $v_d' \sim v_d$. However, under other conditions the rate of deposition can sometimes be limited by the rate of pollutant transfer through Layer B to the vicinity of the surface. During stable conditions, $D_{bl}$ may be small compared to $v_d(h\text{-}z_s)$, and $v_d'$ may be substantially smaller than $v_d$. In the near-field of a source, before the plume has spread through the boundary layer, it is assumed that $v_d' \sim v_d$. This allows the near-field vertical Gaussian distribution to be maintained.

The resistances in the layers below the reference height in the surface constant-flux layer determine $v_d$. The parameterization of these resistances is discussed separately for gases and particles in Sections 2.7.2 and 2.7.3, respectively. Once $v_d$ is determined, $v_d'$ is computed from Eqn. (2-234). Each time step, the mass of the pollutant in the puff is adjusted to account for the dry removal:

$$Q_m(t + \Delta t) = Q_m(t) \exp\left[-\left(v_d' \, dt / \Delta s\right) \int_{s}^{s+\Delta s} g\left(s'\right)ds'\right] \qquad (2\text{-}235)$$

where,  $Q_m$     is the mass (g) of the pollutant in the puff below the mixing height (h) at time t
            and t+$\Delta$t,

   $\Delta$t      is the time step (s),

   s,s+$\Delta$s   are the positions of the puff at the beginning and end of the time step, and

   g(s)     is the vertical term of the Gaussian puff equation.  For a puff uniformly mixed in
            the vertical, g(s) = 1/h.

If user-specified deposition velocities are used for any of the pollutants, the effective deposition velocity, $v_d'$, is set equal to the user specified value read from the VD.DAT file.

2.7.2    Resistance Deposition Model For Gases

At the reference height, $z_s$, the deposition velocity for gases is expressed (Wesely and Hicks, 1977; Hicks, 1982) as the inverse of a sum of three resistances.

$$v_d = \left( r_a + r_d + r_c \right)^{-1}$$    (2-236)

where,  $r_a$     is the atmospheric resistance (s/m) through the surface layer,

   $r_d$      is the deposition layer resistance (s/m), and

   $r_c$      is the canopy (vegetation layer) resistance (s/m).

**Atmospheric Resistance**

The atmospheric resistance is obtained by integration of the micrometeorological flux-gradient relationships (Wesely and Hicks, 1977):

$$r_a = \frac{1}{k \, u_*} \left[ \ln\left( z_s / z_o \right) - \varphi_H \right]$$    (2-237)

where,  $z_s$     is the reference height (m),

   $z_o$      is the surface roughness length (m),

   k       is the von Karman constant (~ 0.4),

   $u_*$     is the friction velocity (m/s),

   $\varphi_H$    is a stability correction term, and

   L       is the Monin-Obukhov length (m).

The stability correction term accounts for the effects of buoyancy on the eddy diffusivity of the pollutant. It is assumed that the pollutant transfer is similar to that for heat (Wesely and Hicks, 1977).  A gridded field of surface roughness lengths is passed to the model in the output file of the meteorological model, CALMET.  In CALMET, the surface roughness length is either estimated from the predominant land use of each grid cell, or, if available, based on actual values entered by the user.  Over water, due to the effect of

the wind on wave height, the surface roughness length varies as a function of wind speed, and is computed internally within CALPUFF using the parameterization of Hosker (1974)

$$z_0 = 2.0 \ x \ 10^{-6} \ u^{2.5}$$

(2-238)

where u is the wind speed (m/s) at 10 m, and $z_0$ is in meters.

**Deposition Layer Resistance**

Due to the importance of molecular diffusion to the transport through the laminar deposition layer, the deposition layer resistance for gaseous pollutants is parameterized in terms of the Schmidt number:

$$r_d = d_1 S_c^{d_2} / (k \ u_*)$$

(2-239)

where,  $S_c$      is the Schmidt number ($\upsilon/D$),

      $\upsilon$      is the kinematic viscosity of air ($0.15 \times 10^{-4}$ m²/s),

      D      is the molecular diffusivity of the pollutant (m²/s), and

      $d_1, d_2$      are empirical parameters.

Experimental studies summarized by Hicks (1982) suggest a range of values for the empirical variables of 1.6 to 16.7 for $d_1/k$ and 0.4 to 0.8 for $d_2$. Intermediate values of $d_1 = 2$ (or $d_1/k$ of 5), and $d_2 = 2/3$ are recommended based on Shepherd (1974), Slinn et al. (1978), and Hicks (1982).

**Canopy Resistance**

The canopy resistance is the resistance for gases in the vegetation layer. There are three main pathways for uptake/reaction of the pollutant within the vegetation or surface:

     (1)      Transfer through the stomatal pore and dissolution or reaction in the mesophyll cells.

     (2)      Reaction with or transfer through the leaf cuticle.

     (3)      Transfer into the ground/water surface.

In the resistance model, these pathways are treated as three resistances in parallel.

$$r_c = \left[ LA \ I / r_f + LA \ I / r_{cut} + 1 / r_g \right]^{-1}$$

(2-240)

where,  $r_f$      is the internal foliage resistance (s/m) (Pathway 1),

      $r_{cut}$      is the cuticle resistance (s/m), (Pathway 2),

      $r_g$      is the ground or water surface resistance (s/m), (Pathway 3), and

      LAI      is the leaf area index (ratio of leaf surface area divided by ground surface area).

              The LAI is specified in the model as a function of land use type.

The first pathway is usually the most important for uptake of soluble pollutants in vegetated areas. The internal foliage resistance consists of two components:

$$r_f = r_s + r_m \qquad (2\text{-}241)$$

where, $r_s$     is the resistance (s/m) to transport through the stomatal pore, and

$r_m$     is the resistance (s/m) to dissolution or reaction of the pollutant in the mesophyll (spongy parenchyma) cells.

Stomatal action imposes a strong diurnal cycle on the stomatal resistance, and, due to its important role in determining deposition rates for gaseous soluble pollutants such as $SO_2$, on the deposition velocity, as well. Stomatal opening/closing is a response to the plant's competing needs for uptake of $CO_2$ and prevention of water loss from the leaves.

The stomatal resistance can be written (O'Dell et al., 1977) as:

$$r_s = p / (bD) \qquad (2\text{-}242)$$

where, $p$     is a stomatal constant ($\approx 2.3 \times 10^{-8}$ m$^2$),

$b$     is the width of the stomatal opening (m), and

$D$     is the molecular diffusivity of the pollutant (m$^2$/s).

The width of the stomatal opening is a function of the radiation intensity, moisture availability, and temperature. The variation of b during periods when vegetation is active can be represented (Pleim et al., 1984) as:

$$b = b_{max}\left[S / S_{max}\right] + b_{min} \qquad (2\text{-}243)$$

where, $b_{max}$     is the maximum width (m) of the stomatal opening ($\sim 2.5 \times 10^{-6}$ m) (Padro et al., 1991),

$b_{min}$     is the minimum width (m) of the stomatal opening ($\sim 0.1 \times 10^{-6}$ m),

$S$     is the solar radiation (W/m$^2$) received at the ground, and

$S_{max}$     is the solar radiation (W/m$^2$) at which full opening of the stomata occur.

However, during periods of moisture stress, the need to prevent moisture loss becomes critical, and the stomata close. It can be assumed that $b = b_{min}$ for unirrigated vegetation under moisture stress conditions. When vegetation is inactive (e.g., during the seasonal dry periods in much of California), the internal foliage resistance becomes very large, essentially cutting off Pathway 1. In CALPUFF, the state of the unirrigated vegetation is specified as one of these states: (A) active and unstressed, (B) active and stressed, or (C) inactive.

The effect of temperature on stomatal activity has been reviewed by Pleim et al. (1984). The most significant effects are due to temperature extremes. During cold periods (T < 10° C), metabolic activity slows, and b is set equal to $b_{min}$. During hot weather conditions (T > ~ 35° C), the stomata are fully open (b = $b_{max}$) to allow evaporative cooling of the plant (assuming the vegetation is in state A - active and unstressed). These temperature effects provide additional bounds on the value of $r_s$ given by Eqn. (2-242).

### Mesophyll Resistance

The mesophyll resistance depends on the solubility and reactivity of the pollutant. It is an input parameter supplied to the deposition model for each gaseous species. O'Dell et al. (1977) estimate the mesophyll resistance for several pollutants. For soluble pollutants such as HF, $SO_2$, $Cl_2$ and $NH_3$, $r_m$ ~ 0.0. The mesophyll resistance can be large for less soluble pollutants such as $NO_2$ (~ 500 s/cm) and NO (9400 s/cm). For other pollutants, $r_m$ can be estimated based on the solubility and reactivity characteristics of the pollutant.

### Cuticle Resistance

The second pathway for deposition of gases in the vegetation layer is via the leaf cuticle. This includes potential direct passage through the cuticle or reaction of the pollutant on the cuticle surface. Hicks (1982) notes that measurements of $SO_2$ deposition to wheat (Fowler and Unsworth, 1979) show significant cuticle deposition. However, Hosker and Lindberg (1982) suggest that passage of gases through the cuticle is negligible. Therefore, the cuticle deposition is likely to be controlled by the pollutant reactivity. Pleim et al. (1984) parameterize $r_{cut}$ as a function of the pollutant reactivity of the depositing gas relative to the reference values for $SO_2$.

$$r_{cut} = \left( A_{ref} / A \right) r_{cut}(ref)$$

(2-244)

where, A            is the reactivity parameter for the depositing gas,
       $A_{ref}$        is the reference reactivity of $SO_2$ (~ 8.0), and
       $r_{cut}(ref)$     is the empirically determined reference cuticle resistance (s/m) of $SO_2$.

Padro et al. (1991) suggest $r_{cut}(ref)$ is about 30 s/cm. Reactivity values for other pollutants are estimated at 8.0 ($NO_2$), 15.0 ($O_3$), 18.0 ($HNO_3$), and 4.0 (PAN).

### Ground/Water Resistance

The third pathway through the "vegetation layer" involves deposition directly to the ground or water surface. In moderately or heavily vegetated areas, the internal foliage and cuticle resistances usually control the total canopy resistance. However, in sparsely vegetated areas, deposition directly to the surface may be an important pathway. Over water, deposition of soluble pollutants can be quite rapid.

The ground resistance, $r_g$, over land surfaces can be expressed (Pleim et al., 1984) relative to a reference value for $SO_2$:

$$r_g = \left(A_{ref}/A\right)r_g(ref) \tag{2-245}$$

where, $r_g(ref)$ is the reference ground resistance of $SO_2$ (~ 10 s/cm) (Padro et al., 1991).

Slinn et al. (1978) parameterize the liquid phase resistance of the depositing pollutant as a function of its solubility and reactivity characteristics. Their results can be expressed as:

$$r_g = H/\left(\alpha_* \, d_3 \, u_*\right) \tag{2-246}$$

where, H      is the Henry's law constant, which is the ratio of gas to liquid phase concentration of the pollutant, (H ~ $4 \times 10^{-2}$ ($SO_2$), $4 \times 10^{-7}$ ($H_2O_2$), $8 \times 10^{-8}$ ($HNO_3$), $2 \times 10^0$ ($O_3$), $3.5 \times 10^0$ ($NO_2$), $1 \times 10^{-2}$ (PAN), and $4 \times 10^{-6}$ (HCHO)),

      $\alpha_*$      is a solubility enhancement factor due to the aqueous phase dissociation of the pollutant ($\alpha_*$ ~ $10^3$ for $SO_2$, ~ 1 for $CO_2$), and

      $d_3$      is a constant (~ $4.8 \times 10^{-4}$).

## 2.7.3    Resistances for Particulate Matter

Because particulate matter does not interact with vegetation in the same way as gaseous pollutants, particle deposition velocities are commonly expressed only in terms of $r_a$, $r_d$ and a gravitational settling term. The atmospheric resistance, $r_a$, for a particle is the same as for a gas (Eqn. 2-237). The resistance in the vegetation layer ($r_c$) is not a factor because once penetrating the deposition layer, particles are usually assumed to stick to the surface (e.g., Voldner et al., 1986). Therefore, their behavior is similar to highly soluble/reactive gases with $r_c$ ~ 0. Based on an assumption of steady-state conditions, the deposition velocity for particles can be expressed (Slinn and Slinn, 1980; Pleim et al., 1984) as:

$$v = \left(r_a + r_d + r_a r_d v_g\right)^{-1} + v_g \tag{2-247}$$

where $v_g$ is the gravitational settling speed (m/s) of the particle.

In CALPUFF, the puff centerline height at each receptor is adjusted to account for the cumulative effects of gravitational settling. The puff centerline height is assumed to decrease by an amount given by:

$$\Delta h_g = -v_g \cdot t_{tot} \tag{2-248}$$

where, $\Delta h$      is the change in puff height (m) due to settling effects,

      $v_g$      is the gravitational settling velocity (m/s), and

      $t_{tot}$      is the total travel time (s) from the source to the receptor.

There are three major mechanisms for transport of particles across the deposition layer. Small particles ( < 0.1 μm diameter) are transported through the laminar deposition layer primarily by Brownian diffusion. This process becomes less efficient as the particle diameter increases. Particles in the 2-20 μm diameter range tend to penetrate the deposition layer by inertial impaction. The stopping time, t, defined as the settling velocity divided by the acceleration due to gravity, is a measure of tendency of a particle to impact. Inertial impaction is most effective in the 2-20 μm diameter range. Larger particles are dominated by gravitational settling effects. The effect of the terms involving $v_g$ in Eqn. (2-247) always is to increase the deposition velocity. Particles in the range of 0.1-2 μm diameter range, such as sulfate, have very small settling velocities and are not efficiently transported across the deposition layer by either the Brownian diffusion or the inertial impaction mechanism. As a result, these particles have the lowest deposition velocities.

The deposition layer resistance can be parameterized (e.g., Pleim et al., 1984) in terms of the Schmidt number (Sc = υ/D, where υ is the viscosity of air, and, for particles, D is the Brownian diffusivity of the pollutant in air) and the Stokes number (St = $(v_g/g)(u_*^2/υ)$, where $v_g$ is the gravitational settling velocity and g is the acceleration due to gravity).

$$r_d = \left( Sc^{-2/3} + 10^{-3/St} \right)^{-1} u_*^{-1} \qquad (2\text{-}249)$$

The diffusivity of a particle in air, D, is a function of the particle size. Smaller particles tend to be more efficiently transported by Brownian motion, and therefore have higher diffusivities. The Stokes number is a measure of the likelihood of impaction of the particle. It increases with increasing particle size.

The gravitational settling velocity is a function of the particle size, shape, and density. For spheres, the settling velocity is given by the Stokes equation:

$$v_g = \left[ (d_p)^2 \, g \left( \rho_p - \rho_g \right) C \right] / (18 \, υ) \qquad (2\text{-}250)$$

where, $d_p$    is the particle diameter (m)
$\rho_p$    is the particle density (g/m³),
$\rho_g$    is the air density (g/m³), and
C    is the Cunningham correction for small particles.

This correction given by:

$$C = 1 + \left( 2 \, \lambda / d_p \right) \left[ a_1 + a_2 \exp \left( -a_3 d_p / \lambda \right) \right] \qquad (2\text{-}251)$$

where, $\lambda$    is the mean free path of air molecules (6.53 x 10⁻⁶ cm), and
$a_1, a_2, a_3$    are constants (1.257, 0.40, 0.55, respectively).

Because of the sensitivity of the deposition velocity to particle size, the effective deposition velocity is computed for a number of individual size categories, and then weighted by the actual size distribution. The

particle size distribution is specified in terms of the geometric mass mean diameter and geometric standard deviation of the distribution.  For sulfate, the geometric mass mean diameter is approximately 0.5 μm with a geometric standard deviation of approximately 2 μm.

2.8     Chemical Transformation

One of the design criteria of the CALPUFF model required the capability of modeling linear chemical transformation effects in a manner consistent with the puff formulation of the model.  The CALPUFF chemical module contains four options for dealing with chemical processes:

- A pseudo-first-order chemical reaction mechanism for the conversion of $SO_2$ to $SO_4^=$ and $NO_x$ ($NO + NO_2$) to $NO_3^-$.  This mechanism is based on the chemical transformation scheme used in the MESOPUFF II model (Scire et al., 1984b) and incorporates the most significant dependencies of spatially and temporally varying environmental conditions on the transformation rates.
- The RIVAD/ARM3 scheme (Morris et al., 1988), which treats the NO and $NO_2$ conversion process in addition to the $NO_2$ to total $NO_3$ and $SO_2$ to $SO_4$ conversions, with equilibrium between gaseous $HNO_3$ and ammonium nitrate aerosol.
- User-specified 24-hour cycles of transformation rates.  This option allows simulation of the diurnal, time-dependent behavior of the transformation rates.  However, the transformation rates with this option are spatially uniform.
- No chemical transformation.  An option is provided to completely bypass the chemical transformation calculations.  This will reduce computer requirements for situations or pollutants for which chemical transformation effects are not significant.

The user selects one of the above options by specifying a mechanism flag in the CALPUFF control flag (see Section 4.1).  The MESOPUFF II mechanism (Option 1) and the RIVAD/ARM3 mechanism (Option 3) use ozone concentrations (along with radiation intensity) as surrogates for the OH concentration during the day when gas phase free radical chemistry is active.  With either of these options, hourly observations of ozone concentrations at one or more monitoring stations can be read from a data file (OZONE.DAT) to provide the necessary estimates of ozone concentrations (see Section 4.8).

If "user-specified" transformation rates are used (Option 2), the user must prepare a data file (CHEM.DAT) with a 24-hour diurnal cycle of typical transformation rates for each species (see Section 4.9).

2.8.1    Description of the MESOPUFF II Chemical Mechanism

The chemical processes included in the MESOPUFF II mechanism (Option 1) are the conversion of sulfur dioxide to sulfate and the conversion of nitrogen oxides to nitrate aerosol.  Figures 2-31 and 2-32 illustrate the chemical pathways for $SO_2$ and $NO_x$ oxidation and aerosol formation.  Oxidation may occur by gas and
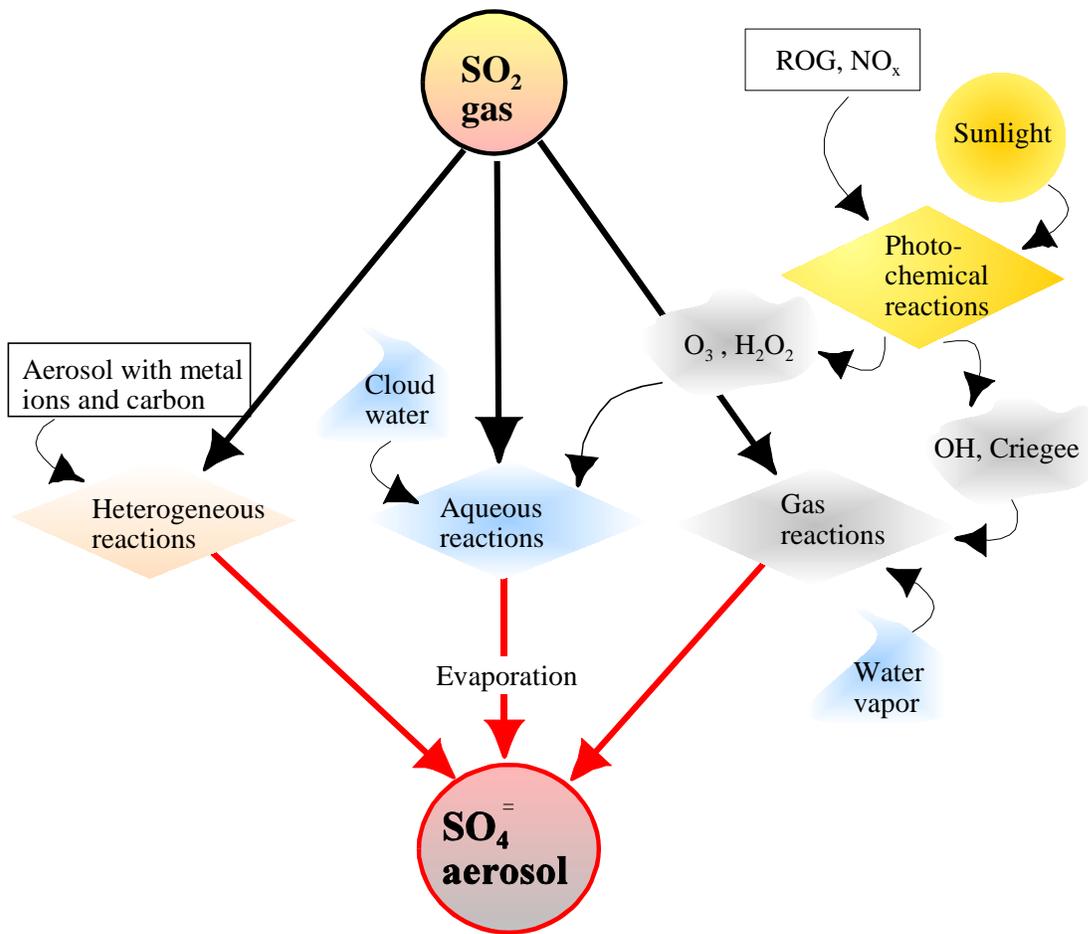
Figure 2-31.       $SO_2$ oxidation pathways (from Scire et al., (1984b)).

aqueous phase reactions. The gas phase reactions for both $SO_x$ and $NO_x$ involve free radical photochemistry and, therefore, are coupled to the oxidation of reactive organic gases (ROG).

Homogeneous gas phase reaction is the dominant $SO_2$ oxidation pathway during clear, dry conditions (Calvert et al., 1978). Ozone and hydrogen peroxide are believed to be the principal oxidants for aqueous-phase oxidation of $SO_2$.

The oxidation of $NO_x$ is dependent on gas phase $ROG/NO_x/O_3$ photochemistry. It is generally more rapid than $SO_2$ oxidation. As shown in Figure 2-32, $NO_x$ can be oxidized to nitric acid ($HNO_3$) and organic nitrates ($RNO_3$) such as peroxyacetylnitrate (PAN). Nitric acid combines with ammonia gas to form solid or aqueous ammonium nitrate ($NH_4NO_3$). Unlike sulfate formation, the nitrate process is reversible. Equilibrium is established between nitric acid, ammonia, and ammonium nitrate:

$$NH_4NO_3 \quad HNO_3 \text{ (g)} + NH_3 \text{ (g)} \tag{2-252}$$

The equilibrium constant for this reaction ($K = [NH_3][HNO_3]/[NH_4NO_3]$) is a nonlinear function of temperature and relative humidity as shown in Figure 2-33 (Stelson and Seinfeld, 1982). The equilibrium constant can vary several orders of magnitude over a typical diurnal cycle. Given fixed amounts of total nitrate, ammonia, and water vapor, higher $NH_4NO_3$ concentrations are expected at night due to lower nighttime temperatures and higher relative humidities. Thus, the nitrate aerosol cannot be considered a stable product like sulfate. Also, unlike sulfate, the ambient concentration of nitrate is limited by the availability of ammonia which is preferentially scavenged by sulfate (Stelson et al., 1983).

The transformation pathways for the five active pollutants ($SO_2$, $SO_4^=$, $NO_x$, $HNO_3$, and $NO_3^-$) included in the MESOPUFF II scheme are shown in Figure 2-34. Transformation rate expressions were developed by statistically analyzing hourly transformation rates produced by a photochemical model. The photochemical model employed the $RHC/NO_x/SO_x$ chemical mechanism of Atkinson et al. (1982). Plume $SO_x/NO_x$ dispersing into background air containing ozone and reactive hydrocarbons was simulated over a wide range of conditions representing different solar radiation intensities, temperatures, dispersion conditions, background ozone and RHC concentrations, plume $NO_x$ concentrations and emission times. The following transformation rate expressions, representing curve fits to the daytime hourly conversion rates predicted by the photochemical model, were determined:

$$k_1 \; = \; 36 \, R^{0.55} \left[ O_3 \right]^{0.71} \; S^{-1.29} \; + \; k_{1(aq)} \tag{2-253}$$

$$k_2 \; = \; 1206 \left[ O_3 \right]^{1.5} \; S^{-1.41} \left[ NO_x \right]^{-0.33} \tag{2-254}$$

$$k_3 \; = \; 1261 \left[ O_3 \right]^{1.45} \; S^{-1.34} \left[ NO_x \right]^{-0.12} \tag{2-255}$$
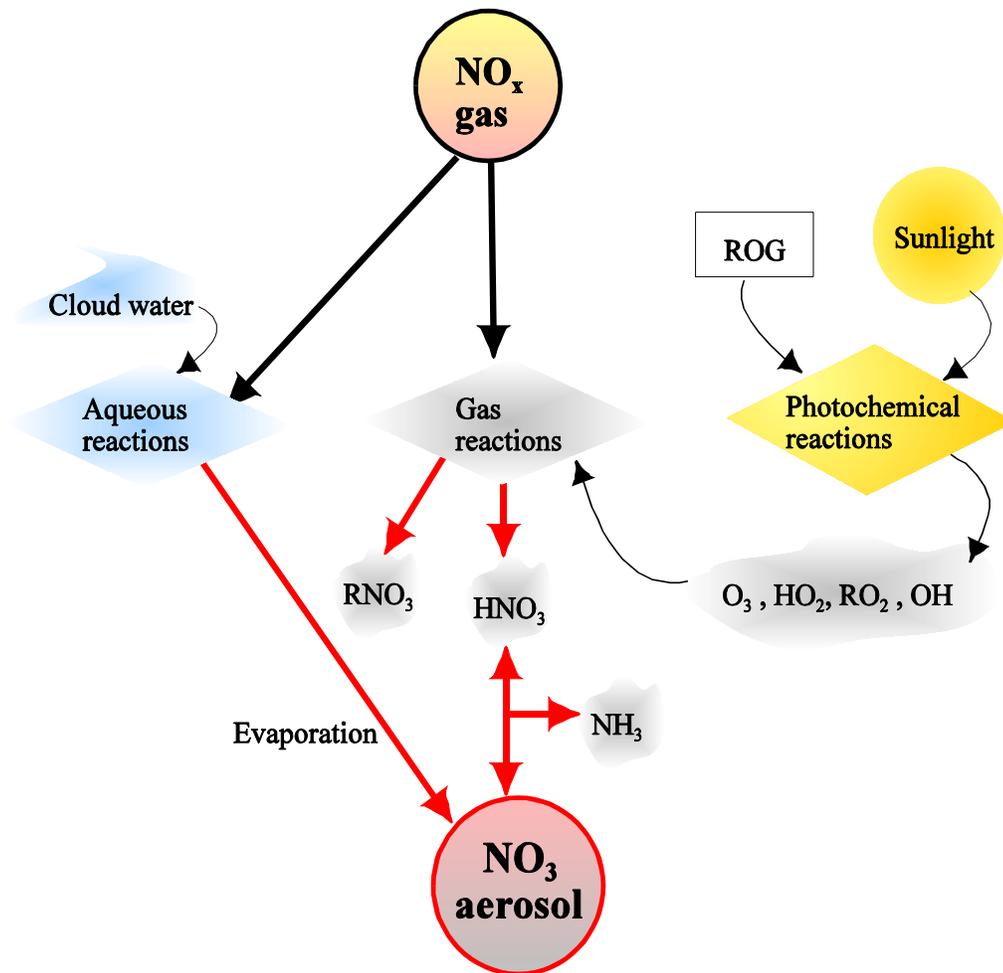
Figure 2-32. $NO_x$ oxidation pathways (from Scire et al., (1984b)).
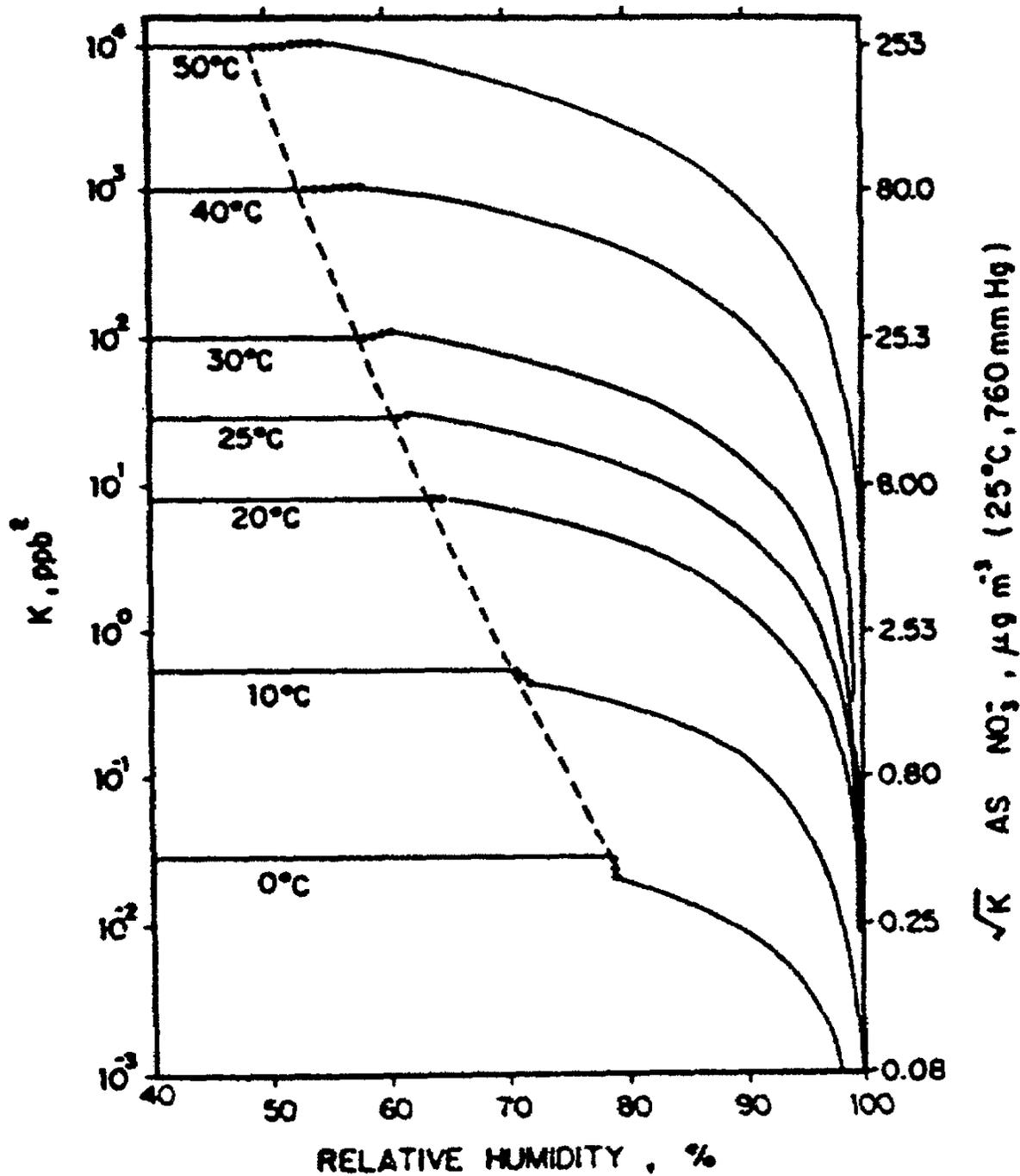
Figure 2-33. $NH_4NO_3$ dissociation constant as a function of temperature and relative humidity (from Stelson and Seinfeld, (1982)).

POLLUTANT 1    $\xrightarrow{\quad k_1 \quad}$    POLLUTANT 2
(SO₂)                                     ($SO_4^=$)

POLLUTANT 3    $\xrightarrow{\quad k_2 \quad}$    ALL PRODUCTS
($NO_x$)

                   $\xrightarrow{\quad k_3 \quad}$    POLLUTANT 4
                                              ($HNO_3$)

POLLUTANT 4    $\underset{\longleftarrow}{\overset{NH_3}{\longrightarrow}}$    POLLUTANT 5
($HNO_3$)                                   ($NO_3$)
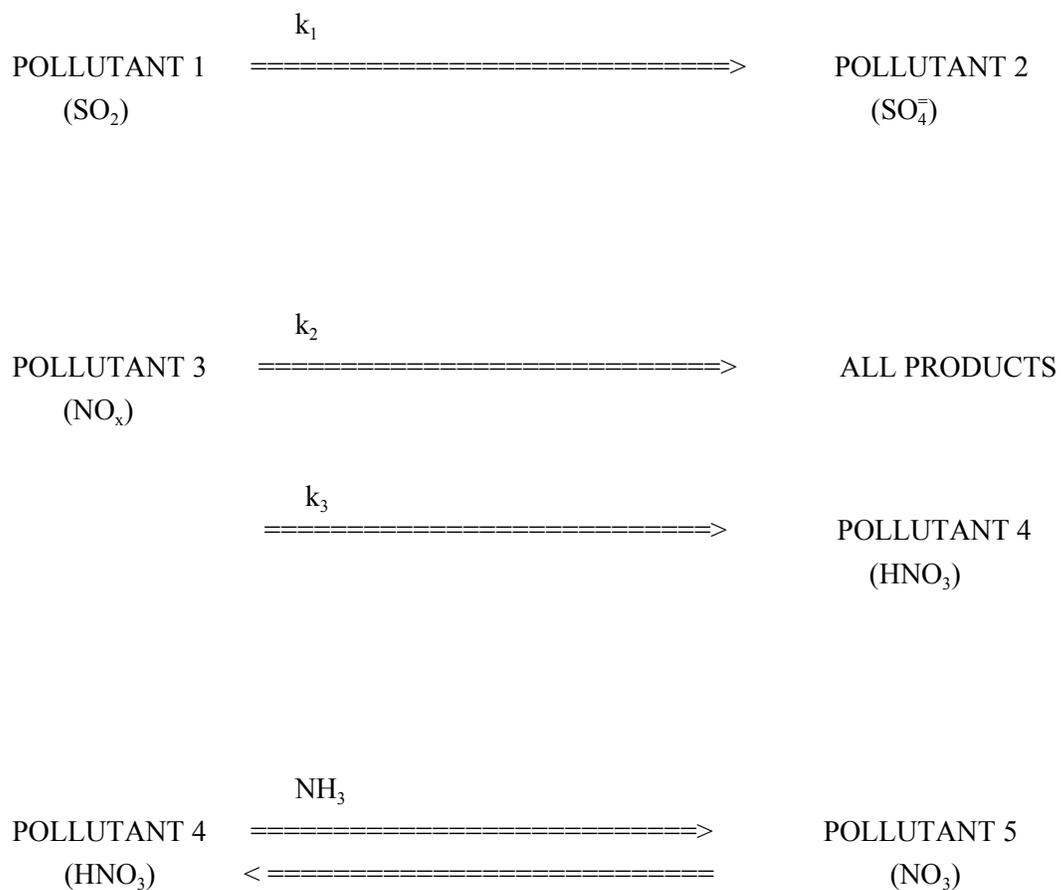
Figure 2-34.     Schematic representation of chemical pathways in the five-pollutant system assumed with the MESOPUFF II chemical mechanism.

where the aqueous phase component of the $SO_2$ conversion rate is parameterized as:

$$k_{1(aq)} = 3 \ x \ 10^{-8} \ RH^4 \tag{2-256}$$

and,  $k_1$     is the $SO_2$ to $SO_4$ transformation rate (percent/hour),

$k_2$     is the $NO_x$ to $HNO_3 + RNO_3$ transformation rate (percent/hour),

$k_3$     is the $NO_x$ to $HNO_3$ (only) transformation rate (percent/hour),

R     is the total solar radiation intensity (kw/m$^2$),

S     is a stability index ranging from 2 to 6 (PGT class A and B=2, C=3, D=4, E=5,

F=6),

RH     is the relative humidity (percent),

$[O_3]$     is the background ozone concentration (ppm), and

$[NO_x]$   is the plume $NO_x$ concentration (ppm).

Eqns. (2-253) to (2-255) apply only during daytime periods when gas phase free radical chemistry is active. The use of the ozone concentration and the radiation intensity as surrogates for the OH concentration, as in the above equations, is appropriate only during the day. At night, $SO_2$ and $NO_x$ oxidation rates resulting from heterogeneous reactions are generally much lower than typical daytime rates (Wilson, 1981; Forrest et al., 1981). Nighttime oxidation rates of 0.2% and 2.0% for $SO_2$ and $NO_x$, respectively, are used as default values in the model.

Two options are provided for the specification of ozone concentrations:  (1) hourly ozone data from a network of stations (OZONE.DAT, see Section 4.8), or (2) a single, user-specified background ozone value may be used. The background ammonia concentration required for the $HNO_3/NH_4NO_3$ equilibrium calculation can be user-specified or a default value will be assumed.

The parameterized $NO_x$ oxidation rate depends on the $NO_x$ concentration. In situations where puffs overlap, it is necessary to estimate the total $NO_x$ concentration at a particular point to properly determine $k_2$ and $k_3$. Similarly, the nitrate equilibrium relationship requires knowledge of the total (local average) $SO_4$, $NO_x$, and total nitrate ($HNO_3 + NO_x$) concentrations. Because of the preferential scavenging of ammonia by sulfate, the available ammonia is computed as total ammonia minus sulfate. The local average concentrations within a puff are estimated as the sum of contributions from the puff's own pollutants plus those of nearby puffs. Local average concentrations are separately computed for puffs within and above the mixed-layer.

2.8.2    Description of the RIVAD/ARM3 Chemical Mechanism

The second mechanism available in CALPUFF is the RIVAD condensed pseudo-first-order chemical scheme, as prepared for ARM3 (Morris et al., 1988). Because the mechanism assumes low  background concentrations of VOCs, the authors suggest that it is best suited for relatively clear non-urban areas.

In the RIVAD scheme, the rate of sulfate and nitrate production is estimated by calculating the steady-state concentration of hydroxyl radical, $OH^-$ , which is the primary oxidizer of $SO_2$ and $NO_2$. Within a puff, the steady-state equations for $0('D)$ and $OH^-$ are:

$$[O('D)] = \frac{k_{34}(hv)[O_3]}{k_{35} + k_{36}[H_2O]}$$

(2-257)

$$\frac{d[OH\cdot]}{dt} = 2\ K_{36}[0('D)][H_2O] - K_{37}[OH\cdot][SO_2] - K_{38}[OH\cdot][NO_2]$$

(2-258)

$$[OH\cdot] = \frac{2\ K_{36}[O('D)][H_2O]}{K_{37}[SO_2] + K_{38}[NO_2]}$$

(2-259)

With this steady-state concentration, pseudo-first-order $SO_2$-to-$SO_4$ and $NO_2$-to-$HNO_3 + NO_3^-$ conversion rates are calculated as:

$$-\frac{1}{[SO_2]}\frac{d[SO_2]}{dt} = K_{37}[OH\cdot]$$

(2-260)

$$-\frac{1}{[NO_2]}\frac{d[NO_2]}{dt} = K_{38}[OH\cdot]$$

(2-261)

where,

$$K_{34} = 1.3\ x\ 10^{-3}\left(\cos Z_s\right)^{2.74}\ ppm^{-1}\ min^{-1}$$

(2-262)

$$k_{35} = 4.45\ x\ 10^{10}\ ppm^{-1}\ min^{-1}$$

(2-263)

$$k_{36} = 3.4\ x\ 10^5\ ppm^{-1}\ min^{-1}$$

(2-264)

$$k_{37} = 2.0\ x\ 10^3\ ppm^{-1}\ min^{-1}$$

(2-265)

$$k_{38} = 1.4\ x\ 10^4\ ppm^{-1}\ min^{-1}$$

(2-266)

and $\cos(Z_s)$ is the cosine of the solar zenith angle. The MESOPUFF II scheme is used to determine the equilibrium between nitric acid, ammonia, and ammonium nitrate. Ozone concentrations and background ammonia data are provided as described in 2.8.1.

The RIVAD chemical mechanism does not explicitly calculate the aqueous-phase oxidation of $SO_2$ to sulfates. The RIVAD chemistry assumes a constant heterogeneous oxidation rate of $SO_2$ of 0.2 %/hr that is added to the homogeneous rate.

2.9    Wet Removal

Many studies have shown that during rain events, wet scavenging of soluble or reactive pollutants can be of the order of tens of percent per hour (Barrie, 1981; Slinn et al., 1978; Levine and Schwartz, 1982; Scire and Venkatram, 1985). Gaseous pollutants are scavenged by dissolution into cloud droplets and precipitation. For $SO_2$, aqueous-phase oxidation can be an important removal pathway. Particulate pollutants are removed by both in-cloud scavenging (rainout) and below-cloud scavenging (washout). Over source-receptor distances of tens to hundreds of kilometers, wet scavenging can deplete a substantial fraction of the pollutant material from the puff.

$k_{1(aq)}$    is the aqueous phase $SO_2$ oxidation term (percent/hour).

A simple approach that has been shown (e.g., Maul, 1980) to yield realistic long-term estimates of wet removal is the empirically-based scavenging coefficient method. The depletion of a pollutant is represented as:

$$\chi_{t+dt} = \chi_t \exp\left[- \Lambda \Delta t\right] \tag{2-267}$$

where, $\chi$      is the concentration ($g/m^3$) at time t and t + $\Delta$t, and
        $\Lambda$      is the scavenging ratio.
The scavenging ratio can be expressed as:

$$\Lambda = \lambda \left(R / R_1\right) \tag{2-268}$$

where, $\lambda$      is the scavenging coefficient ($s^{-1}$),
        R      is the precipitation rate (mm/hr), and
        $R_1$      is a reference precipitation rate of 1 mm/hr.

The scavenging coefficient depends on the characteristics of the pollutant (e.g., solubility and reactivity) as well as the nature of the precipitation. Table 2-10 contains the default values of the scavenging coefficient for $SO_2$, $SO_4^=$, $NO_x$, $HNO_3$, and $NO_3^-$. A precipitation code determined from the hourly surface meteorological observations of precipitation type (i.e., CD144 data) is used to determine if the value of $\lambda$ for liquid or frozen precipitation is most appropriate. The reported precipitation code is related to precipitation type as shown in Table 2-11. The liquid precipitation values of $\lambda$ are used for precipitation codes 1-18. The frozen precipitation values are used for precipitation codes 19-45.

Table 2-10

Default Values of the Scavenging Coefficient, $\lambda(s^{-1})$

| Pollutant | Liquid Precipitation | Frozen Precipitation |
|-----------|---------------------|---------------------|
| $SO_2$ | $3 \times 10^{-5}$ | 0.0 |
| $SO_4^=$ | $1 \times 10^{-4}$ | $3 \times 10^{-5}$ |
| $NO_x$ | 0.0 | 0.0 |
| $HNO_3$ | $6 \times 10^{-5}$ | 0.0 |
| $NO_3^-$ | $1 \times 10^{-4}$ | $3 \times 10^{-5}$ |

Table 2-11

Conversion of Reported Precipitation Type/Intensity To Precipitation Codes

| Precipitation Code | Type | Intensity |
|---|---|---|
| Liquid Precipitation | | |
| 1 | Rain | Light |
| 2 | Rain | Moderate |
| 3 | Rain | Heavy |
| 4 | Rain Showers | Light |
| 5 | Rain Showers | Moderate |
| 6 | Rain Showers | Heavy |
| 7 | Freezing Rain | Light |
| 8 | Freezing Rain | Moderate |
| 9 | Freezing Rain | Heavy |
| 10 | Not Used | - |
| 11 | Not Used | - |
| 12 | Not Used | - |
| 13 | Drizzle | Light |
| 14 | Drizzle | Moderate |
| 15 | Drizzle | Heavy |
| 16 | Freezing Drizzle | Light |
| 17 | Freezing Drizzle | Moderate |
| 18 | Freezing Drizzle | Heavy |
| **Frozen Precipitation** | | |
| 19 | Snow | Light |
| 20 | Snow | Moderate |
| 21 | Snow | Heavy |
| 22 | Snow Pellets | Light |
| 23 | Snow Pellets | Moderate |
| 24 | Snow Pellets | Heavy |
| 25 | Not Used | - |
| 26 | Ice Crystals | * |
| 27 | Not Used | - |
| 28 | Snow Showers | Light |
| 29 | Snow Showers | Moderate |
| 30 | Snow Showers | Heavy |
| 31 | Not Used | - |
| 32 | Not Used | - |
| 33 | Not Used | - |
| 34 | Snow Grains | Light |
| 35 | Snow Grains | Moderate |
| 36 | Snow Grains | Heavy |
| 37 | Ice Pellets | Light |
| 38 | Ice Pellets | Moderate |
| 39 | Ice Pellets | Heavy |
| 40 | Not Used | - |
| 41 | Hail | * |
| 42 | Not Used | - |
| 43 | Not Used | - |
| 44 | Small Hail | * |
| 45 | Not Used | - |

---

* Intensity not currently reported for ice crystals, hail and small hail.

The user can override the default values of the scavenging coefficient by entering new values in the CALPUFF control file (see Section 4.1).  An option is provided in the model to completely by-pass the wet removal calculation for pollutants or time periods for which it is not of importance.


2.10    Odor Modeling


A simple averaging-time scaling factor can be used to estimate short-term peak concentrations for applications such as assessing the perception of odor.  Such adjustments are necessary because the averaging time associated with dispersion curves used to compute mean concentrations are 3 to 60 minutes, while odors are perceived on time scales of a few seconds.  This adjustment primarily addresses the effect of meandering (fluctuations in the wind about the mean flow for the hour) on the average lateral distribution of material.  The scaling factor used to adjust the lateral dispersion coefficient (Turner, 1970) for averaging time is the $1/5^{th}$ power law:

$$f(t, t_o) = (t_o/t)^{0.2} \tag{2-269}$$

 where (t) is the averaging time (min.) of interest, and ($t_0$) is the averaging time consistent with the dispersion rates used to obtain the mean concentration.


Two methods may be used to incorporate this scaling factor.  When the PG dispersion curves are used, an averaging time (min.) can be specified by the variable AVET in Input Group 1 of the control file.  PG $\sigma_y$ values used for the dispersion due to ambient turbulence will then be adjusted by the scaling factor (assuming $t_o$ to be 60 minutes in CALPUFF and 3 minutes in AUSPUFF).  Any initial source influences on $\sigma_y$ will not be adjusted.  Using a short averaging time therefore reduces $\sigma_y$ , which increases the "centerline" concentrations simulated, but decreases the lateral spread (adjusted concentrations at receptors to the side of the "centerline" may decrease).  In CALPUFF, the notion of a "centerline" concentration must be recognized to be a "trajectory centerline" concentration.


In the second method, the scaling factor is applied directly to the mean concentrations.  This is best accomplished by applying the scaling factor at the postprocessing stage (CALPOST).  All concentrations will then be increased for short averaging times.


The difference in these two methods requires interpretation.  In the first, the lateral turbulence is given an averaging time much shorter than the averaging time associated with the mean wind.  One obtains a representation of the peak concentrations that are consistent with that turbulence, but may not obtain a characterization of the lateral extent of the area that is affected by those concentrations during an hour.  This concentration field may be thought of as a short-term "snapshot" for the most probable trajectory during the hour.  In the second, one still obtains a representation of the peak concentrations, but the off-centerline concentrations need to be interpreted as probability-weighted short-term peak concentrations.  The "snapshot" distribution meanders about its mean trajectory during the hour, and the concentrations reported

away from the most probable trajectory are, on average, less likely to be as large as those in the "snapshot" distribution.

2.11    Area Sources

A specialized algorithm is used to simulate concentrations within and downwind of area sources.  The original CALPUFF model approximated all area sources using the virtual point source method in which the overall size of the area source was represented by an initial $\sigma_y$.  While such an approach is reasonable far from the area source, it becomes a poor approximation nearby, or for receptors embedded within, a large area source.  The ISCST model overcame a similar limitation by including an algorithm for explicit 2-dimensional integration over an arbitrary, polygon-shaped area source.

The ISCST 2-dimensional integration was carried out to a predetermined accuracy for an arbitrary n-sided convex polygon using a series of steps, including:

•       transformation to the (along-wind, cross-wind) coordinate frame by simply transforming each of the polygon vertices to this frame,
•       evaluation of the cross-wind integral exactly in terms of the difference of two error functions, and
•       integration in the along-wind direction using as many samples as is necessary to meet some desired convergence accuracy criteria.

This third step actually involves an iteration of three distinct steps:

•       trapezoidal rule integration using an increasing number (i.e., doubling) of sampling points in the along-wind direction,
•       use of the Romberg method, involving polynomial extrapolation, to estimate the value of the integral in the limit of an integrand sampling interval of zero, and
•       testing on the convergence (i.e., robustness) of this estimated integral value.

The use of the Romberg method to extrapolate the value of the integral, rather than work with the raw trapezoidal rule estimates, constitutes a more efficient and rapidly converging quadrature algorithm and was developed and tested for the ISCST2 Model.

The extension of the slug formalism to include polygon area sources uses the same basic steps, and even several of the same subroutines (with minor interface related modifications); however, the integration is over the slug integrand rather than over the steady-state Gaussian plume integrand as in ISCST.  As developed in the Section 2.1.2, the slug integrand is generally more complex than the Gaussian plume expression, but for the case of time-averaged concentrations produced by freshly emitted material and given by Eqn.(2-16), the crosswind, "Y term" is identical and therefore enables the same conversion of a 2-d integral to a 1-d integral of an analytic expression to be invoked.  More specifically, one begins with the

formal expression of the 2-d integral of Eqn.(2-16) as:

$$\overline{C}_p \;=\; \int_p \int \; dxdy \; \overline{C}(x,y)$$

(2-270)

where $\overline{C}_p$ denotes the time-averaged concentration resulting from the polygon area source, the double integral over the polygon is computed in the cross-wind (y) and along-wind (x) frame, and $\overline{C}(x,y)$ is simply Eqn. (2-16) adjusted for the fact that q is now the areal emission rate expressed as $(g/m^2/s)$. Inserting Eqn. (2-16) into (2-270) and regrouping terms one obtains

$$\overline{C}_p \;=\; \frac{q}{u}\int_p^{dx} \overline{F}(x)g(x)\cdot\frac{u}{\sqrt{2\pi}\,u'\,\sigma_y(x)}\int_{d_{cl}}^{d_{cr}} dy \; \exp\left[\frac{-y^2}{2\sigma_y^2(x)}\,\frac{u^2}{u'^2}\right]$$

(2-271)

where $d_{cl}$ and $d_{cr}$ are the x-dependent left and right (i.e., as seen from the receptor) cross-wind limits of the polygon source, and $\overline{F}(x)$ and $g(x)$, defined in Eqs.(2-17) and (2-2) respectively, are now functions of along-wind distance from the specific point within the polygon source. Similarly, one notes that other $\overline{F}(x)$ related variables, defined by Eqs. (2-18) thru (2-20), are now all x-dependent. Finally, one notes that the cross-wind integral in Eqn. (2-271) can be performed, yielding the difference of two error functions, and one obtains the final analytic result,

$$\overline{C}_p \;=\; \frac{q}{u} \int_p dx \; \overline{F}(x)g(x) \; Y(x)$$

(2-272)

where

$$Y(x) \;=\; \frac{1}{2}\left[ erf\left[\frac{d_{cr}(x)u}{\sqrt{2}\sigma_y(x)u'}\right] \;-\; erf\left[\frac{d_{cl}(x)u}{\sqrt{2}\sigma_y(x)u'}\right]\right].$$

(2-273)

The remaining x integration of Eqn. (2-272) must now be performed numerically by the Romberg integration method outlined above. This procedure involves evaluating the integrand of Eqn. (2-272) at numerous x values until the Romberg estimated value of $\overline{C}_p$, estimated in the limit of $\Delta x \to 0$, displays appropriate robustness.

The formalism detailed above deals only with the case of slugs involving new emissions (i.e., IAGE=0) from polygon area sources. As mentioned previously, the biggest differences between the virtual point source and integral approaches occurs near the area source; hence, emphasis was placed on the IAGE=0 case. For old slugs of material (i.e., IAGE > 0), the problem becomes significantly more complicated, and an approximate treatment is employed.

An old slug is any slug whose younger end is not attached to the source during a sampling step. It is a "non-emitting" slug. Thus old slugs may be as young as one sampling step old. For area sources, a collection of

emitting slugs is employed in the integration procedure just described in order to represent the mass release distribution in the along-wind direction. Recall that the initial cross-wind distribution for each emitting slug is that of a line source. One slug replaces this collection in subsequent sampling steps. It is released from the center of the area source, and is given an initial $\sigma_{ys}$ that is derived from the cross-wind length of the area source. Note, however, that this initial $\sigma$ is not used to define a virtual point source, but is added in quadrature to the ambient $\sigma$ (see Eqn. 2-37). This is equivalent to treating the initial distribution as a group of independent point sources, where the source strengths are distributed with a sigma of $\sigma_{ys}$.

With this effective $\sigma_y$, old slugs are transported and sampled in the normal way, but the concentrations obtained in the cross-slug direction are adjusted to account for the initial line source distribution, rather than the effective Gaussian distribution. The adjustment factor is the ratio of the cross-wind line source distribution to the point source distribution:

$$
F_r = \frac{\sigma_{yr}}{\sigma_{ys}} \; \frac{erf\left(\dfrac{y_r + L_c/2}{\sqrt{2}\;\sigma_{ya}}\right) - erf\left(\dfrac{y_r - L_c/2}{\sqrt{2}\;\sigma_{ya}}\right)}{2\;\exp\left(-\dfrac{y_r^2}{2\;\sigma_{yr}^2}\right)}
\tag{2-274}
$$

where

$\sigma_{yr}$    is the receptor-specific $\sigma_y$ (m),

$\sigma_{ys}$    is the $\sigma_y$ (m) associated with the cross-wind scale of the area source, $= L_c / (2\pi)^{\frac{1}{2}}$,

$\sigma_{ya}^2$    $= \sigma_{yr}^2 - \sigma_{ys}^2$ ,

$L_c$    is the cross-wind scale of the area source (m), and

$y_r$    is the receptor-specific cross-slug distance (m)

When the slug sampling requires the numerical integration technique, the adjustment $F_r$ is applied to the individual snapshot slug distributions.

The same approximate treatment applies to all puffs released from an area source. Because the puff is symmetric, there is no "cross-puff" orientation, so the distance $y_r$ is simply the minimum distance from the center of the puff to the receptor during the sampling step. The puff is sampled in the normal way, and the concentration obtained is multiplied by $F_r$.

2.12    Buoyant Line Sources

CALPUFF contains specialized algorithms to simulate concentrations from buoyant line sources using techniques from the Buoyant Line and Point (BLP) source dispersion model (Schulman and Scire, 1980). Line source attributes used in BLP define the geometry of one or more long buildings associated with the

emissions. The coordinates of the beginning and ending locations of each line are used to determine the points of release, and the orientation of the lines. In addition, for a group of such buildings, the average source attributes (Figure 2-35) are needed:

  L      is the average building (line) length (m),
  $H_B$    is the average building height (m),
  $W_M$    is the average line source width (m),
  $W_B$    is the average building width (m),
  $\delta_x$    is the average spacing between buildings (m), and
  F'      is the average line source buoyancy parameter ($m^4/s^3$)

where

$$F^{\prime} = \frac{g \ L \ W_M \ w \ (T_s - T_a)}{T_s}$$

(2-275)

and

  g      is the gravitational acceleration ($m/s^2$),
  w      is the exit velocity (m/s),
  $T_s$    is the exit temperature (K), and
  $T_a$    is the ambient air temperature (K)

Generally, the buoyancy parameter is computed for each line and then averaged.

There is usually strong asymmetry to groups of line sources, so their properties appear to change with wind direction. Figure 2-36 illustrates the effective cross-wind length $L_e$ and along-wind length $X_{FB}$ for a wind direction at an angle to the long side of the lines. For a single line,

$$\begin{aligned} L_e &= |L \ \sin\theta| + |W_M \ \cos\theta| \\ X_{FB} &= |L \ \cos\theta| + |W_M \ \sin\theta| \end{aligned}$$

(2-276)

For a group of lines, $L_e$ is a weighting of the line length for perpendicular winds (L) and the length for parallel winds ($L_v$):

$$L_e = |L \ \sin\theta| + |L_v \ \cos\theta|$$

(2-277)

where $L_v$ is the length that produces a combined plume width that matches the composite width of the plumes from the individual lines at the point that these individual plumes merge. See Schulman and Scire (1980) for more details. The buildings also induce downwash effects. This is incorporated by using a
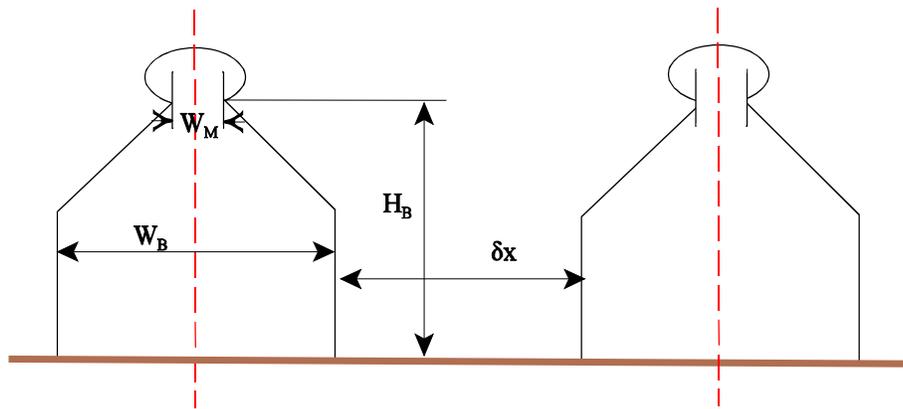
Figure 2-35.  Cross-section of adjacent buildings with dimensions defined for BLP  (from Schulman and Scire, (1980)).
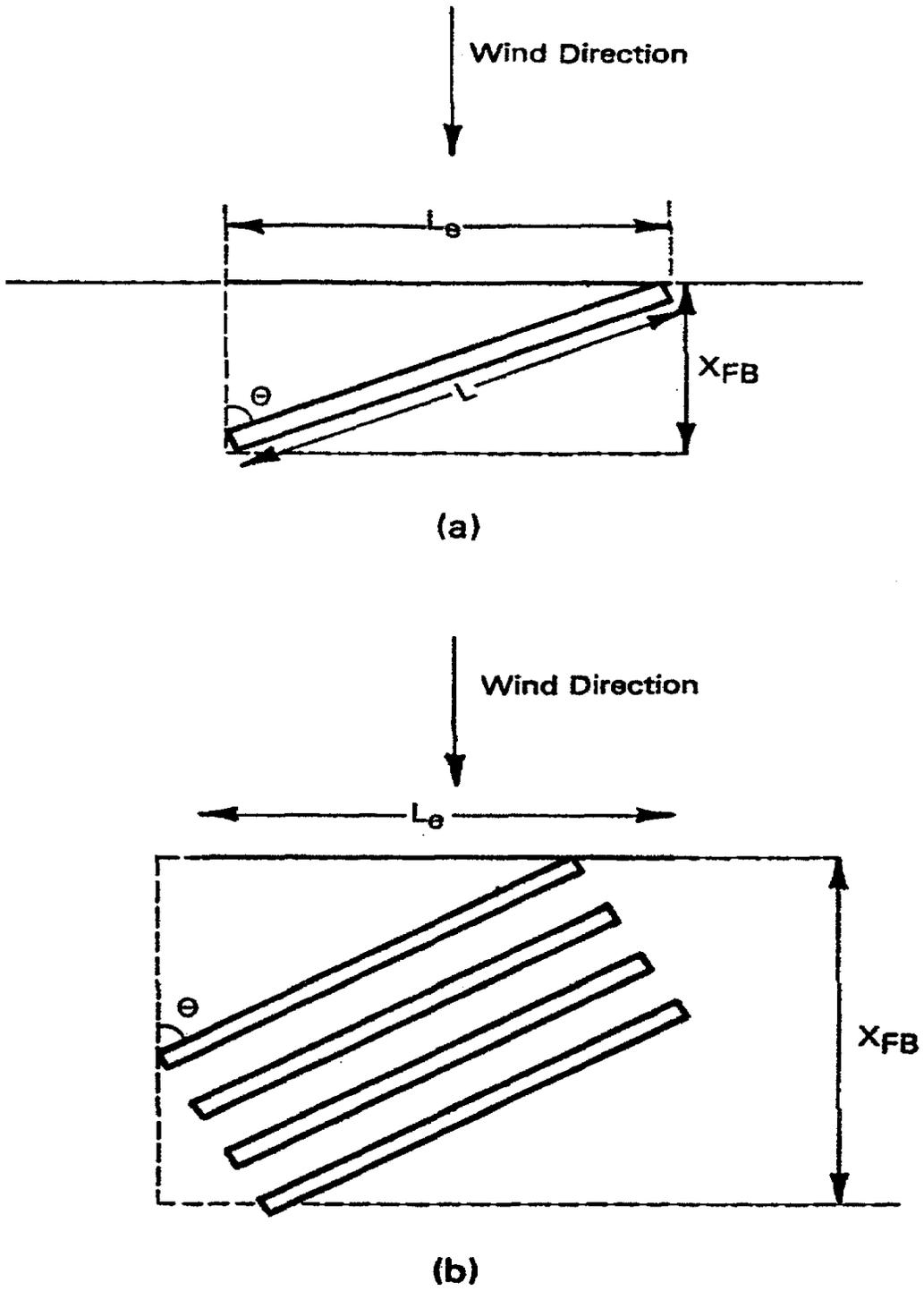
Figure 2-36. Illustration of effective line length and the along-wind distance to full buoyancy (from Schulman and Scire, (1980)).

downwash length scale $L_d$ in addition to an initial dilution radius $R_o$ in the equations for plume rise from a finite line:

$$
\begin{aligned}
L_d &= |L_e \sin\theta| \\
R_o &= MIN(H_B \, , \, L_d)
\end{aligned}
$$

(2-278)

With these scales defined, the BLP plume rise $z_L$ is computed for neutral-unstable conditions as:

$$
z_L^3 + \left[ 3L_e / (\pi\beta_1) \right] z_L^2 + \left[ 3R_o z_L / \beta_1 + 6R_o L_d / (\pi\beta_1^2) + 3R_o^2 / \beta_1^2 \right] z_L =
$$

$$
\frac{F'_T \, x^3}{2\pi \, \beta_1^2 \, X_{FB} \, u_e^3} \qquad\qquad x < X_{FB}
$$

(2-279)

$$
\frac{3F'_T}{2\pi \, \beta_1^2 \, u_e^3} \left( X_{FB}^2 / 3 + x^2 - x X_{FB} \right) \qquad x \geq X_{FB}
$$

and, for final stable plume rise:

$$
z_L^3 + \left[ 3L_e / (\pi\beta_1) \right] z_L^2 + \left[ 3R_o z_L / \beta_1 + 6R_o L_d / (\pi\beta_1^2) + 3R_o^2 / \beta_1^2 \right] z_L =
$$

$$
\frac{6F'_T}{\pi \, \beta_2^2 \, u_e \, S}
$$

(2-280)

where $F'_T$ is the total or sum of the buoyancy parameters for the lines, $u_e$ is the effective wind speed, either the stack-top speed or the mean speed adjusted for wind shear. See Section 2.4.1 for definitions of the other parameters. Note that the neutral rise equation is used to compute transitional rise for stable conditions.

Plume rise is tabulated for distances from the most upwind part of the group of line sources to the distance of final rise. Each line is then subdivided into segments (the maximum number may be set via the input control file), and each segment releases a puff (or slug). In the case of puffs, all are modeled using the virtual point source method in which the initial $\sigma_{y0}$ is obtained from the projection of the line segment across the wind. For slugs, each line is modeled as an area source during the first sampling step (emitting slugs), using the full numerical integration described in Section 2.11. Slugs in subsequent sampling steps are modeled using the virtual point source method.

## 2.13    Visibility Modeling

The CALPUFF system can be used to assess changes in regional visibility.  In a particular application, CALPUFF provides hourly concentrations of sulfates and/or nitrates and/or other particulates resulting from emissions from specific sources, and the postprocessor CALPOST computes and summarizes the corresponding light extinction coefficient ($b_{ext}$), relative to the background light extinction.  The light extinction coefficient includes both scattering and absorption components, and is a measure of the attenuation of light over a unit distance, expressed in inverse megameters (1/Mm) where a megameter is one million meters.  Another measure derived from $b_{ext}$ is also computed to indicate perceived visibility on a linear scale.  The deciview is defined as:

$$dv = 10 \ln\left[\frac{b_{ext}}{10}\right] \tag{2-281}$$

Here, a reference extinction coefficient of 10 (Mm$^{-1}$) in the denominator of the log corresponds to a 'pristine' environment, and a deciview of zero.

Because visibility degradation is a relative quantity, the absolute $b_{ext}$ is not sufficient by itself to quantify the perceived effects of particular sources.  A given $b_{ext}$ that may go largely unnoticed against a hazy background may be acutely apparent against a pristine background.  A fractional measure made up of the modeled extinction coefficient ($b_{ext-m}$) and the current background extinction coefficient ($b_{ext-0}$) is needed for this.  Two such measures are computed, the fractional (percent) change in extinction and the change in deciview (delta-deciview):

$$\Delta b/b \ (\%) = 100 \ (b_{ext-m} \ / \ b_{ext-0}) \tag{2-282}$$

$$\begin{aligned} \Delta dv &= 10 \ \ln((b_{ext-m}+b_{ext-0})/10) - 10 \ \ln(b_{ext-0}/10) \\ &= 10 \ \ln(1+b_{ext-m}/b_{ext-0}) \end{aligned} \tag{2-283}$$

The extinction coefficient may be expressed as the sum of a hygroscopic component and a non-hygroscopic component.  Sulfate and nitrate aerosols are hygroscopic, and have greater extinction efficiencies at larger relative humidity.  Absorption and scattering by other constituents are taken to be independent of the humidity, so that:

$$b_{ext} = b_{SN} \ f(RH) + b_{dry} \tag{2-284}$$

where $b_{SN}$ is the combined scattering coefficient for sulfates and nitrates ($b_{SO4}+b_{NO3}$) at RH=0%, and f(RH) is the humidity adjustment factor ( $\geq 1$).  Two versions of f(RH) are available in CALPOST.  The first is adapted from the factor suggested in the IWAQM 1993 guidance, and the second is the FLAG tabulation

which provides the factor for every whole % in the range 0-99%. These are shown in Figure 2-37. The non-hygroscopic extinction coefficient $b_{dry}$ is made up of the sum of scattering due to other fine particulates including organic aerosols ($b_{OC}$) and soil ($b_{soil}$), scattering due to coarse particles sized between 2.5 µm and 10 µm ($b_{PMC}$), and the Rayleigh scattering from air molecules ($b_{Ray}$); and also from absorption, largely from elemental carbon particles ($b_{EC}$) -- "soot".

Individual scattering coefficients are computed as the product of an extinction efficiency ($m^2/g$) and a concentration ($\mu g/m^3$):

$$
\begin{aligned}
b_{SO4} &= 3 \; [(NH_4)_2 \; SO_4] \\
b_{NO3} &= 3 \; [NH_4 \; NO_3] \\
b_{OC} &= 4 \; [OC] \\
b_{soil} &= 1 \; [Soil] \\
b_{PMC} &= 0.6 \; [Coarse \; Mass] \\
b_{EC} &= 10 \; [EC]
\end{aligned}
\tag{2-285}
$$

Note that the extinction efficiency for sulfates is based on ammonium sulfate, and that for nitrates is based on ammonium nitrate. Sulfate and nitrate concentrations are converted to ammonium sulfate and ammonium nitrate by the respective molecular weight factors 1.374 and 1.29.

Eqns. 2-284 and 2-285 are used for all modeled species to obtain the hourly $b_{ext-m}$ at each receptor, although typically only sulfates and nitrates are modeled. The corresponding hourly background extinction $b_{ext-0}$ at each receptor may be computed from these equations using monthly, seasonal, or length-of run concentrations, or may be derived from hourly measurements. Five distinct methods are provided in CALPOST. The visibility measures in Eqns. 2-282 and 2-283 are computed from daily averages of the hourly $b_{ext-m}$ and $b_{ext-0}$ at each receptor.

METHOD 1

A single "dry" background extinction coefficient ($b_{BAK}$) is specified (e.g. Eqn. 2-284 with f(RH)=1), along with a fraction $F_H$ that denotes the portion of this background that is hygroscopic. Then $b_{ext-0}$ is computed using Eqn. 2-284 with $b_{SN}$ equal to $F_H b_{BAK}$ and $b_{dry}$ equal to $(1- F_H) b_{BAK}$. This extinction coefficient changes hourly at each receptor as the humidity at the nearest surface meteorological data station varies. Extinction coefficients for modeled species are explicitly computed from the concentrations and Eqn. 2-285.

The humidity factor used for this method is identified as the "method 1" line in Figure 2-37 (IWAQM, 1993). The factor is capped at 16.0, the value listed for RH=98%, unless a smaller value is specified for the maximum allowed relative humidity (RHMAX). When the relative humidity exceeds the maximum allowed, the hourly $b_{ext-0}$ for the receptor is computed from Eqn. 2-284 with f(RHMAX).

METHOD 2

Speciated measurements are used to provide monthly values of background particulate concentrations for use in Eqn. 2-285 when computing $b_{ext-0}$ . Furthermore, the relative humidity factor is obtained from the curve identified as "method 2-5" in Figure 2-37. The minimum value is 1.0, and the maximum at 99% is 21.37.  As in method 1, f(RH) is capped at f(RHMAX), where RHMAX is 98% unless a smaller value is specified. Extinction coefficients for modeled species are explicitly computed from the concentrations and Eqn. 2-285.

METHOD 3

Speciated measurements are used to provide monthly values of background particulate concentrations for use in Eqn. 2-285 when computing $b_{ext-0}$ and the relative humidity factor is obtained from the curve identified as "method 2-5" in Figure 2-37.  However, unlike method 2, the hourly background and modeled extinction are invalidated at any receptor at which the relative humidity exceeds RHMAX, where RHMAX is 98% unless a smaller value is specified.  Rather than using f(RHMAX), the receptor-hour is dropped. When 24-hour visibility measures are computed, no fewer than 6 valid hours are accepted at each receptor. Days for which no receptor has a valid 24-hour average are tabulated as "missing".

METHOD 4

Hourly transmissometer measurements are used to provide the background extinction coefficient $b_{ext-0}$ at all receptors.   The relative humidity factor obtained from the curve identified as "method 2-5" in Figure 2-37 is used when computing the modeled extinction $b_{ext-m}$ as in method 3.  If the hourly transmissometer data are invalid (missing, high relative humidity reported at the transmissometer location, or other interference is noted), the hour is removed from the daily average (all receptors).  If the hourly relative humidity exceeds RHMAX at a receptor, the hourly modeled extinction is invalidated at that receptor, where RHMAX is 98% unless a smaller value is specified.  Rather than using f(RHMAX), the receptor-hour is dropped.  When 24-hour visibility measures are computed, no fewer than 6 valid hours are accepted at each receptor.  Days for which no receptor has a valid 24-hour average are tabulated as "missing".

METHOD 5

Hourly nephelometer measurements are used to provide the background extinction coefficient $b_{ext-0}$ at all receptors.  Because these measurements do not include Rayleigh scattering, a constant $b_{Ray}$ is added to the hourly measurements   The relative humidity factor obtained from the curve identified as "method 2-5" in Figure 2-37 is used when computing the modeled extinction $b_{ext-m}$ as in method 3.  If the hourly transmissometer data are invalid (missing, high relative humidity reported at the transmissometer location, or other interference is noted), the hour is removed from the daily average (all receptors).  If the hourly relative humidity exceeds RHMAX at a receptor, the hourly modeled extinction is invalidated at that receptor, where RHMAX is 98% unless a smaller value is specified.  Rather than using f(RHMAX), the

receptor-hour is dropped.  When 24-hour visibility measures are computed, no fewer than 6 valid hours are accepted at each receptor.  Days for which no receptor has a valid 24-hour average are tabulated as "missing".

2.14    Treatment of Calm Periods

Calm periods are those in which the puff transport speed is less than a user-supplied threshold speed (default = 0.5 m/s).  When ISC-type meteorological data are used, the associated meteorological preprocessors that reformat airport wind speeds explicitly identify calms by reporting a speed of 0.0 m/s.  All non-calm hours are given a minimum speed of 1.0 m/s.  Therefore, all puffs and slugs are immobile during these calm periods.  CALMET winds can prescribe transport speeds less than 1 m/s, and so the default calm threshold speed is used to identify periods when the transport distances are minimal, but not zero.

While no special module is required in CALPUFF to simulate calm periods, several adjustments are made to the normal algorithms.  These adjustments alter the way slugs are released, the way gradual rise is addressed, the way near-source effects are simulated, and the way the puff size changes during each sampling step.  These adjustments are consistent with the conceptual model in which fresh releases rise virtually straight up from a source, and disperse as a function of time due to wind fluctuations about a mean of zero, while existing emissions stagnate, and disperse as a function of time due to wind fluctuations about a mean of zero.  Methods for computing plume rise during calms (wind speed less than 1 m/s) are stated in Section 2.4.1.

Adjustments made to puffs that are released into a calm period include:
- slugs are released as puffs (slug length is zero)
- all mass for the period (hour) is placed into 1 puff
- distance to final rise is set to zero (no gradual rise)
- no building downwash effects are included
- growth of $\sigma_y$ and $\sigma_z$ is based on time (not distance traveled) during the sampling step, regardless of the dispersion option selected in the control file
- minimum values of the turbulence velocities $\sigma_v$ and $\sigma_w$ are imposed

Adjustments made to puffs released prior to encountering a calm period include:
- distance to final rise is set to zero (no gradual rise)
- growth of $\sigma_y$ and $\sigma_z$ is based on time (not distance traveled) during the sampling step, regardless of the dispersion option selected in the control file
- minimum values of the turbulence velocities $\sigma_v$ and $\sigma_w$ are imposed

When ISC-type meteorological data are used and the mean speed is zero, the implied $u_*$ is also zero and the PGT stability class is the only parameter available for estimating turbulence for such periods.  When CALMET data are used, $u_*$ and $w_*$ may be available even when the puff transport speed is less than the threshold, so that the turbulence can be estimated.  However, this may not be a robust procedure if the wind

data used by CALMET include true calms. During calm conditions, estimates of the turbulence velocities $\sigma_v$ and $\sigma_w$ can be indeterminate. CALPUFF relies on these velocities to grow puffs (using the time-dependent dispersion formulas) during periods that are considered calm, so this is a matter of practical significance. Calm periods can be associated with very stable as well as convective boundary layers, with their distinctly different turbulence properties.

Given these concerns, CALPUFF allows the use of stability-dependent minimum turbulence velocities. These velocities are used whenever the velocities otherwise obtained (measured or predicted) are less than the tabulated minimums. For routine applications, default values are based on the effective turbulence intensity implied by the PGT curves, as prescribed by Briggs (1973), which are listed in Table 2-12. The leading factor in these curves behaves as a turbulence intensity, i.e. as the ratio of the turbulence velocity to the mean speed. Because these curves have been historically applied for wind speeds of 1.0 m/s and greater, we estimate the minimum turbulence velocity $\sigma_w$ corresponding to $I_z$ by assuming a speed of 1.0 m/s. The lateral turbulence velocity could be estimated in the same way, using the $I_y$ values, but this would ignore the influence of meander during calm conditions. Hanna et al. (1986) suggest an appropriate minimum one-hour average $\sigma_v$ value is $\approx 0.5$ m/s. Therefore, the default minimum $\sigma_v = 0.5$ m/s for all stability classes.

When CALPUFF is applied with detailed wind and turbulence measurements, care must be used to ensure that valid measurements are not superceded by the minimum turbulence values. The minimum speed used as the calm threshold, and the individual turbulence minima should reflect the characteristics of the wind sensors and the data collection system used.

Table 2-12
Turbulence Intensity Implied by
the Briggs (1973) Dispersion Curves

| PG Class | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| $I_z$ | .20 | .12 | .08 | .06 | .03 | .016 |
| $I_y$ | .22 | .16 | .11 | .08 | .06 | .04 |

# 3. CALPUFF MODEL STRUCTURE

## 3.1 Memory Management

A flexible memory management system is used in CALPUFF which facilitates the user's ability to alter the dimension of the major arrays within the code. Arrays dealing with the number of horizontal or vertical grid cells, meteorological stations, chemical species, puffs, sources, and several other internal variables are dimensioned throughout the code with parameter statements. The declaration of the values of the parameters are stored in a file called "PARAMS.PUF." This file is automatically inserted into any CALPUFF subroutine or function requiring one of its parameters via FORTRAN "include" statements. Thus, a global redimensioning of all of the model arrays dealing with the number of vertical layers, for example, can be accomplished simply by modifying the PARAMS.PUF file and recompiling the program.

The parameter file contains variables which set the array dimensions or the maximum allowed number of vertical layers, or horizontal grid cells, etc. The actual value of the variables for a particular run is set within the user input file (i.e., the control file), and can be less than the maximum value set in the parameter file.

A sample parameter file is shown in Table 3-1. In addition to the parameters specifying the maximum array dimensions of the major model arrays, the parameter file also contains variables determining the Fortran I/O unit numbers associated with each input and output file. For example, the input control file (IO5) and output list file (IO6) are normally associated with unit numbers 5 and 6. However, if these units are reserved on a particular computer system, these files can be redirected to other non-reserved units by setting IO5 and IO6 equal to 1 and 2, for example, as in the sample PARAMS.PUF file.

## 3.2 Structure of the CALPUFF Modules

Execution of the CALPUFF model is divided into three major phases: setup, computational, and termination (see Figure 3-1). In the setup phase of the model execution, a variety of initialization and one-time I/O and computational operations are performed, including the following:

· Processing the command line argument.

· Opening input and output files.

Table 3-1

Sample CALPUFF Parameter File

```
c----------------------------------------------------------------------
c --- PARAMETER statements                                       CALPUFF
c----------------------------------------------------------------------
c --- Specify model version
      character*12 mver, mlevel, mmodel
      parameter(mver='5.2',mlevel='991104')
      parameter(mmodel='CALPUFF')
c
c --- Specify parameters
      parameter(mxpuff=40000)
      parameter(mxspec=20)
      parameter(mxnx=50,mxny=50,mxnz=12)
      parameter(mxnxg=50,mxnyg=50,mxrec=2000)
      parameter(mxss=150,mxus=20,mxps=60)
      parameter(mxpt1=100,mxpt2=100,mxarea=100,mxvert=5)
      parameter(mxlines=20,mxlngrp=1,mxvol=20)
      parameter(mxrise=10)
      parameter(mxpdep=9,mxint=9)
      parameter(mxoz=20)
      parameter(mxhill=20,mxtpts=25,mxrect=1000,mxcntr=21)
      parameter(mxprfz=50)
      parameter(mxent=10,mxntr=50,mxnw=5000)
      parameter(mxvalz=10)
      parameter(mxcoast=10,mxptcst=5000)
      parameter(mxbndry=10,mxptbdy=5000)   ! keep mxbndry LE 20
      parameter(mxmetdat=12)
      parameter(mxsg=30,mxvar=60,mxcol=132)
      parameter(io3=3,io4=4,io5=1,io6=2,io7=7,io8=8,io9=9)
      parameter(io10=10,io11=11,io16=16)
      parameter(io17=17,io18=18,io19=19,io20=20,io22=22,io24=24)
      parameter(io25=25,io28=28,io29=29,io30=30,io31=31,io32=32)
      parameter(io35=35,io36=36,io37=37)
      parameter(iomesg=0)
c
c
c --- Compute derived parameters
      parameter(mxnzp1=mxnz+1)
      parameter(mxvertp1=mxvert+1)
      parameter(mxnxy=mxnx*mxny)
      parameter(mxnxyg=mxnxg*mxnyg)
      parameter(mxgsp=mxnxg*mxnyg*mxspec)
      parameter(mxrsp=mxrec*mxspec)
      parameter(mxcsp=mxrect*mxspec)
      parameter(mx2=2*mxspec,mx5=5*mxspec,mx7=7*mxspec)
      parameter(mxp2=2+mxspec,mxp3=3+mxspec,mxp6=6+mxspec)
      parameter(mxp7=7+mxspec,mxp8=8+mxspec,mxp14=mxspec+14)
      parameter(mxpuf6=6*mxpuff)
      parameter(mxlev=mxprfz)
      parameter(mxprfp1=mxprfz+1)
      parameter(mxentp1=mxent+1)
      parameter(mxgrup=mxspec)
      parameter(mxql2=mxspec*(mxpt1+mxarea)*2)
      parameter(mxspar=mxspec*mxarea,mxspln=mxspec*mxlines)
      parameter(mxsppt1=mxspec*mxpt1,mxspvl=mxspec*mxvol)
c
c --- Specify parameters for sizing GUI:
      parameter(mxavar=1)
      parameter(mxlvar=1)
      parameter(mxpvar=1)
      parameter(mxvvar=1)
c
c --- GENERAL PARAMETER definitions:
c        MXPUFF - Maximum number of active puffs allowed on the
c                 computational grid at one time
c        MXSLUG - Maximum number of active slugs allowed on the
c                 computational grid at one time (can be set to
c                 one if the slug option is not used)
c        MXSPEC - Maximum number of chemical species.  N.B.: Changes
c                 to MXSPEC may also require code changes to BLOCK DATA
c                 and READCF.
c        MXGRUP - Maximum number of Species-Groups.  Results for grouped
c                 species are added together and reported using the
c                 name of the group, rather than the name of one of the
c                 species in the group. (MXGRUP = MXSPEC since specie
c                 names are used as group names whenever group names are
c                 not provided)
c          MXNX - Maximum number of METEOROLOGICAL grid cells in
c                 the X direction
c          MXNY - Maximum number of METEOROLOGICAL grid cells in
```

Table 3-1 (Continued)
Sample CALPUFF Parameter File

```
c               the Y direction
c        MXNZ - Maximum number of vertical layers in
c               the METEOROLOGICAL grid
c       MXNXG - Maximum number of SAMPLING grid cells in
c               the X direction
c       MXNYG - Maximum number of SAMPLING grid cells in
c               the Y direction
c       MXREC - Maximum number of non-gridded receptors
c        MXSS - Maximum number of surface meteorological stations
c               in the CALMET data
c        MXUS - Maximum number of upper air stations in the CALMET
c               data
c        MXPS - Maximum number of precipitation stations in the
c               CALMET data
c       MXPT1 - Maximum number of point sources with constant
c               emission parameters
c       MXPT2 - Maximum number of point sources with time-varying
c               emission parameters
c      MXAREA - Maximum number of polygon area sources with constant
c               emission parameters (i.e., non-gridded area sources)
c      MXVERT - Maximum number of vertices in polygon area source
c      MXLINES- Maximum number of line sources
c      MXLNGRP- Maximum number of groups of line sources
c       MXVOL - Maximum number of volume sources
c      MXRISE - Maximum number of points in computed plume rise
c               tabulation for buoyant area and line sources
c      MXPDEP - Maximum number of particle species dry deposited
c       MXINT - Maximum number of particle size intervals used
c               in defining mass-weighted deposition velocities
c        MXOZ - Maximum number of ozone data stations (for use in the
c               chemistry module)
c      MXHILL - Maximum number of subgrid-scale (CTSG) terrain
c               features
c      MXTPTS - Maximum number of points used to obtain flow
c               factors along the trajectory of a puff over the hill
c      MXRECT - Maximum number of complex terrain (CTSG) receptors
c      MXCNTR - Maximum number of hill height contours (CTDM ellipses)
c      MXPRFZ - Maximum number of vertical levels of met. data in
c               CTDM PROFILE file
c       MXLEV - Maximum number of vertical levels of met. data
c               allowed in the CTSG module (set to MXPRFZ in the
c               current implementation of CALPUFF)
c       MXENT - Maximum number of perturbed entrainment coefficients
c               entered
c       MXNTR - Maximum number of downwind distances for which
c               numerical plume rise will be reported
c        MXNW - Maximum number of downwind distances for numerical
c               plume rise integration (should be set equal to
c               SLAST/DS)
c      MXVALZ - Maximum number of heights above ground at which valley
c               widths are found for each grid cell
c     MXCOAST - Maximum number of coasts provided in COASTLN.DAT file
c     MXPTCST - Maximum number of points used to store all coastlines
c     MXBNDRY - Maximum number of boubaries provided in FLUXBDY.DAT file
c     MXPTBDY - Maximum number of points used to store all boundaries
c     MXMETDAT - Maximum number of CALMET.DAT files used in run
c       MXQ12 - Maximum number of groups of 12 emission rate scaling
c               factors.  Factors come in groups of 12,24,36, or 96.
c               These are specified for source-species combinations,
c               but not all combinations will be filled.  Default
c               value of MXQ12 assumes that no more than 24 factors
c               are provided for each source-species combination for
c               point and area sources.
c
c --- CONTROL FILE READER definitions:
c        MXSG - Maximum number of input groups in control file
c       MXVAR - Maximum number of variables in each input group
c       MXCOL - Maximum length (bytes) of a control file input record
c
c --- FORTRAN I/O unit numbers:
c         IO3 - Restart file (RESTARTB.DAT)   - input  - unformatted
c         IO4 - Restart file (RESTARTE.DAT)   - output - unformatted
c         IO5 - Control file (CALPUFF.INP)    - input  - formatted
c         IO6 - List file (CALPUFF.LST)       - output - formatted
c
c         IO7 - Meteorological data file      - input  - unformatted
c               (CALMET.DAT)
c
```

Table 3-1 (Continued)
Sample CALPUFF Parameter File

```
c          IO8 - Concentration output file    - output - unformatted
c                (CONC.DAT)
c          IO9 - Dry flux output file         - output - unformatted
c                (DFLX.DAT)
c         IO10 - Wet flux output file         - output - unformatted
c                (WFLX.DAT)
c         IO11 - Visibility output file       - output - unformatted
c                (VISB.DAT)
c         IO16 - Pt. source emissions file    - input  - unformatted
c                (PTEMARB.DAT) with arbitrarily
c                varying point source emissions
c         IO17 - Buoyant area sources file    - input  - free format
c                (BAEMARB.DAT) with arbitrarily
c                varying location & emissions
c         IO18 - Gridded volume source        - input  - unformatted
c                emissions file (VOLEM.DAT)
c         IO19 - Buoyant line sources file    - input  - free format
c                (LNEMARB.DAT) with arbitrarily
c                varying location & emissions
c         IO20 - User-specified deposition    - input  - formatted
c                velocities (VD.DAT)
c         IO22 - Hourly ozone monitoring data - input  - formatted
c                (OZONE.DAT)
c         IO24 - User-specified chemical      - input  - formatted
c                transformation rates
c                (CHEM.DAT)
c         IO25 - User-specified coast line(s) - input  - free format
c                for sub-grid TIBL module
c                (COASTLN.DAT)
c         IO28 - CTSG hill specifications from - input  - formatted
c                CTDM terrain processor
c                (HILL.DAT)
c         IO29 - CTSG receptor specifications  - input  - formatted
c                from CTDM receptor generator
c                (RECS.DAT)
c         IO30 - Tracking puff/slug data       - output - formatted
c                (DEBUG.DAT)
c         IO31 - CTDM "tower" data            - input  - formatted
c                (PROFILE.DAT)
c         IO32 - CTDM surface layer parameters - input  - formatted
c                (SURFACE.DAT)
c         IO35 - User-specified boundary lines(s)- input- free format
c                for mass flux calculations
c                (FLUXBDY.DAT)
c         IO36 - Mass flux data               - output - formatted
c                (MASSFLX.DAT)
c         IO37 - Mass balance data            - output - formatted
c                (MASSBAL.DAT)
c       IOMESG - Fortran unit number for screen- output - formatted
c                output (NOTE: This unit is
c                NOT opened -- it must be a
c                preconnected unit to the screen
c                -- Screen output can be suppressed
c                by the input "IMESG" in the
c                control file)
c
c
c --- GUI memory control parameters:  variable emissions scaling factors
c     for areas, lines, points, and volumes require much memory in GUI.
c     To reduce GUI memory requirement, set one or more of the
c     following parameters to ZERO when such scaling is not required.
c     These parameters have no effect on CALPUFF, but are read by the
c     GUI at execution time.
c
c       MXAVAR - Using scaled area sources?   (1:yes, 0:no)
c       MXLVAR - Using scaled line sources?   (1:yes, 0:no)
c       MXPVAR - Using scaled point sources?  (1:yes, 0:no)
c       MXVVAR - Using scaled volume sources? (1:yes, 0:no)
c
c
c ----------------------------------------------------------------
```

```
Start
   .
   .
   .
   .
SETUP -    Setup phase - Initialization and program setup operations.
   .
   .

COMP  -    Computational phase - basic time loop with time-dependent I/O and all
   .           scientific modules.
   .
   .
FIN   -    Termination phase - program termination functions.
   .
   .
   .
STOP
```
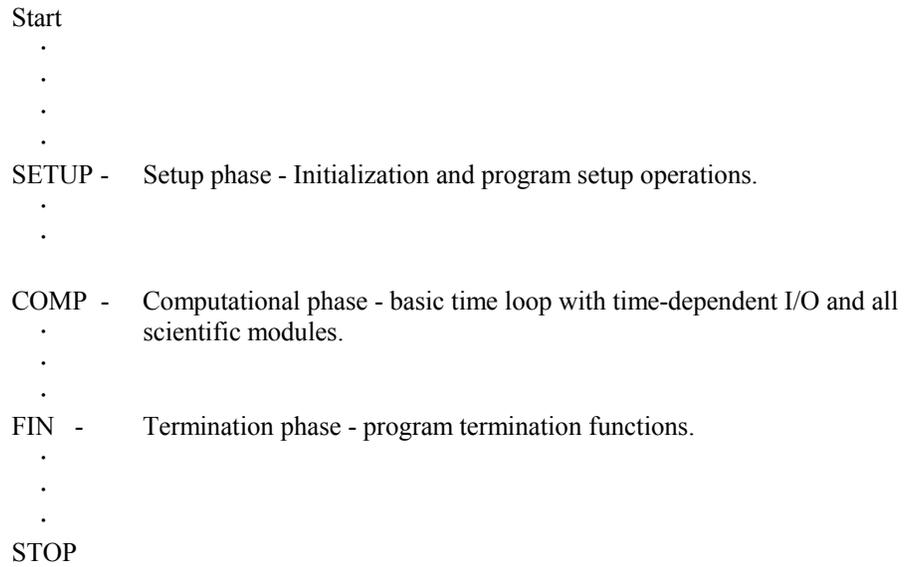
Figure 3-1.    Flow diagram showing the calling sequence of major routines in the CALPUFF MAIN
               program.

- Reading and processing the control file inputs which includes model option flags and run control variables.

- Reading and processing the time-invariant data records of the model's input data bases (i.e., meteorological data file, optional emissions files, ozone data files, and user-specified deposition velocities and transformation rate files).

- Performing consistency checks of the input data base information versus the control file inputs.

- Performing initialization and setup operations for the terrain, chemistry, dry deposition, dispersion, plume rise, sub-grid scale TIBL, and puff-sampling modules.

- Writing the header records to the model's output concentration and dry/wet deposition files.

The computational phase of the model includes the basic time loop within which the hourly concentrations and deposition fluxes are computed and, if appropriate, time averaged. The functions performed in the computation phase include the following:

- Initializing puff array data read from a "restart" file from a previous run (optional).

- Retrieving and processing time-averaging data from the meteorological, emissions, and ozone data files.

- Emitting, transporting, and removing puffs from the computation grid.

- Evaluating the effects of dispersion, chemical transformation, wet removal, dry deposition, and subgrid scale complex terrain.

- Sampling the puffs to determine concentrations and deposition fluxes at gridded and discrete receptors.

- Time-averaging and storing concentrations and deposition flux results to the appropriate output files.

The final phase of the model execution deals with run termination functions. The termination phase includes the closing of any active data files, computation of model run time, and printing of summary or normal termination messages.

A flow diagram for the setup module is provided in Figure 3-2. The flow diagram contains the name of each subroutine or function called by the setup module along with a brief description of the routine's purpose. A flow diagram for the main computational routine, subroutine COMP, is shown in Figure 3-3. As illustrated in the figure, COMP contains the basic time loop and calls to all of the technical modules.

At the beginning of the hour loop, the data files containing meteorological fields, time-varying emissions, and ozone observations are read and related fields are computed for the current conditions. Existing puffs are evaluated for the potential of splitting, and new puffs are defined for each emitting source in the hour. This definition includes the time of emission (puffs may be released throughout the hour), initial size, and plume rise features. Then, a loop over puffs is entered which determines the initial advective wind for the puff, and the initial length of the sampling step. Plume dispersion, advection, chemical transformation, wet deposition, dry deposition, terrain effects, and puff/slug sampling are performed within the innermost loop over sampling steps for the hour.

Detailed programmer information on the model code and structure is provided in Appendices A and B. Appendix A contains a tree diagram showing the calling structure of every routine (subroutine or function) in the code. The sequence of calls and the calls to lower level subroutines are shown in the diagram. The second part of Appendix A lists for each subroutine or function the routine from which it is called and any routines that are called by it. Appendix B contains a description of each routine in CALPUFF along with its type (function or subroutine).

**Enter SETUP**
.
.
.

DATETM   -   Get date and time from the system clock.
.
.

COMLINE   -   Get the I/O file name from the command line
.
.

READCF   -   Read the control file inputs, including the control file name and the list file
.
.

WRFILES   -   Write the file names used in this run to the list file
.
.

SETCOM   -   Set miscellaneous common block parameters (grid parameters, etc.)
.
.

OPENOT   -   Open all other input and output files.
.
.

MET1   -   Read the header records for the meteorological data file
MET2           (MET1 for CALMET.DAT, MET2 for ISCMET.DAT, MET3 for PLMMET.DAT,
MET3           MET4 for PROFILE.DAT).
MET4
.
.

RDHDEM2   -   Read header records for the PTEMARB.DAT emission file (arbitrarily-
.           varying point source emissions).
.

RDHDEM3   -   Read header records for the BAEMARB.DAT emission file (arbitrarily-
.           varying buoyant area source emissions).
.

RDHDEM4   -   Read header records for the VOLEM.DAT emissions file (gridded volume source
.           emissions).
.

RDHDEM5   -   Read header records for the LNEMARB.DAT emissions file (arbitrarily-
.           varying buoyant line source emissions).
.

CHEMI   -   Perform setup operations for the chemistry module.
.
.

EMQA   -   Perform QA checks on emission header record data, set up cross-referencing
.           arrays.
.

RDTIEM2   -   Read the time-invariant data from the PTEMARB.DAT file (arbitrarily-
.           varying point source emissions).
.

RDTIEM3   -   Read the time-invariant data from the BAEMARB.DAT file (arbitrarily-
.           varying area source emissions).
.
.

(Continued)

Figure 3-2.          Flow diagram showing the calling sequence of major routines in subroutine SETUP
(Setup Phase).

RDTIEM5 - Read the time-invariant data from the LNEMARB.DAT file (arbitrarily-
         varying buoyant line source emissions).
·
ELEVI - Interpolate the elevations from the meteorological grid to the gridded
        receptor points.
·
SIGSET - Perform setup operations for the dispersion coefficient module.
·
·
SLUGI - Perform setup operations for the slug sampling function.
·
·
DRYI - Perform setup operations for the dry deposition module.
·
·
TRELIEF - Perform setup computations for the MCTADJ=2 terrain option.
·
·
VWIDTH - Compute the valley width at each cell for the MCTADJ=2 terrain option.
·
·
CTINIT - Perform setup computations for the subgrid-scale complex terrain module (CTSG).
·
·
NUMPR1 - Perform setup computations for the numerical plume rise module.
·
·
RESTARTQ - Perform QA on information provided in the restart file for continuation runs.
·
·
TIBLSET - Perform setup computations for the sub-grid TIBL module.
·
·
MFLXSET - Perform setup computations for the diagnostic mass flux module.
·
·
MFLXHDR - Write header records to diagnostic mass flux output file (MASSFLX.DAT).
·
·
MBALHDR - Write header records to diagnostic mass balance output file (MASSBAL.DAT).
·
·
WROUT1 - Write the header records to the CONC.DAT (concentrations), DFLX.DAT
         (dry deposition flux), and WFLX.DAT (wet deposition flux) output files.
·
·
·
Return to MAIN PROGRAM

Figure 3-2.        Flow diagram showing the calling sequence of major routines in subroutine SETUP
                   (Setup Phase).  (Concluded).

**Enter COMP**
.
.

JULDAY     -     Compute the Julian day from the Gregorian date.
.
.

RESTARTI   -     Initialize puff arrays with data from end of previous run.
.
.

Begin Hour Loop
.
.

RDMET,     -   Read an hour of meteorological data (RDMET for CALMET.DAT data,
RDISC,          RDISC for ISCMET.DAT data, RDPLM for PLMMET.DAT data, RDMET4 for
RDPLM,        SURFACE.DAT and PROFILE.DAT data).
RDMET4
.

RDPROF    -   Read data from PROFILE.DAT file if needed (e.g, if using turbulence $\sigma$s).
.
.

SUNDATA  -   Compute cloud and zenith data at surface meteorology stations.
.
.

RDOZ       -   Read hourly ozone data from the OZONE.DAT file (if using
.            MESOPUFF II chemistry).
.

INITR2D   -   Initialize concentrations and deposition flux arrays at the beginning of
.            each averaging period.
.

MFLXINI  -   Initialize mass flux arrays.
.
.

MBALINI  -   Initialize mass balance arrays.
.
.

GETPRFP,  -   Compute ratio of wind speed to Brunt-Vaisala frequency and the
GETPRFM,     dividing streamline height for the CTSG module.
HDUN
.
.

SPLIT      -   Split selected puffs to respond to vertical shear.
.
.

INITPUF   -   Perform all initialization operations for new puffs.  Read time-varying
.            emissions data (from PTEMARB.DAT, BAEMARB.DAT, VOLEM.DAT,
.            LNEMARB.DAT).
.

Begin Loop Over Puffs
.
.

ZFIND       - Find the vertical layer containing the puff before and after rise.
.
.

(Continued)

Figure 3-3.    Flow diagram showing the calling sequence of major routines in Subroutine COMP
(Computational Phase).

```
|  |  |         PUFFDZ              - Find the top and the bottom of the puff.
|  |  |           .
|  |  |           .
|  |  |         ADVECT              - Obtain advection speed and direction for puff.
|  |  |           .
|  |  |           .
|  |  |      Determine puff codes.
|  |  |           .
|  |  |      Determine the sampling parameters for this puff.
|  |  |           .
|  |  |           .
|  |  |         MBALSUM             - Update mass balance for new emissions..
|  |  |           .
|  |  |           .
|  |  ┌──── Begin Loop Over Sampling Steps
|  |  |           .
|  |  |           .
|  |  |           PUFFDZ            - Find the top and the bottom of the puff.
|  |  |             .
|  |  |             .
|  |  |           ADVECT            - Obtain plume-averaged advective winds for sampling step.
|  |  |             .
|  |  |             .
|  |  |           RISEWIND          - Revise average wind for the rise stage.
|  |  |             .
|  |  |             .
|  |  |         Configure sampling substep.
|  |  |             .
|  |  |             .
|  |  |           GETOZ             - Determine the appropriate ozone concentration to use in
|  |  |             .                 the chemistry eqns. for the puff.
|  |  |             .
|  |  |           TIBLON            - Check for initiating sub-grid TIBL this sampling step
|  |  |             .
|  |  |             .
|  |  |           TIBLGRO           - Compute TIBL arrays for this step.
|  |  |             .
|  |  |             .
|  |  |           EXMET             - Transfer this hour's surface meteorological variables.
|  |  |             .
|  |  |             .
|  |  |           VMASS             - Set vertical distribution of pollutant mass for this
|  |  |             .                   time step.
|  |  |             .
|  |  |           TURBSET           - Determine plume turbulence values.
```

(Continued)

Figure 3-3.    Flow diagram showing the calling sequence of major routines in Subroutine COMP
               (Computational Phase).

```
        .
        .
PDFVARS          - Set PDF variables.
        .
        .
PTLAPS           - Compute local Brunt-Vaisala frequency.
        .
        .
SETPUF           - Set the remaining parameters for puffs.
        .
        .
SETSLG           - Set the remaining parameters for slugs.
        .
        .
CHEM             - Determine the chemical transformation rates for this puff
        .          (compute internally or extract from user-specified array
        .           of values) and apply to puff.
        .
        .
MBALSUM          - Update mass balance for chemical transformation.
        .
        .
WET              - Compute the wet scavenging coefficients and apply to puff.
        .
        .
MBALSUM          - Update mass balance for wet removal.
        .
        .
DRY              - Determine the deposition velocity for the puff (compute
        .          internally using the resistance model or extract from user-
        .          specified array of values) and apply to puff.
        .
        .
MBALSUM          - Update mass balance for dry removal.
        .
        .
TRACK            - Write puff data to the DEBUG.DAT file (if requested).
        .
        .
MFLXCMP          - Update mass flux totals.
        .
        .
 If puff is treated as circular puff,
                        .
                CALCPF    -    Compute the concentrations and deposition fluxes
                        .      at each non-CTSG receptor using the integrated
                        .      puff model.
                        .
        (Continued)
```

Figure 3-3.      Flow diagram showing the calling sequence of major routines in Subroutine COMP (Computational Phase).

End circular puff section.

.
.

If puff is treated as an elongated slug,

.
.

CALCSL -    Compute the concentrations and deposition fluxes
.           at each non-CTSG receptor using the slug model.
.

End elongated slug section.

.
.

For circular puff at CTSG receptors,

.
.

PUFSCRN   -   Screen out receptors too far away.
.
.

PUFRECS   -   Obtain receptor-specific puff information.
.
.

CTSG   -   Compute concentrations at CTSG receptors.
.
.

End circular puff section for CTSG.

.
.

For elongated slugs at CTSG receptors,

.
.

SLG2PUF   -   If using slugs, generate circular puffs to represent
.             the slug for the CTSG module ("plugs").
.

PLGRECS   -   Compute sigmas for plugs.
.
.

PUFSCRN   -   Screen out receptors too far away.
.
.

PLGRECS   -   Obtain receptor-specific puff information.
.
.

CTSG -    Compute concentrations at the CTSG receptors.
.

(Continued)

Figure 3-3.    Flow diagram showing the calling sequence of major routines in Subroutine COMP
(Computational Phase).

.
End elongated slug section for CTSG.
.

    MBALSUM          - Update mass balance for advection out of domain.
    .
End Sampling Loop
.
.

    MBALSUM          - Update mass balance for total mass in domain.
    .
    .
End Puff Loop
.
.

    OUTPUT    - Output time-averaged concentrations and deposition fluxes to disk files
    .            list file.
    .
    RESTARTO - Output puff arrays to restart file every NRESPD hours, or at the end of the run.
    .
    .
    INCR      - Increment the hour and Julian day.
    .
    .
    GRDAY     - Convert the updated Julian day to a Gregorian date.
    .
    .
End Hour Loop
    .
    .
Return to MAIN PROGRAM
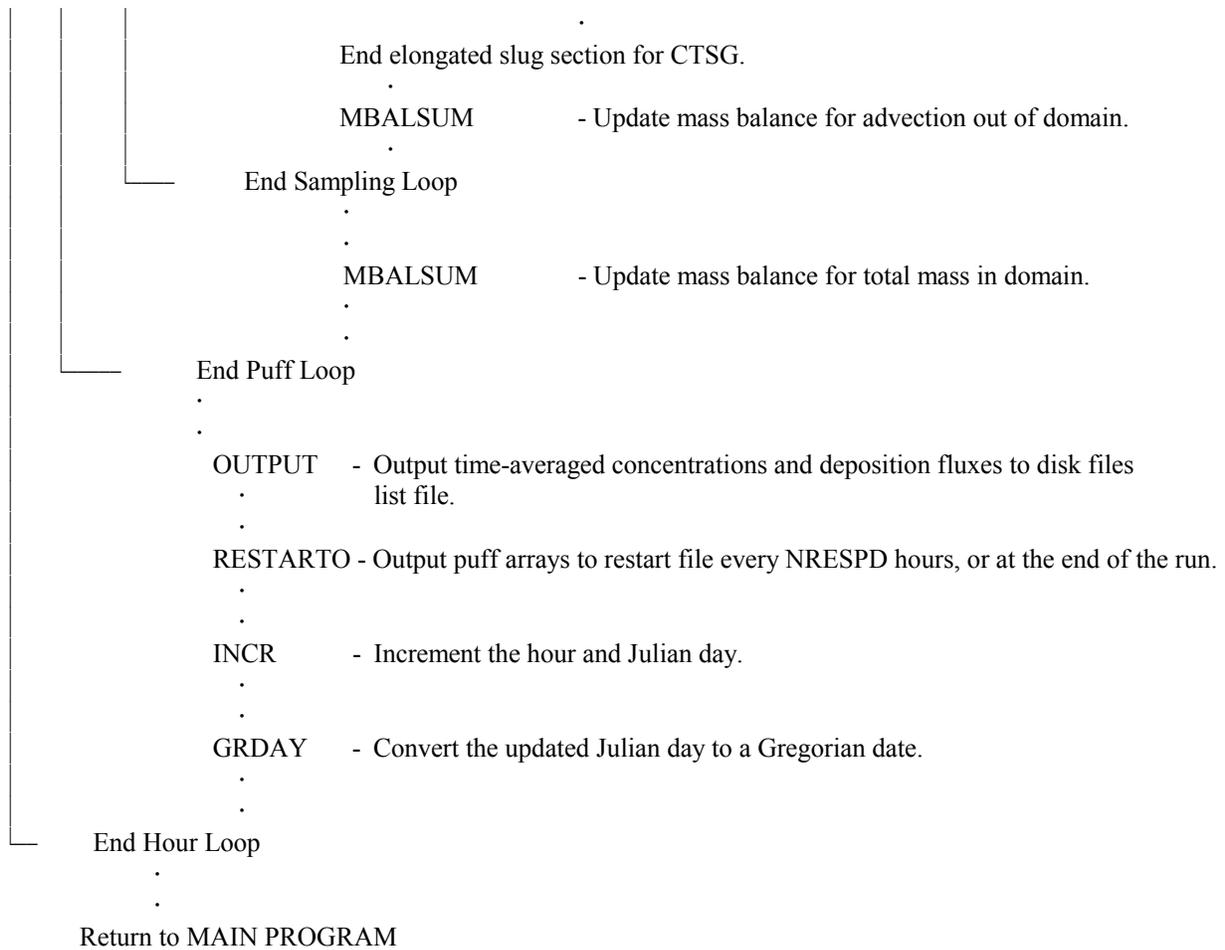
Figure 3-3.  Flow diagram showing the calling sequence of major routines in Subroutine
            COMP (Computational Phase).  (Concluded).

# 4.  USER'S INSTRUCTIONS

The CALPUFF model obtains information about sources, receptors, meteorological data, geophysical data, and model control parameters from a series of input files.  These files are listed in Table 1-2.  The model creates several output files, which are listed in Table 1-4.  Detailed information on the structure and content of each of the input and output files is provided in this section.

Tables 1-2 and 1-4 show the Fortran unit numbers associated with each file.  These unit numbers are specified in the parameter file (PARAMS.PUF).  They can be easily modified to accommodate system-dependent restrictions on allowable unit numbers.  Any changes to variables in the parameter file are automatically modified throughout the CALPUFF Fortran code.  The code must be re-compiled for changes in the parameter file to take effect, since the parameter values are set at the program compilation stage rather than at program execution.  An example PARAMS.PUF file was presented in Table 3-1.

The name and full path of each CALPUFF file (except one) is assigned in the control file (CALPUFF. INP).  The exception, the control filename itself, is assigned on the command line.  For example, on a DOS system,

> CALPUFF   d:\CALPUFF\CALPUFF.INP

will execute the CALPUFF code (CALPUFF.EXE), and read the input and output filenames for the current run from the file CALPUFF.INP in the directory d:\CALPUFF.  If the control filename is not specified on the command line, the default control filename (i.e., CALPUFF.INP in the current working directory) will be used.  The path and filename can be up to 70 characters long.

The utility routine that delivers a command line argument is system dependent.  The function that provides the system clock time and system CPU time are also system or compiler-specific.  All system-dependent or compiler-specific routines in CALPUFF are isolated into a file called DATETM.xxx, where the file extension (.xxx) indicates the system for which the code is designed.  For example, DATETM.HP contains code for Hewlett-Packard Unix systems, DATETM.SUN is for Sun Unix systems, DATETM.LAH is for Lahey-compiled PC-applications, and DATETM.MS is for Microsoft-compiled PC applications.  By appending the correct system-dependent DATETM file onto the main CALPUFF code, the code should run without any modifications.

## 4.1      User Control File (CALPUFF.INP)

The selection and control of CALPUFF options are determined by user-specified inputs contained in a file called the control file.  This file, which has the default name CALPUFF.INP, contains all of the information necessary to define a model run (e.g., starting date, run length, grid specifications, technical

options, output options, etc.).  CALPUFF.INP may be created/edited directly using a conventional editor, or it may be created/edited indirectly by means of the PC-based, Windows-compatible Graphical User Interface (GUI) developed for CALPUFF.

The CALPUFF GUI not only prepares the control file, it also executes the model and facilitates file management functions;  and it contains an extensive help system that makes much of the information in this manual available to the user on-line.  When using the GUI, the source data and receptor information required for a CALPUFF run can be entered through the edit screens or read from external ASCII files (spreadsheet-compatible).  Each source type (points, areas, volumes, and lines) contains an external ASCII file format description and sample file in the help system.

Although the model can be set up and run entirely within the GUI system, the interface is designed to always create the ASCII CALPUFF.INP file.  This allows runs to be set up on PC-based systems and the control file transferred to a workstation or a mainframe computer for computationally intensive applications.  The ASCII CALPUFF.INP file should be directly transportable to virtually any non-PC system.

When CALPUFF is setup and run entirely on a non-PC system, or if the GUI is not used on a PC, the control file CALPUFF.INP may be configured by using a conventional editor.  This is facilitated by the extensive self-documenting statements contained in the standard file.  As explained further below, more comments can be readily added by the user to document specific parameter choices used in the run. These comments remain in the file, and are reported to the CALPUFF list file when CALPUFF is executed from the command line.  Note, however, that the GUI always writes the standard comments to CALPUFF.INP, and ignores any additional text.  Furthermore, the control file is always updated by the GUI, even if the GUI is only used to run CALPUFF without altering the technical content of the control file.  Thus, the user must save the control file to another filename prior to using the GUI if non-standard comments are to be saved.  This feature of the GUI can be used to create a new copy of the standard control file by merely saving a "new file" to disk, so a fresh version of the control file is always available.

The control file is organized into 18 major Input Groups and a variable number of subgroups within several of the major Input Groups.  The first three lines of the input file consist of a run title.  As shown in Table 4-1, the major Input Groups are defined along functional lines (e.g., technical options, output options, subgrid scale, complex terrain inputs, etc.).  Each subgroup contains a set of data such as source variables, subgrid scale hill descriptions, or discrete receptor information.  The number of subgroups varies with the number of sources, hills, etc., in the model run.

A sample control file is shown in Table 4-2.  The control file is read by a set of Fortran text processing routines contained within CALPUFF which allow the user considerable flexibility in designing and

customizing the input file.  An unlimited amount of optional descriptive text can be inserted within the control file to make it self-documenting.  For example, the definition, allowed values, units, and default value of each input variable can be included within the control file.

The control file processor searches for pairs of special delimiter characters (!).  All text outside the delimiters is assumed to be optional documentation and is echoed back but otherwise ignored by the input module.  Only data within the delimiter characters is processed.  The input data consists of a leading delimiter followed by the variable name, equals sign, input value or values, and a terminating delimiter (e.g., !XX = 12.5 !).  The variable name can be lower or upper case, or a mixture of both (i.e., XX, xx, Xx are all equivalent).  The variable type can be real, integer, logical, or character and it can be an array or a scalar.  The use of repetition factors for arrays is allowed (e.g., ! XARRAY = 3 * 1.5 ! instead of ! XARRAY = 1.5, 1.5, 1.5 !).  <u>Different values must be separated by commas</u>.  Spaces within the delimiter pair are ignored.  Exponential notation (E format) for real numbers is allowed.  However, the optional plus sign should be omitted (e.g., enter +1.5E+10 as 1.5E10).  The data may be extended over more than one line (except for character variables, which must be entirely on one line).  The line being continued must end with a comma.  Each leading delimiter must be paired with a terminating delimiter.  All text between the delimiters is assumed to be data, so no optional documentation is allowed to appear within the delimiters.  The inclusion in the control file of any variable that is being assigned its default value is optional.  The control file reader expects that logical variables will be assigned using only a one character representation (i.e., 'T' or 'F').

The major Input Groups must appear in order, i.e., Input Group 0 followed by Input Group 1 followed by Input Group 2, etc.  However, the variables within an Input Group may appear in any order.  The variable names in each Input Group are independent, so that the same name can be repeated in different Input Groups (e.g., as shown in the sample control file, species names (SO2, SO4) are used in several Input Groups).  Each Input Group and subgroup must end with an Input Group terminator consisting of the word END between two delimiters (i.e., !END!).  Every major Input Group, even blank Input Groups (i.e., one in which no variables are included) must end with an Input Group terminator in order to signal the end of that Input Group and the beginning of another.

The control file module has a list of variable names and array dimensions for each Input Group.  Checks are performed to ensure that the proper variable names are used in each Input Group, and that no array dimensions are exceeded.  Error messages result if an unrecognized variable name is encountered or too many values are entered for a variable.

As an example, the first group (Group 0) identifies all of the I/O files to be used in the run, except for the control file which is specified on the command line.  Each CALPUFF input and output file has a default name and path (i.e., the current working directory).  If the filename is not specified, the default name will be assumed.  Each filename must be less than or equal to 70 characters long.

All text except that between the delimiters (i.e., ! characters) is treated as optional documentation, and is ignored by the input module. Between the delimiters, the character filename variables (e.g., METDAT, PUFLST, CONDAT, etc.) must be entered as shown in the sample file. The control file reader is case insensitive. The filename is placed between the equals sign and the right delimiter character (!). Files that are not used or are not to be changed from their default names can be omitted from the I/O file. For example, by replacing the delimiter characters ("!"s) with "*"s, the line becomes a comment, and will not be interpreted by the program as data:

! CONDAT = conc.dat     !       - this line sets the file name of the output concentration file

* CONDAT = conc.old     *       - this line is a comment that does nothing

* PUFLST =            *       - this line is OK (interpreted as a comment)

! PUFLST =            !       - this is not OK (delimiters present, so file must be specified)

Blanks within the delimiters are ignored, and all delimiters must appear in pairs. If the optional CALPUFF GUI is being used, the control file will automatically be correctly formatted and written to disk for use by CALPUFF.

Table 4-1

Input Groups in the CALPUFF Control File

| Input Group | Description |
|---|---|
| * | Run title<br>First three lines of control file (up to 80 characters/line) |
| 0 | Input and Output filenames |
| 1 | General run control parameters<br>Starting date and hour, run length, time step.<br>Number of species.<br>Model restart configuration for making a series of continuation runs.<br>Meteorological data format and averaging time adjustment. |
| 2 | Technical options<br>Control variables determining methods for treating chemistry, wet deposition, dry deposition, dispersion, plume rise, complex terrain, and near-field puff sampling methods |
| 3 a,b | Species list<br>Species names, flags for determining which species are modeled, advected, emitted, and dry deposited |
| 4 | Grid control parameters<br>Specification of meteorological, computational, and sampling grids, number of cells, vertical layers, and reference coordinates. |
| 5 | Output options<br>Printer control variables, disk output control variables |
| 6a,b,c | Subgrid scale complex terrain (CTSG) inputs<br>Information describing subgrid scale hill location, shape and height.  Complex terrain receptor locations and elevations. |
| 7 | Dry deposition parameters - Gases<br>Pollutant diffusivity, dissociation constant, reactivity, mesophyll resistance, Henry's law coefficient |

Table 4-1 (Concluded)

Input Groups in the CALPUFF Control File

| Input Group | Description |
|---|---|
| 8 | Dry deposition parameters - Particles<br>Geometric mass mean diameter, geometric standard deviation |
| 9 | Miscellaneous dry deposition parameters<br>Reference cuticle and ground resistances, reference pollutant reactivity, vegetation state |
| 10 | Wet deposition parameters<br>Scavenging coefficients for each pollutant and precipitation type (liquid and frozen precipitation) |
| 11 | Chemistry parameters<br>Control variables for input of ozone data, background ozone and ammonia concentrations, nighttime transformation rates |
| 12 | Miscellaneous dispersion parameters and computational parameters<br>Vertical dispersion constants, dispersion rate above the boundary layer, crossover distance to time-dependent dispersion coefficients, land use associated with urban dispersion, site characterization parameters for single-point meteorological data files, sampling constraints, puff-splitting controls, plume path coefficients, wind speed power-law exponents, default temperature gradients and wind speed classes |
| 13a,b,c,d | Point source parameters<br>Point source data including source location, elevation, stack parameters, emissions, units, building dimensions, variable emissions cycle |
| 14a,b,c,d | Area source parameters<br>Area source data including source location, effective height, elevation, initial sigmas, emissions, units, variable emissions cycle |
| 15a,b,c | Line source parameters<br>Buoyant line source data including source location, elevation, line length, buoyancy parameters, release height, emissions, units, variable emissions cycle |
| 16a,b,c | Volume source parameters<br>Volume source data including source location, elevation, effective height, initial size data, emissions, units, variable emissions cycle |
| 17a,b | Non-gridded (discrete) receptor information<br>Receptor coordinates and ground elevation |

Table 4-2

Sample CALPUFF Control File (CALPUFF.INP)

Input Group 0

```
CALPUFF Example
40 x 40 meteorological grid
All source types represented;  CTSG hill
--------------- Run title (3 lines) ------------------------------------------

                    CALPUFF MODEL CONTROL FILE
                    --------------------------


-------------------------------------------------------------------------------

INPUT GROUP: 0 -- Input and Output File Names

     Number of CALMET.DAT files for run (NMETDAT)
                                   Default: 1       ! NMETDAT =   1   !

--------------
Default Name  Type          File Name
------------  ----         ---------
CALMET.DAT    input    ! METDAT =CALMET.DAT   !
    or
ISCMET.DAT    input    * ISCDAT =            *
    or
PLMMET.DAT    input    * PLMDAT =            *
    or
PROFILE.DAT   input    * PRFDAT =            *
SURFACE.DAT   input    * SFCDAT =            *
RESTARTB.DAT  input    * RSTARTB=            *
-------------------------------------------------------------------------------
CALPUFF.LST   output   ! PUFLST =CALPUFF2.LST  !
CONC.DAT      output   ! CONDAT =CONC2.DAT     !
DFLX.DAT      output   ! DFDAT  =DFLX2.DAT     !
WFLX.DAT      output   * WFDAT  =            *

VISB.DAT      output   * VISDAT =            *
RESTARTE.DAT  output   * RSTARTE=            *
-------------------------------------------------------------------------------
Emission Files
--------------
PTEMARB.DAT   input    * PTDAT  =            *
VOLEM.DAT     input    * VOLDAT =            *
BAEMARB.DAT   input    * ARDAT  =            *
LNEMARB.DAT   input    * LNDAT  =            *
-------------------------------------------------------------------------------
Other Files
-----------
OZONE.DAT     input    * OZDAT  =            *
VD.DAT        input    * VDDAT  =            *
CHEM.DAT      input    * CHEMDAT=            *
HILL.DAT      input    * HILDAT=             *
HILLRCT.DAT   input    * RCTDAT=             *
COASTLN.DAT   input    * CSTDAT=             *
FLUXBDY.DAT   input    * BDYDAT=             *
DEBUG.DAT     output   * DEBUG =             *
MASSFLX.DAT   output   * FLXDAT=             *
MASSBAL.DAT   output   * BALDAT=             *
-------------------------------------------------------------------------------
All file names will be converted to lower case if LCFILES = T
Otherwise, if LCFILES = F, file names will be converted to UPPER CASE
        T = lower case      ! LCFILES = F !
        F = UPPER CASE
NOTE: (1) file/path names can be up to 70 characters in length

!END!

-------------
Subgroup (0a)
-------------


  The following CALMET.DAT filenames are processed in sequence if NMETDAT>1

Default Name  Type          File Name
------------  ----         ---------
 none         input    * METDAT=     **END*
```

--------------------------------------------------------------------------------

INPUT GROUP: 1 -- General run control parameters
--------------

```
    Option to run all periods found
    in the met. file      (METRUN)   Default: 0       ! METRUN =   0  !

         METRUN = 0 - Run period explicitly defined below
         METRUN = 1 - Run all periods in met. file

     Starting date:   Year (IBYR) -- No default       ! IBYR =  1994  !
     (used only if   Month (IBMO) -- No default        ! IBMO =  11  !
      METRUN = 0)      Day (IBDY) -- No default         ! IBDY =  1  !
                      Hour (IBHR) -- No default         ! IBHR =  10  !

     Length of run (hours) (IRLG) -- No default        ! IRLG =  2  !

     Number of chemical species (NSPEC)
                                       Default: 5       ! NSPEC =  8   !

     Number of chemical species
     to be emitted  (NSE)             Default: 3        ! NSE =  7  !

     Flag to stop run after
     SETUP phase (ITEST)             Default: 2         ! ITEST =  2   !
     (Used to allow checking
     of the model inputs, files, etc.)
           ITEST = 1 - STOPS program after SETUP phase
           ITEST = 2 - Continues with execution of program
                       after SETUP

     Restart Configuration:

        Control flag (MRESTART)      Default: 0         ! MRESTART =  0   !

           0 = Do not read or write a restart file
           1 = Read a restart file at the beginning of
               the run
           2 = Write a restart file during run
           3 = Read a restart file at beginning of run
               and write a restart file during run

        Number of periods in Restart
        output cycle (NRESPD)        Default: 0         ! NRESPD =  0   !

           0 = File written only at last period
          >0 = File updated every NRESPD periods

     Meteorological Data Format (METFM)
                                       Default: 1        ! METFM =  1   !

           METFM = 1 - CALMET binary file (CALMET.MET)
           METFM = 2 - ISC ASCII file (ISCMET.MET)
           METFM = 3 - AUSPLUME ASCII file (PLMMET.MET)
           METFM = 4 - CTDM plus tower file (PROFILE.DAT) and
                       surface parameters file (SURFACE.DAT)

     PG sigma-y is adjusted by the factor (AVET/PGTIME)**0.2
     Averaging Time (minutes) (AVET)
                                       Default: 60.0     ! AVET = 60. !
     PG Averaging Time (minutes) (PGTIME)
                                       Default: 60.0     ! PGTIME = 60. !


 !END!
```

--------------------------------------------------------------------------------

INPUT GROUP: 2 -- Technical options
-------------

```
    Vertical distribution used in the
    near field (MGAUSS)                  Default: 1      ! MGAUSS =  1   !
       0 = uniform
       1 = Gaussian

    Terrain adjustment method
    (MCTADJ)                             Default: 3      ! MCTADJ =  0    !
       0 = no adjustment
       1 = ISC-type of terrain adjustment
       2 = simple, CALPUFF-type of terrain
           adjustment
       3 = partial plume path adjustment

    Subgrid-scale complex terrain
    flag (MCTSG)                         Default: 0      ! MCTSG =  1   !
       0 = not modeled
       1 = modeled

    Near-field puffs modeled as
    elongated 0 (MSLUG)                  Default: 0      ! MSLUG =  1   !
       0 = no
       1 = yes (slug model used)

    Transitional plume rise modeled ?
    (MTRANS)                             Default: 1      ! MTRANS =  0    !
       0 = no  (i.e., final rise only)
       1 = yes (i.e., transitional rise computed)

    Stack tip downwash? (MTIP)           Default: 1      ! MTIP =  0   !
       0 = no  (i.e., no stack tip downwash)
       1 = yes (i.e., use stack tip downwash)

    Vertical wind shear modeled above
    stack top? (MSHEAR)                  Default: 0      ! MSHEAR =  0   !
       0 = no  (i.e., vertical wind shear not modeled)
       1 = yes (i.e., vertical wind shear modeled)

    Puff splitting allowed? (MSPLIT)     Default: 0      ! MSPLIT =  0   !
       0 = no (i.e., puffs not split)
       1 = yes (i.e., puffs are split)

    Chemical mechanism flag (MCHEM)      Default: 1      ! MCHEM =  0   !
       0 = chemical transformation not
           modeled
       1 = transformation rates computed
           internally (MESOPUFF II scheme)
       2 = user-specified transformation
           rates used
       3 = transformation rates computed
           internally (RIVAD/ARM3 scheme)

    Wet removal modeled ? (MWET)         Default: 1      ! MWET =  1   !
       0 = no
       1 = yes

    Dry deposition modeled ? (MDRY)      Default: 1      ! MDRY =  1   !
       0 = no
       1 = yes
       (dry deposition method specified
        for each species in Input Group 3)
```

```
Method used to compute dispersion
coefficients (MDISP)                   Default: 3      ! MDISP =  3   !

   1 = dispersion coefficients computed from measured values
       of turbulence, sigma v, sigma w
   2 = dispersion coefficients from internally calculated
       sigma v, sigma w using micrometeorological variables
       (u*, w*, L, etc.)
   3 = PG dispersion coefficients for RURAL areas (computed using
       the ISCST multi-segment approximation) and MP coefficients in
       urban areas
   4 = same as 3 except PG coefficients computed using
       the MESOPUFF II eqns.
   5 = CTDM sigmas used for stable and neutral conditions.
       For unstable conditions, sigmas are computed as in
       MDISP = 3, described above.  MDISP = 5 assumes that
       measured values are read

Sigma-v/sigma-theta, sigma-w measurements used? (MTURBVW)
(Used only if MDISP = 1 or 5)          Default: 3      ! MTURBVW =  3   !
   1 = use sigma-v or sigma-theta measurements
       from PROFILE.DAT to compute sigma-y
       (valid for METFM = 1, 2, 3, 4)
   2 = use sigma-w measurements
       from PROFILE.DAT to compute sigma-z
       (valid for METFM = 1, 2, 3, 4)
   3 = use both sigma-(v/theta) and sigma-w
       from PROFILE.DAT to compute sigma-y and sigma-z
       (valid for METFM = 1, 2, 3, 4)
   4 = use sigma-theta measurements
       from PLMMET.DAT to compute sigma-y
       (valid only if METFM = 3)

Back-up method used to compute dispersion
when measured turbulence data are
missing (MDISP2)                       Default: 3      ! MDISP2 =  4   !
(used only if MDISP = 1 or 5)
   2 = dispersion coefficients from internally calculated
       sigma v, sigma w using micrometeorological variables
       (u*, w*, L, etc.)
   3 = PG dispersion coefficients for RURAL areas (computed using
       the ISCST multi-segment approximation) and MP coefficients in
       urban areas
   4 = same as 3 except PG coefficients computed using
       the MESOPUFF II eqns.

PG sigma-y,z adj. for roughness?       Default: 0      ! MROUGH =  0   !
(MROUGH)
   0 = no
   1 = yes

Partial plume penetration of           Default: 1      ! MPARTL =  1   !
elevated inversion?
(MPARTL)
   0 = no
   1 = yes

Strength of temperature inversion      Default: 0      ! MTINV =  0    !
provided in PROFILE.DAT extended records?
(MTINV)
   0 = no (computed from measured/default gradients)
   1 = yes

PDF used for dispersion under convective conditions?
                                       Default: 0      ! MPDF =  0   !
(MPDF)
   0 = no
   1 = yes
```

```
Sub-Grid TIBL module used for shore line?
                                    Default: 0      ! MSGTIBL = 0  !
(MSGTIBL)
   0 = no
   1 = yes

Test options specified to see if
they conform to regulatory
values? (MREG)                      Default: 1      ! MREG =  0    !

   0 = NO checks are made
   1 = Technical options must conform to USEPA values
                 METFM     1
                 AVET      60. (min)
                 MGAUSS    1
                 MCTADJ    3
                 MTRANS    1
                 MTIP      1
                 MCHEM     1 (if modeling SOx, NOx)
                 MWET      1
                 MDRY      1
                 MDISP     3
                 MROUGH    0
                 MPARTL    1
                 SYTDEP    550. (m)
                 MHFTSZ    0


!END!
```

```
--------------------------------------------------------------------------------

INPUT GROUP: 3a, 3b -- Species list
-------------------

------------
Subgroup (3a)
------------

  The following species are modeled:

! CSPEC =          SO2 !          !END!
! CSPEC =          NOX !          !END!
! CSPEC =      PMSIZE1 !          !END!
! CSPEC =      PMSIZE2 !          !END!
! CSPEC =      PMSIZE3 !          !END!
! CSPEC =      PMSIZE4 !          !END!
! CSPEC =      PMSIZE5 !          !END!
! CSPEC =      PMSIZE6 !          !END!

                                                 Dry              OUTPUT GROUP
       SPECIES          MODELED        EMITTED    DEPOSITED          NUMBER
        NAME          (0=NO, 1=YES)  (0=NO, 1=YES)  (0=NO,         (0=NONE,
      (Limit: 12                                   1=COMPUTED-GAS      1=1st CGRUP,
       Characters                                  2=COMPUTED-PARTICLE 2=2nd CGRUP,
       in length)                                  3=USER-SPECIFIED)   3= etc.)

!         SO2  =        1,             1,             1,              0   !
!         NOX  =        1,             1,             1,              0   !
!      PMSIZE1  =        1,             1,             2,              1   !
!      PMSIZE2  =        1,             1,             2,              1   !
!      PMSIZE3  =        1,             1,             2,              1   !
!      PMSIZE4  =        1,             1,             2,              1   !
!      PMSIZE5  =        1,             1,             2,              1   !
!      PMSIZE6  =        1,             1,             2,              1   !

!END!


-------------
Subgroup (3b)
-------------
  The following names are used for Species-Groups in which results
  for certain species are combined (added) prior to output.  The
  CGRUP name will be used as the species name in output files.
  Use this feature to model specific particle-size distributions
  by treating each size-range as a separate species.
  Order must be consistent with 3(a) above.

! CGRUP =          PM10 !     !END!
```

--------------------------------------------------------------------------------

INPUT GROUP: 4 -- Grid control parameters
--------------

METEOROLOGICAL grid:

```
           No. X grid cells (NX)      No default     ! NX =  40   !
           No. Y grid cells (NY)      No default     ! NY =  40   !
      No. vertical layers (NZ)        No default     ! NZ =  10   !

        Grid spacing (DGRIDKM)        No default     ! DGRIDKM = 0.5 !
                                      Units: km

            Cell face heights
                 (ZFACE(nz+1))        No defaults
                                      Units: m
  ! ZFACE = 0., 20., 50., 100., 200., 400., 600., 1000., 1500., 2000.,
         3000. !

            Reference Coordinates
            of SOUTHWEST corner of
                grid cell(1, 1):

        X coordinate (XORIGKM)        No default     ! XORIGKM = -10. !
        Y coordinate (YORIGKM)        No default     ! YORIGKM = -10. !
                                      Units: km

            UTM zone (IUTMZN)         No default     ! IUTMZN =  19   !

  Reference coordinates of CENTER
      of the domain (used in the
  calculation of solar elevation
                        angles)

        Latitude  (deg.) (XLAT)       No default     ! XLAT  = 42.  !
        Longitude (deg.) (XLONG)      No default     ! XLONG = 75.  !
            Time zone        (XTZ)    No default     ! XTZ   = 5.0  !
    (PST=8, MST=7, CST=6, EST=5)
```

Computational grid:

```
     The computational grid is identical to or a subset of the MET. grid.
     The lower left (LL) corner of the computational grid is at grid point
     (IBCOMP, JBCOMP) of the MET. grid.  The upper right (UR) corner of the
     computational grid is at grid point (IECOMP, JECOMP) of the MET. grid.
     The grid spacing of the computational grid is the same as the MET. grid.

        X index of LL corner (IBCOMP)      No default     ! IBCOMP = 1   !
                (1 <= IBCOMP <= NX)

        Y index of LL corner (JBCOMP)      No default     ! JBCOMP = 1   !
                (1 <= JBCOMP <= NY)


        X index of UR corner (IECOMP)      No default     ! IECOMP =  40   !
                (1 <= IECOMP <= NX)

        Y index of UR corner (JECOMP)      No default     ! JECOMP =  40   !
                (1 <= JECOMP <= NY)
```

```
SAMPLING GRID (GRIDDED RECEPTORS):

    The lower left (LL) corner of the sampling grid is at grid point
    (IBSAMP, JBSAMP) of the MET. grid.  The upper right (UR) corner of the
    sampling grid is at grid point (IESAMP, JESAMP) of the MET. grid.
    The sampling grid must be identical to or a subset of the computational
    grid.  It may be a nested grid inside the computational grid.
    The grid spacing of the sampling grid is DGRIDKM/MESHDN.

        Logical flag indicating if gridded
        receptors are used (LSAMP)          Default: T     ! LSAMP = T !
        (T=yes, F=no)

        X index of LL corner (IBSAMP)       No default     ! IBSAMP = 1   !
         (IBCOMP <= IBSAMP <= IECOMP)

        Y index of LL corner (JBSAMP)       No default     ! JBSAMP = 1   !
         (JBCOMP <= JBSAMP <= JECOMP)


        X index of UR corner (IESAMP)       No default     ! IESAMP =  40   !
         (IBCOMP <= IESAMP <= IECOMP)

        Y index of UR corner (JESAMP)       No default     ! JESAMP =  40   !
         (JBCOMP <= JESAMP <= JECOMP)


       Nesting factor of the sampling
        grid (MESHDN)                       Default: 1     ! MESHDN =  1  !
        (MESHDN is an integer >= 1)

    !END!
```

```
--------------------------------------------------------------------------------
INPUT GROUP: 5 -- Output Options
--------------
                                      *                          *
    FILE                     DEFAULT VALUE            VALUE THIS RUN
    ----                     -------------            --------------

  Concentrations (ICON)            1                 !  ICON =  1   !
  Dry Fluxes (IDRY)                1                 !  IDRY =  1   !
  Wet Fluxes (IWET)                1                 !  IWET =  0   !
  Relative Humidity (IVIS)         1                 !  IVIS =  0   !
   (relative humidity file is
    required for visibility
    analysis)
  Use data compression option in output file?
  (LCOMPRS)                     Default: T           ! LCOMPRS = T !


   *
   0 = Do not create file, 1 = create file

   DIAGNOSTIC MASS FLUX OUTPUT OPTIONS:

      Mass flux across specified boundaries
      for selected species reported hourly?
      (IMFLX)                     Default: 0         ! IMFLX =  0  !
        0 = no
        1 = yes (FLUXBDY.DAT and MASSFLX.DAT filenames
                 are specified in Input Group 0)

      Mass balance for each species
      reported hourly?
      (IMBAL)                     Default: 0         ! IMBAL =  0  !
        0 = no
        1 = yes (MASSBAL.DAT filename is
             specified in Input Group 0)


   LINE PRINTER OUTPUT OPTIONS:

      Print concentrations (ICPRT)  Default: 0       ! ICPRT =  1   !
      Print dry fluxes (IDPRT)      Default: 0       ! IDPRT =  0   !
      Print wet fluxes (IWPRT)      Default: 0       ! IWPRT =  0   !
      (0 = Do not print, 1 = Print)

      Concentration print interval
      (ICFRQ) in hours              Default: 1       ! ICFRQ =  1   !
      Dry flux print interval
      (IDFRQ) in hours              Default: 1       ! IDFRQ =  1   !
      Wet flux print interval
      (IWFRQ) in hours              Default: 1       ! IWFRQ =  1   !

      Units for Line Printer Output
      (IPRTU)                       Default: 1       ! IPRTU =  1   !
                       for            for
                  Concentration    Deposition
          1 =        g/m**3         g/m**2/s
          2 =        mg/m**3        mg/m**2/s
          3 =        ug/m**3        ug/m**2/s
          4 =        ng/m**3        ng/m**2/s
          5 =      Odour Units

      Messages tracking progress of   Default: 1     ! IMESG =  1   !
      run written to the screen ?
      (IMESG) -- 0=no, 1=yes
```

```
      SPECIES (or GROUP for combined species) LIST FOR OUTPUT OPTIONS

              ---- CONCENTRATIONS ----   ------ DRY FLUXES ------   ------ WET FLUXES ------   -- MASS FLUX
--
   SPECIES
   /GROUP      PRINTED?  SAVED ON DISK?  PRINTED?  SAVED ON DISK?  PRINTED?  SAVED ON DISK?  SAVED ON
DISK?
   -------     ----------------------   ----------------------   ----------------------
---------------
!       SO2 =   1,            1,           0,            1,           0,            0,           0   !
!       NOX =   1,            1,           0,            1,           0,            0,           0   !
!      PM10 =   1,            1,           0,            1,           0,            0,           0   !

      OPTIONS FOR PRINTING "DEBUG" QUANTITIES (much output)

        Logical for debug output
        (LDEBUG)                               Default: F     ! LDEBUG = F !

        First puff to track
        (IPFDEB)                               Default: 1     ! IPFDEB =  1  !

        Number of puffs to track
        (NPFDEB)                               Default: 1     ! NPFDEB =  1  !

        Met. period to start output
        (NN1)                                  Default: 1     ! NN1 =  1   !

        Met. period to end output
        (NN2)                                  Default: 10    ! NN2 =  10  !

   !END!
```

--------------------------------------------------------------------------------

INPUT GROUP: 6a, 6b, & 6c -- Subgrid scale complex terrain inputs
-------------------------

---------------
Subgroup (6a)
---------------
```
        Number of terrain features (NHILL)      Default: 0     ! NHILL = 1   !

        Number of special complex terrain
        receptors  (NCTREC)                     Default: 0     ! NCTREC = 9   !

        Terrain and CTSG Receptor data for
        CTSG hills input in CTDM format ?
        (MHILL)                                 No Default     ! MHILL = 2   !
        1 = Hill and Receptor data created
            by CTDM processors & read from
            HILL.DAT and HILLRCT.DAT files
        2 = Hill data created by OPTHILL &
            input below in Subgroup (6b);
            Receptor data in Subgroup (6c)

        Factor to convert horizontal dimensions  Default: 1.0   ! XHILL2M = 1. !
        to meters (MHILL=1)

        Factor to convert vertical dimensions    Default: 1.0   ! ZHILL2M = 1. !
        to meters (MHILL=1)

        X-origin of CTDM system relative to      No Default     ! XCTDMKM = 0.0E00 !
        CALPUFF coordinate system, in Kilometers (MHILL=1)

        Y-origin of CTDM system relative to      No Default     ! YCTDMKM = 0.0E00 !
        CALPUFF coordinate system, in Kilometers (MHILL=1)

! END !
```

---------------
Subgroup (6b)
---------------

```
                  1 **
      HILL information
```

| HILL | XC | YC | THETAH | ZGRID | RELIEF | EXPO 1 | EXPO 2 | SCALE 1 | SCALE 2 | AMAX1 AMAX2 |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NO. | (km) | (km) | (deg.) | (m) | (m) | (m) | (m) | (m) | (m) | (m) (m) |
| ---- | ---- | ---- | ------ | ----- | ------ | ------ | ------ | ------- | ------- | ----- ----- |
| 1!HILL = | 0., | 0., | 0., | 25., | 100., | 2., | 2., | 800., | 400., | 1132., 566. !   !END! |

---------------
Subgroup (6c)
---------------

```
    COMPLEX TERRAIN RECEPTOR INFORMATION
```

| | XRCT (km) | YRCT (km) | ZRCT (m) | XHH | |
| --- | --- | --- | --- | --- | --- |
| | ------ | ----- | ------ | ---- | |
| 1 !CTREC = | -0.2, | 0., | 95.0, | 1.0 ! | !END! |
| 2 !CTREC = | -0.2, | -0.1, | 93.5, | 1.0 ! | !END! |
| 3 !CTREC = | -0.2, | -0.2, | 89.3, | 1.0 ! | !END! |
| 4 !CTREC = | -0.2, | -0.3, | 82.9, | 1.0 ! | !END! |
| 5 !CTREC = | -0.2, | -0.4, | 75.0, | 1.0 ! | !END! |
| 6 !CTREC = | -0.2, | -0.5, | 66.4, | 1.0 ! | !END! |
| 7 !CTREC = | -0.2, | -0.6, | 57.8, | 1.0 ! | !END! |
| 8 !CTREC = | -0.2, | -0.7, | 49.4, | 1.0 ! | !END! |
| 9 !CTREC = | -0.2, | -0.8, | 41.7, | 1.0 ! | !END! |

```
-------------------
1
     Description of Complex Terrain Variables:
          XC, YC  = Coordinates of center of hill
          THETAH  = Orientation of major axis of hill (clockwise from
                    North)
          ZGRID   = Height of the  0  of the grid above mean sea
                    level
          RELIEF  = Height of the crest of the hill above the grid elevation
          EXPO 1  = Hill-shape exponent for the major axis
          EXPO 2  = Hill-shape exponent for the major axis
          SCALE 1 = Horizontal length scale along the major axis
          SCALE 2 = Horizontal length scale along the minor axis
          AMAX    = Maximum allowed axis length for the major axis
          BMAX    = Maximum allowed axis length for the major axis

          XRCT, YRCT = Coordinates of the complex terrain receptors
          ZRCT    = Height of the ground (MSL) at the complex terrain
                    Receptor
          XHH     = Hill number associated with each complex terrain receptor
                    (NOTE: MUST BE ENTERED AS A REAL NUMBER)

   **
     NOTE: DATA for each hill and CTSG receptor are treated as a separate
           input subgroup and therefore must end with an input group terminator.
```

```
--------------------------------------------------------------------------------

INPUT GROUP: 7 -- Chemical parameters for dry deposition of gases
-------------

      SPECIES    DIFFUSIVITY    ALPHA STAR    REACTIVITY   MESOPHYLL RESISTANCE    HENRY'S LAW
COEFFICIENT
      NAME       (cm**2/s)                                       (s/cm)           (dimensionless)
      -------    ----------     ----------    ----------    --------------------
----------------------

!       SO2 =     0.1509,        1000.,          8.,               0.,               0.04 !
!       NOX =     0.1656,        1.,             8.,               5.,               3.5  !

!END!


--------------------------------------------------------------------------------


INPUT GROUP: 8 -- Size parameters for dry deposition of particles
-------------

     For SINGLE SPECIES, the mean and standard deviation are used to
     compute a deposition velocity for NINT (see group 9) size-ranges,
     and these are then averaged to obtain a mean deposition velocity.

     For GROUPED SPECIES, the size distribution should be explicitly
     specified (by the 'species' in the group), and the standard deviation
     for each should be entered as 0.  The model will then use the
     deposition velocity for the stated mean diameter.

     SPECIES    GEOMETRIC MASS MEAN       GEOMETRIC STANDARD
      NAME          DIAMETER                  DEVIATION
                    (microns)                 (microns)
     -------    -------------------       ------------------
!    PMSIZE1 =          0.05,                   0.   !
!    PMSIZE2 =          0.1,                    0.   !
!    PMSIZE3 =          0.2,                    0.   !
!    PMSIZE4 =          0.4,                    0.   !
!    PMSIZE5 =          0.8,                    0.   !
!    PMSIZE6 =          1.6,                    0.   !

!END!


--------------------------------------------------------------------------------


INPUT GROUP: 9 -- Miscellaneous dry deposition parameters
-------------

     Reference cuticle resistance (s/cm)
     (RCUTR)                          Default: 30    ! RCUTR = 30. !
     Reference ground resistance  (s/cm)
     (RGR)                            Default: 10    !   RGR = 10. !
     Reference pollutant reactivity
     (REACTR)                         Default: 8     ! REACTR = 8. !

     Number of particle-size intervals used to
     evaluate effective particle deposition velocity
     (NINT)                           Default: 9     !   NINT = 9 !

     Vegetation state in unirrigated areas
     (IVEG)                           Default: 1     !  IVEG = 1   !
        IVEG=1 for active and unstressed vegetation
        IVEG=2 for active and stressed vegetation
        IVEG=3 for inactive vegetation

!END!
```

```
--------------------------------------------------------------------------------

INPUT GROUP: 10 -- Wet Deposition Parameters
---------------


                    Scavenging Coefficient -- Units: (sec)**(-1)

        Pollutant     Liquid Precip.     Frozen Precip.
        ---------     --------------     --------------
!        SO2 =          3.0E-05,            0.0E00  !
!        NOX =          0.0,                0.0     !
!     PMSIZE1 =         1.0E-04,            3.0E-05 !
!     PMSIZE2 =         1.0E-04,            3.0E-05 !
!     PMSIZE3 =         1.0E-04,            3.0E-05 !
!     PMSIZE4 =         1.0E-04,            3.0E-05 !
!     PMSIZE5 =         1.0E-04,            3.0E-05 !
!     PMSIZE6 =         1.0E-04,            3.0E-05 !

!END!


--------------------------------------------------------------------------------


INPUT GROUP: 11 -- Chemistry Parameters
---------------

     Ozone data input option (MOZ)     Default: 1           ! MOZ =  0   !
     (Used only if MCHEM = 1 or 3)
        0 = use a constant background ozone value
        1 = read hourly ozone concentrations from
            the OZONE.DAT data file

     Background ozone concentration
     (BCKO3) in ppb                    Default: 80.         ! BCKO3 = 80. !
     (Used only if MCHEM = 1 or 3 and
      MOZ = 0 or (MOZ = 1 and all hourly
      O3 data missing)

     Background ammonia concentration
     (BCKNH3) in ppb                   Default: 10.         ! BCKNH3 = 10. !

     Nighttime SO2 loss rate (RNITE1)
     in percent/hour                   Default: 0.2         ! RNITE1 = 0.2 !

     Nighttime NOx loss rate (RNITE2)
     in percent/hour                   Default: 2.0         ! RNITE2 = 2. !

     Nighttime HNO3 formation rate (RNITE3)
     in percent/hour                   Default: 2.0         ! RNITE3 = 2. !

!END!
```

--------------------------------------------------------------------------------

INPUT GROUP: 12 -- Misc. Dispersion and Computational Parameters
--------------

```
    Horizontal size of puff (m) beyond which
    time-dependent dispersion equations (Heffter)
    are used to determine sigma-y and
    sigma-z (SYTDEP)                        Default: 550.    ! SYTDEP = 1.0E04 !

    Switch for using Heffter equation for sigma z
    as above (0 = Not use Heffter; 1 = use Heffter
    (MHFTSZ)                                Default: 0       ! MHFTSZ =  1   !

    Stability class used to determine plume
    growth rates for puffs above the boundary
    layer (JSUP)                            Default: 5       ! JSUP =  5    !

    Vertical dispersion constant for stable
    conditions (k1 in Eqn. 2.7-3)  (CONK1)  Default: 0.01    ! CONK1 = 0.01 !

    Vertical dispersion constant for neutral/
    unstable conditions (k2 in Eqn. 2.7-4)
    (CONK2)                                 Default: 0.1     ! CONK2 = 0.1 !

    Factor for determining Transition-point from
    Schulman-Scire to Huber-Snyder Building Downwash
    scheme (SS used for Hs < Hb + TBD * HL)
    (TBD)                                   Default: 0.5     ! TBD = 0.5 !
       TBD < 0   ==> always use Huber-Snyder
       TBD = 1.5 ==> always use Schulman-Scire
       TBD = 0.5 ==> ISC Transition-point

    Range of land use categories for which
    urban dispersion is assumed
    (IURB1, IURB2)                          Default: 10      ! IURB1 =  10  !
                                                     19      ! IURB2 =  19  !

    Site characterization parameters for single-point Met data files ---------
    (needed for METFM = 2,3,4)

       Land use category for modeling domain
       (ILANDUIN)                           Default: 20      ! ILANDUIN =  20  !

       Roughness length (m) for modeling domain
       (Z0IN)                               Default: 0.25    ! Z0IN = 0.25 !

       Leaf area index for modeling domain
       (XLAIIN)                             Default: 3.0     ! XLAIIN = 3. !

       Elevation above sea level (m)
       (ELEVIN)                             Default: 0.0     ! ELEVIN = 0. !

       Latitude (degrees) for met location
       (XLATIN)                             Default: -999.   ! XLATIN = 0. !

       Longitude (degrees) for met location
       (XLONIN)                             Default: -999.   ! XLONIN = 0. !

    Specialized information for interpreting single-point Met data files -----

       Anemometer height (m) (Used only if METFM = 2,3)
       (ANEMHT)                             Default: 10.     ! ANEMHT = 10. !

       Form of lateral turbulance data in PROFILE.DAT file
       (Used only if METFM = 4 or MTURBVW = 1 or 3)
       (ISIGMAV)                            Default: 1       ! ISIGMAV =  1 !
          0 = read sigma-theta
          1 = read sigma-v

       Choice of mixing heights (Used only if METFM = 4)
       (IMIXCTDM)                           Default: 0       ! IMIXCTDM =  0 !
          0 = read PREDICTED mixing heights
          1 = read OBSERVED mixing heights

    Maximum length of a slug (met. grid units)
    (XMXLEN)                                Default: 1.0     ! XMXLEN = 1. !
```

```
Maximum travel distance of a puff/slug (in
grid units) during one sampling step
(XSAMLEN)                                 Default: 1.0     ! XSAMLEN = 1. !

Maximum Number of slugs/puffs release from
one source during one time step
(MXNEW)                                   Default: 99      ! MXNEW =  99   !

Maximum Number of sampling steps for
one puff/slug during one time step
(MXSAM)                                   Default: 99      ! MXSAM =  99   !

Number of iterations used when computing
the transport wind for a sampling step
that includes gradual rise (for CALMET
and PROFILE winds)
(NCOUNT)                                  Default: 2       ! NCOUNT =  2   !

Minimum sigma y for a new puff/slug (m)
(SYMIN)                                   Default: 1.0     ! SYMIN = 1.  !

Minimum sigma z for a new puff/slug (m)
(SZMIN)                                   Default: 1.0     ! SZMIN = 1.  !

Default minimum turbulence velocities
sigma-v and sigma-w for each
stability class (m/s)
(SVMIN(6) and SWMIN(6))     Default SVMIN : .50,   .50,   .50,   .50,   .50,   .50
                           Default SWMIN : .20,   .12,   .08,   .06,   .03,   .016

                           Stability Class :  A      B      C      D      E      F
                                             ---    ---    ---    ---    ---    ---
                                ! SVMIN = 0.500, 0.500, 0.500, 0.500, 0.500, 0.500!
                                ! SWMIN = 0.200, 0.120, 0.080, 0.060, 0.030, 0.016!

Divergence criterion for dw/dz across puff
used to initiate adjustment for horizontal
convergence (1/s)
Partial adjustment starts at CDIV(1), and
full adjustment is reached at CDIV(2)
(CDIV(2))                                 Default: 0.0,0.0 ! CDIV = 0., 0. !

Minimum wind speed (m/s) allowed for
non-calm conditions. Also used as minimum
speed returned when using power-law
extrapolation toward surface
(WSCALM)                                  Default: 0.5     ! WSCALM = 0.5 !

Maximum mixing height (m)
(XMAXZI)                                  Default: 3000.   ! XMAXZI = 3000. !

Minimum mixing height (m)
(XMINZI)                                  Default: 50.     ! XMINZI = 50. !

Default wind speed classes --
5 upper bounds (m/s) are entered;
the 6th class has no upper limit
(WSCAT(5))                     Default   :
                               ISC RURAL : 1.54, 3.09, 5.14, 8.23, 10,8 (10.8+)

                           Wind Speed Class :  1      2      3      4      5      6
                                             ---    ---    ---    ---    ---    ---
                                ! WSCAT = 1.54, 3.09, 5.14, 8.23, 10.80 !

Default wind speed profile power-law
exponents for stabilities 1-6
(PLX0(6))                      Default   : ISC RURAL values
                               ISC RURAL : .07, .07, .10, .15, .35, .55
                               ISC URBAN : .15, .15, .20, .25, .30, .30

                           Stability Class :  A      B      C      D      E      F
                                             ---    ---    ---    ---    ---    ---
                                ! PLX0 = 0.07, 0.07, 0.10, 0.15, 0.35, 0.55 !

Default potential temperature gradient
for stable classes E, F (degK/m)
(PTG0(2))                      Default: 0.020, 0.035
                                ! PTG0 = 0.020,   0.035 !
```

```
Default plume path coefficients for
each stability class (used when option
for partial plume height terrain adjustment
is selected -- MCTADJ=3)
(PPC(6))                    Stability Class :  A     B     C     D     E     F
                            Default  PPC : .50,  .50,  .50,  .50,  .35,  .35
                                           ---   ---   ---   ---   ---   ---
                                        ! PPC = 0.50, 0.50, 0.50, 0.50, 0.35, 0.35 !

Slug-to-puff transition criterion factor
equal to sigma-y/length of slug
(SL2PF)                                    Default: 10.        ! SL2PF = 10. !

Puff-splitting control variables -----------------------

  Number of puffs that result every time a puff
  is split - nsplit=2 means that 1 puff splits
  into 2
  (NSPLIT)                                 Default:   3        ! NSPLIT =  3 !

  Time(s) of a day when split puffs are eligible to
  be split once again; this is typically set once
  per day, around sunset before nocturnal shear develops.
  24 values: 0 is midnight (00:00) and 23 is 11 PM (23:00)
  0=do not re-split   1=eligible for re-split
  (IRESPLIT(24))                           Default:  Hour 17 = 1
  !  IRESPLIT = 0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0 !

  Split is allowed only if last hour's mixing
  height (m) exceeds a minimum value
  (ZISPLIT)                                Default: 100.       ! ZISPLIT = 100. !

  Split is allowed only if ratio of last hour's
  mixing ht to the maximum mixing ht experienced
  by the puff is less than a maximum value (this
  postpones a split until a nocturnal layer develops)
  (ROLDMAX)                                Default: 0.25       ! ROLDMAX = 0.25 !

Integration control variables -----------------------

  Fractional convergence criterion for numerical SLUG
  sampling integration
  (EPSSLUG)                                Default:   1.0e-04  ! EPSSLUG = 1.0E-04 !

  Fractional convergence criterion for numerical AREA
  source integration
  (EPSAREA)                                Default:   1.0e-06  ! EPSAREA = 1.0E-06 !

  Trajectory step-length (m) used for numerical rise
  integration
  (DSRISE)                                 Default:   1.0      ! DSRISE = 1. !

!END!
```

--------------------------------------------------------------------------------

INPUT GROUPS: 13a, 13b, 13c, 13d -- Point source parameters
--------------------------------

---------------
Subgroup (13a)
---------------

```
     Number of point sources with
     parameters provided below     (NPT1) No default  !  NPT1 =  1  !

     Units used for point source
     emissions below               (IPTU) Default: 1 !  IPTU =   1 !
           1 =        g/s
           2 =        kg/hr
           3 =        lb/hr
           4 =       tons/yr
           5 =       Odour Unit * m**3/s  (vol. flux of odour compound)
           6 =       Odour Unit * m**3/min
           7 =       metric tons/yr

     Number of source-species
     combinations with variable
     emissions scaling factors
     provided below in (13d)        (NSPT1) Default: 0  ! NSPT1 =  1  !

     Number of point sources with
     variable emission parameters
     provided in external file      (NPT2)  No default  !  NPT2 =  0  !

     (If NPT2 > 0, these point
     source emissions are read from
     the file: PTEMARB.DAT)
```

!END!

---------------
Subgroup (13b)
---------------

```
                                    a
           POINT SOURCE: CONSTANT DATA
           ---------------------------
                                                                  b           c
   Source     X UTM      Y UTM     Stack  Base    Stack   Exit  Exit  Bldg. Emission
   No.      Coordinate Coordinate Height Elevation Diameter Vel.  Temp.  Dwash  Rates
             (km)       (km)       (m)    (m)       (m)    (m/s) (deg. K)
   ------   ---------- ---------- ------ ------   -------- ----- -------- ----- --------
   1 ! SRCNAM = BLR1 !
   1 ! X =      0.1,      -3.,     40.,   25.,      2.2,   10.,    450.,   1., 1.7E00,  1.0E00, 1.0E-02,
      1.0E-01, 2.0E-01, 2.4E-01, 2.5E-01, 2.0E-01 !
   1 ! SIGYZI =      3.,      1.5   !
```
!END!

--------

```
  a
   Data for each source are treated as a separate input subgroup
   and therefore must end with an input group terminator.

  b
   0. = No building downwash modeled, 1. = downwash modeled
   NOTE: must be entered as a REAL number (i.e., with decimal point)

  c
   An emission rate must be entered for every pollutant modeled.
   Enter emission rate of zero for secondary pollutants that are
   modeled, but not emitted.  Units are specified by IPTU
   (e.g. 1 for g/s).
```

```
---------------
Subgroup (13c)
---------------

          BUILDING DIMENSION DATA FOR SOURCES SUBJECT TO DOWNWASH
          -------------------------------------------------------
Source                                                                a
 No.      Effective building width and height (in meters) every 10 degrees
------    ----------------------------------------------------------------

 1    ! SRCNAM  =   BLR1 !
 1    ! HEIGHT  = 45.,    45.,    45.,    45.,    45.,    45.,
                  45.,    45.,    45.,    0.,    0.,    0.,
                   0.,    0.,    0.,    0.,    0.,    0.,
                  45.,    45.,    45.,    45.,    45.,    45.,
                  45.,    45.,    45.,    0.,    0.,    0.,
                   0.,    0.,    0.,    0.,    0.,    0.!
 1    ! WIDTH  =  12.5,    12.5,    12.5,    12.5,    12.5,    12.5,
                  12.5,    12.5,    12.5,    0.,    0.,    0.,
                   0.,    0.,    0.,    0.,    0.,    0.,
                  12.5,    12.5,    12.5,    12.5,    12.5,    12.5,
                  12.5,    12.5,    12.5,    0.,    0.,    0.,
                   0.,    0.,    0.,    0.,    0.,    0.!
!END!

--------

     a
   Each pair of width and height values is treated as a separate input
   subgroup and therefore must end with an input group terminator.

---------------
Subgroup (13d)
---------------
                                         a
          POINT SOURCE: VARIABLE EMISSIONS DATA
          -------------------------------------

   Use this subgroup to describe temporal variations in the emission
   rates given in 13b.  Factors entered multiply the rates in 13b.
   Skip sources here that have constant emissions.  For more elaborate
   variation in source parameters, use PTEMARB.DAT and NPT2 > 0.

   IVARY determines the type of variation, and is source-specific:
   (IVARY)                               Default: 0
        0 =        Constant
        1 =        Diurnal cycle (24 scaling factors: hours 1-24)
        2 =        Monthly cycle (12 scaling factors: months 1-12)
        3 =        Hour & Season (4 groups of 24 hourly scaling factors,
                                  where first group is DEC-JAN-FEB)
        4 =        Speed & Stab. (6 groups of 6 scaling factors, where
                                  first group is Stability Class A,
                                  and the speed classes have upper
                                  bounds (m/s) defined in Group 12
        5 =        Temperature   (12 scaling factors, where temperature
                                  classes have upper bounds (C) of:
                                  0, 5, 10, 15, 20, 25, 30, 35, 40,
                                  45, 50, 50+)


 1  ! SRCNAM = BLR1 !
 1  ! IVARY  =  2  !   (12 Months)
 1  ! SO2         = 0.1,0.1,0.5,0.9,2,2.2,
                    2.5,1.5,1.1,0.9,0.5,0.1      !
!END!

--------
     a
   Data for each species are treated as a separate input subgroup
   and therefore must end with an input group terminator.
```

---------------------------------------------------------------------------

INPUT GROUPS: 14a, 14b, 14c, 14d -- Area source parameters
-------------------------------

---------------
Subgroup (14a)
---------------

     Number of polygon area sources with
     parameters specified below (NAR1)      No default  ! NAR1 =  2   !

     Units used for area source
     emissions below          (IARU)       Default: 1  ! IARU =   1  !
           1 =        g/m**2/s
           2 =       kg/m**2/hr
           3 =       lb/m**2/hr
           4 =     tons/m**2/yr
           5 =     Odour Unit * m/s  (vol. flux/m**2 of odour compound)
           6 =     Odour Unit * m/min
           7 =     metric tons/m**2/yr

     Number of source-species
     combinations with variable
     emissions scaling factors
     provided below in (14d)        (NSAR1) Default: 0  !  NSAR1 =  4   !

     Number of buoyant polygon area sources
     with variable location and emission
     parameters (NAR2)                    No default  !  NAR2 = 0    !
     (If NAR2 > 0, ALL parameter data for
     these sources are read from the file: BAEMARB.DAT)

!END!

---------------
Subgroup (14b)
---------------
                                   a
           AREA SOURCE: CONSTANT DATA
           --------------------------
                                                 b
Source          Effect.    Base     Initial    Emission
 No.            Height   Elevation  Sigma z     Rates
                 (m)       (m)        (m)
-------         ------    ------    --------   ---------

   1! SRCNAM = AREA1 !
   1! X =           1.,       0.,         2.5,   8.5E-01,  0.5E00,  0.0E00,
 0.0E00,  0.0E00,  0.0E00,  0.0E00,  0.0E00 !
!END!
   2! SRCNAM = AREA2 !
   2! X =           1.5,      0.,         3.,    0.0E00,  0.0E00, 1.0E-01,
 0.0E00,  0.0E00, 5.0E-01,  1.0E00,  1.3E00 !
!END!

--------
   a
    Data for each source are treated as a separate input subgroup
    and therefore must end with an input group terminator.
   b
    An emission rate must be entered for every pollutant modeled.
    Enter emission rate of zero for secondary pollutants that are
    modeled, but not emitted.  Units are specified by IARU
    (e.g. 1 for g/m**2/s).

```
---------------
Subgroup (14c)
---------------

          COORDINATES (UTM-km) FOR EACH VERTEX(4) OF EACH POLYGON
          -------------------------------------------------------
Source                                                               a
 No.     Ordered list of X followed by list of Y, grouped by source
------    ----------------------------------------------------------

 1    ! SRCNAM  =   AREA1 !
 1       ! XVERT = 0.5,     0.51,    0.51,    0.5!
 1       ! YVERT = 1.61,    1.61,    1.6,     1.6!
!END!
 2    ! SRCNAM  =   AREA2 !
 2       ! XVERT = 0.75,    0.76,    0.76,    0.75!
 2       ! YVERT = 1.81,    1.81,    1.8,     1.8!
!END!

--------
    a
    Data for each source are treated as a separate input subgroup
    and therefore must end with an input group terminator.


---------------
Subgroup (14d)
---------------
                                        a
          AREA SOURCE: VARIABLE EMISSIONS DATA
          ------------------------------------

    Use this subgroup to describe temporal variations in the emission
    rates given in 14b.  Factors entered multiply the rates in 14b.
    Skip sources here that have constant emissions.  For more elaborate
    variation in source parameters, use BAEMARB.DAT and NAR2 > 0.

    IVARY determines the type of variation, and is source-specific:
    (IVARY)                              Default: 0
          0 =       Constant
          1 =       Diurnal cycle (24 scaling factors: hours 1-24)
          2 =       Monthly cycle (12 scaling factors: months 1-12)
          3 =       Hour & Season (4 groups of 24 hourly scaling factors,
                                   where first group is DEC-JAN-FEB
          4 =       Speed & Stab. (6 groups of 6 scaling factors, where
                                   first group is Stability Class A,
                                   and the speed classes have upper
                                   bounds (m/s) defined in Group 12
          5 =       Temperature   (12 scaling factors, where temperature
                                   classes have upper bounds (C) of:
                                   0, 5, 10, 15, 20, 25, 30, 35, 40,
                                   45, 50, 50+)


 2  ! SRCNAM = AREA2 !
 2  ! IVARY  =  4  !    (6 speed classes for each stability)
 2  ! PMSIZE1      = 0.1,0.1,0.5,0.9,1,1.5,
                     0.1,0.1,0.5,0.9,1,1.5,
                     0.1,0.1,0.5,0.9,1,1.5,
                     0.1,0.1,0.5,0.9,1,1.5,
                     0.1,0.1,0.5,0.9,1,1.5,
                     0.1,0.1,0.5,0.9,1,1.5      !
!END!
 2  ! SRCNAM = AREA2 !
 2  ! IVARY  =  4  !    (6 speed classes for each stability)
 2  ! PMSIZE4      = 0.1,0.1,0.5,0.9,1.5,2.2,
                     0.1,0.1,0.5,0.9,1.5,2.2,
                     0.1,0.1,0.5,0.9,1.5,2.2,
                     0.1,0.1,0.5,0.9,1.5,2.2,
                     0.1,0.1,0.5,0.9,1.5,2.2,
                     0.1,0.1,0.5,0.9,1.5,2.2      !
!END!
```

```
 2  ! SRCNAM = AREA2 !
 2  ! IVARY  =  4  !    (6 speed classes for each stability)
 2  ! PMSIZE5      = 0.1,0.1,0.5,0.9,2,2.5,
                     0.1,0.1,0.5,0.9,2,2.5,
                     0.1,0.1,0.5,0.9,2,2.5,
                     0.1,0.1,0.5,0.9,2,2.5,
                     0.1,0.1,0.5,0.9,2,2.5,
                     0.1,0.1,0.5,0.9,2,2.5      !
!END!
 2  ! SRCNAM = AREA2 !
 2  ! IVARY  =  4  !    (6 speed classes for each stability)
 2  ! PMSIZE6      = 0.1,0.1,0.5,0.9,2,2.5,
                     0.1,0.1,0.5,0.9,2,2.5,
                     0.1,0.1,0.5,0.9,2,2.5,
                     0.1,0.1,0.5,0.9,2,2.5,
                     0.1,0.1,0.5,0.9,2,2.5      !
!END!

--------
    a
     Data for each species are treated as a separate input subgroup
     and therefore must end with an input group terminator.
```

--------------------------------------------------------------------------------

INPUT GROUPS: 15a, 15b, 15c -- Line source parameters
--------------------------

---------------
Subgroup (15a)
---------------

```
     Number of buoyant line sources
     with variable location and emission
     parameters (NLN2)                        No default  !  NLN2 =  0   !

     (If NLN2 > 0, ALL parameter data for
      these sources are read from the file: LNEMARB.DAT)

     Number of buoyant line sources (NLINES)    No default   ! NLINES =  2 !

     Units used for line source
     emissions below              (ILNU)       Default: 1 !  ILNU =   1  !
            1 =        g/s
            2 =       kg/hr
            3 =        lb/hr
            4 =      tons/yr
            5 =     Odour Unit * m**3/s  (vol. flux of odour compound)
            6 =     Odour Unit * m**3/min
            7 =     metric tons/yr

     Number of source-species
     combinations with variable
     emissions scaling factors
     provided below in (15c)         (NSLN1) Default: 0 !  NSLN1 =  1  !

     Maximum number of segments used to model
     each line (MXNSEG)                         Default: 7   ! MXNSEG =  7 !

     The following variables are required only if NLINES > 0.  They are
     used in the buoyant line source plume rise calculations.

        Number of distances at which          Default: 6   ! NLRISE =  6  !
        transitional rise is computed

        Average building length (XL)          No default   ! XL = 500. !
                                              (in meters)

        Average building height (HBL)         No default   ! HBL = 22. !
                                              (in meters)

        Average building width (WBL)          No default   ! WBL = 18. !
                                              (in meters)

        Average line source width (WML)       No default   ! WML = 3.2 !
                                              (in meters)

        Average separation between buildings (DXL)  No default   ! DXL = 22. !
                                              (in meters)

        Average buoyancy parameter (FPRIMEL)    No default   ! FPRIMEL = 300. !
                                              (in m**4/s**3)

!END!
```

```
---------------
Subgroup (15b)
---------------

         BUOYANT LINE SOURCE: CONSTANT DATA
         ----------------------------------
                                                                          a
Source     Beg. X      Beg. Y      End. X      End. Y    Release   Base       Emission
  No.    Coordinate  Coordinate  Coordinate  Coordinate  Height    Elevation    Rates
            (km)        (km)        (km)        (km)       (m)       (m)
------   ----------  ----------  ---------  ----------  -------   ---------   ---------
   1! SRCNAM = LINE1 !
   1! X =       12.,        35.,       12.5,        35.,    22.000,      0.000, 2.3E00, 1.1E00, 0.0E00,
 0.0E00, 0.0E00, 0.0E00, 0.0E00, 0.0E00 !
!END!
   2! SRCNAM = LINE2 !
   2! X =       12.,     35.022,       12.5,     35.022,    22.000,      0.000, 2.3E00, 1.1E00, 0.0E00,
 0.0E00, 0.0E00, 0.0E00, 0.0E00, 0.0E00 !
!END!

--------

    a
     Data for each source are treated as a separate input subgroup
     and therefore must end with an input group terminator.

    b
     An emission rate must be entered for every pollutant modeled.
     Enter emission rate of zero for secondary pollutants that are
     modeled, but not emitted.  Units are specified by ILNTU
     (e.g. 1 for g/s).

---------------
Subgroup (15c)
---------------
                                                        a
         BUOYANT LINE SOURCE: VARIABLE EMISSIONS DATA
         --------------------------------------------

    Use this subgroup to describe temporal variations in the emission
    rates given in 15b.  Factors entered multiply the rates in 15b.
    Skip sources here that have constant emissions.

    IVARY determines the type of variation, and is source-specific:
    (IVARY)                                Default: 0
          0 =       Constant
          1 =       Diurnal cycle (24 scaling factors: hours 1-24)
          2 =       Monthly cycle (12 scaling factors: months 1-12)
          3 =       Hour & Season (4 groups of 24 hourly scaling factors,
                                 where first group is DEC-JAN-FEB)
          4 =       Speed & Stab. (6 groups of 6 scaling factors, where
                                 first group is Stability Class A,
                                 and the speed classes have upper
                                 bounds (m/s) defined in Group 12
          5 =       Temperature   (12 scaling factors, where temperature
                                 classes have upper bounds (C) of:
                                 0, 5, 10, 15, 20, 25, 30, 35, 40,
                                 45, 50, 50+)


 1  ! SRCNAM = LINE1 !
 1  ! IVARY  =  1  !    (24 Hours)
 1  ! SO2       = 0.1,0.1,0.1,0.2,0.2,0.3,
                  0.3,0.4,0.4,0.5,0.6,1,
                  1,1,1,1,1,1,
                  0.6,0.4,0.3,0.2,0.1,0.1     !
!END!

--------
    a
     Data for each species are treated as a separate input subgroup
     and therefore must end with an input group terminator.
```

--------------------------------------------------------------------------------

INPUT GROUPS: 16a, 16b, 16c -- Volume source parameters
--------------------------

---------------
Subgroup (16a)
---------------

```
     Number of volume sources with
     parameters provided in 16b,c (NVL1)     No default  ! NVL1 =  1   !

     Units used for volume source
     emissions below in 16b       (IVLU)    Default: 1 ! IVLU =   1  !
           1 =        g/s
           2 =       kg/hr
           3 =       lb/hr
           4 =      tons/yr
           5 =      Odour Unit * m**3/s  (vol. flux of odour compound)
           6 =      Odour Unit * m**3/min
           7 =      metric tons/yr

     Number of source-species
     combinations with variable
     emissions scaling factors
     provided below in (16c)      (NSVL1)   Default: 0 ! NSVL1 =  0  !

     Gridded volume source data
     used ? (IGRDVL)                        No default  ! IGRDVL = 0   !
        0 = no
        1 = yes (gridded volume source
            emissions read from the file:
            VOLEM.DAT)

     The following parameters apply to the data in the
     gridded volume source emissions file (VOLEM.DAT)

       - Effective height of emissions
         (VEFFHT) in meters                 No default  ! VEFFHT = 10. !

       - Initial sigma y (VSIGYI) in
         meters                             No default  ! VSIGYI = 3000. !

       - Initial sigma z (VSIGZI) in
         meters                             No default  ! VSIGZI = 10. !

 !END!
```

---------------
Subgroup (16b)
---------------
```
                                     a
             VOLUME SOURCE: CONSTANT DATA
             ----------------------------
                                                           b
           X UTM      Y UTM     Effect.    Base    Initial   Initial   Emission
         Coordinate Coordinate  Height   Elevation Sigma y   Sigma z    Rates
           (km)       (km)       (m)       (m)       (m)       (m)
         ---------- ---------- ------   ------   --------  --------  --------

     1! SRCNAM = VOLS1 !
 ! X =      -5.6,      -1.2,     10.,       0.,      6.2,      6.2, 2.2E00, 4.0E00, 0.0E00,
  0.0E00, 0.0E00, 0.0E00, 0.0E00, 0.0E00 !
 !END!
```

--------
```
    a
    Data for each source are treated as a separate input subgroup
    and therefore must end with an input group terminator.

    b
    An emission rate must be entered for every pollutant modeled.
    Enter emission rate of zero for secondary pollutants that are
    modeled, but not emitted.  Units are specified by IVLU
    (e.g. 1 for g/s).
```

```
---------------
Subgroup (16c)
---------------
                                             a
           VOLUME SOURCE: VARIABLE EMISSIONS DATA
           ---------------------------------------

    Use this subgroup to describe temporal variations in the emission
    rates given in 16b.  Factors entered multiply the rates in 16b.
    Skip sources here that have constant emissions.  For more elaborate
    variation in source parameters, use VOLEM.DAT and IGRDVL = 1.

    IVARY determines the type of variation, and is source-specific:
    (IVARY)                          Default: 0
        0 =       Constant
        1 =       Diurnal cycle (24 scaling factors: hours 1-24)
        2 =       Monthly cycle (12 scaling factors: months 1-12)
        3 =       Hour & Season (4 groups of 24 hourly scaling factors,
                                 where first group is DEC-JAN-FEB)
        4 =       Speed & Stab. (6 groups of 6 scaling factors, where
                                 first group is Stability Class A,
                                 and the speed classes have upper
                                 bounds (m/s) defined in Group 12
        5 =       Temperature   (12 scaling factors, where temperature
                                 classes have upper bounds (C) of:
                                 0, 5, 10, 15, 20, 25, 30, 35, 40,
                                 45, 50, 50+)



--------
   a
    Data for each species are treated as a separate input subgroup
    and therefore must end with an input group terminator.
```

```
--------------------------------------------------------------------------------

INPUT GROUPS: 17a & 17b -- Non-gridded (discrete) receptor information
-----------------------

---------------
Subgroup (17a)
---------------

     Number of non-gridded receptors (NREC)  No default  !  NREC =  3   !

!END!

---------------
Subgroup (17b)
---------------
                                         a
            NON-GRIDDED (DISCRETE) RECEPTOR DATA
            -----------------------------------

               X UTM       Y UTM      Ground      Height   b
Receptor     Coordinate  Coordinate  Elevation  Above Ground
  No.          (km)        (km)        (m)          (m)
--------     ----------  ----------  ---------  ------------
    1 ! X =        1.,         1.,     12.500,      0.000!   !END!
    2 ! X =        2.5,        4.2,    28.100,      0.000!   !END!
    3 ! X =        2.89,       3.2,    39.600,      0.000!   !END!


-------------
   a
    Data for each receptor are treated as a separate input subgroup
    and therefore must end with an input group terminator.

   b
    Receptor height above ground is optional.  If no value is entered,
    the receptor is placed on the ground.
```

Table 4-3
CALPUFF Control File Inputs - Input Group 0
Input and Output File Names

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| NMETDAT | integer | Number of CALMET files; if more than 1 CALMET file is used, all names must be placed in Subgroup 0a | 1 |
| | | Input Files | |
| METDAT | character*70 | Meteorological data file created by CALMET | CALMET.DAT |
| ISCDAT | character*70 | Meteorological data file in ISC3 format or extended ISC3 format | ISCMET.DAT |
| PLMDAT | character*70 | Meteorological data file in AUSPLUME format or extended AUSPLUME format | PLMMET.DAT |
| PRFDAT | character*70 | Meteorological data file in CTDM profile format | PROFILE.DAT |
| SFCDAT | character*70 | Meteorological data file in CTDM surface format | SURFACE.DAT |
| RSTARTB | character*70 | Model restart file read at beginning of run | RESTARTB.DAT |
| PTDAT | character*70 | Arbitrarily-varying point source emissions file | PTEMARB.DAT |
| VOLDAT | character*70 | Arbitrarily-varying gridded volume source emissions file | VOLEM.DAT |
| ARDAT | character*70 | Arbitrarily-varying buoyant area source emissions file | BAEMARB.DAT |
| LNDAT | character*70 | Arbitrarily-varying buoyant line source emissions file | LNEMARB.DAT |
| OZDAT | character*70 | Hourly ambient ozone measurement file | OZONE.DAT |
| VDDAT | character*70 | User-specified deposition velocity file | VD.DAT |
| CHEMDAT | character*70 | User-specified chemical transformation rate file | CHEM.DAT |
| HILLDAT | character*70 | Subgrid-scale terrain (hill) file in CTDM format | HILL.DAT |
| RCTDAT | character*70 | Subgrid-scale terrain receptor file in CTDM format | HILLRCT.DAT |
| CSTDAT | character*70 | Subgrid-scale coastal boundary file | COASTLN.DAT |
| BDYDAT | character*70 | Mass flux boundary file | FLUXBDY.DAT |
| | | Output Files | |
| PUFLST | character*70 | CALPUFF list file | CALPUFF.LST |
| CONDAT | character*70 | CALPUFF output concentration file | CONC.DAT |
| DFDAT | character*70 | CALPUFF output dry deposition flux file | DFLX.DAT |
| WFDAT | character*70 | CALPUFF output wet deposition flux file | WFLX.DAT |
| VISDAT | character*70 | Output relative humidity file (needed for visibility calculations in CALPOST) | VISB.DAT |

Table 4-3 (Continued)
CALPUFF Control File Inputs - Input Group 0
Input and Output File Names

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| RSTARTE | character*70 | Model restart file written during run | RESTARTE.DAT |
| DEBUG | character*70 | Puff-tracking data file (created only if LDEBUG = .TRUE. - see Input Group 5) | DEBUG.DAT |
| FLXDAT | character*70 | Mass flux output (hourly) | MASSFLX.DAT |
| BALDAT | character*70 | Mass balance output (hourly) | MASSBAL.DAT |

Input Group 0 consists of two parts.  The first part contains the control variable NMETDAT and all of the filenames listed above.  The second part, Input Group 0a, is only needed when more than one CALMET file is used in the simulation.  If a number of separate CALMET simulations are made to span the full modeling period, this feature allows a single application of CALPUFF to use all of the CALMET simulations in sequence.  This feature is signaled by an NMETDAT value greater than one.

If you have no CALMET file (i.e., you are using one of the other options for providing meteorological data to CALPUFF such as ISC meteorological data), set NMETDAT=0:

```
INPUT GROUP: 0 -- Input and Output File Names

     Number of CALMET.DAT files for run (NMETDAT)
                                   Default: 1        ! NMETDAT =   0   !

--------------
Default Name  Type          File Name
------------  ----          ---------
CALMET.DAT    input    * METDAT =              *
    or
ISCMET.DAT    input     ! ISCDAT = ISCMET.DAT  !
```

If you have a single CALMET file, set NMETDAT=1:

```
INPUT GROUP: 0 -- Input and Output File Names

     Number of CALMET.DAT files for run (NMETDAT)
                                   Default: 1        ! NMETDAT =   1   !

--------------
Default Name  Type          File Name
------------  ----          ---------
CALMET.DAT    input    ! METDAT = CALMET.DAT   !
     or
ISCMET.DAT     input     * ISCDAT =               *
```

If you have 3 CALMET files, set NMETDAT=3:

```
INPUT GROUP: 0 -- Input and Output File Names

     Number of CALMET.DAT files for run (NMETDAT)
                                   Default: 1        ! NMETDAT =   3   !

--------------
Default Name  Type          File Name
------------  ----          ---------
CALMET.DAT    input    * METDAT =            *
     or
ISCMET.DAT     input     * ISCDAT =                *
```

and provide all of the CALMET file names in Input Group 0a:

```
-------------
Subgroup (0a)
-------------

  The following CALMET.DAT filenames are processed in sequence if NMETDAT>1

Default Name Type         File Name
------------ ----         ---------
 none        input    ! METDAT= CALMET1.DAT    !         !END!
 none         input    ! METDAT= CALMET2.DAT     !          !END!
 none         input    ! METDAT= CALMET3.DAT     !          !END!
```

Note that each filename entered in Input Group 0a is treated as a separate input subgroup and therefore must end with the input group terminator (!END!). A total of NMETDAT lines assigning the CALMET file names must be present, and the names must be ordered in the proper sequence (e.g., CALMET results for June must not precede CALMET results for February).

Table 4-3 (Continued)
CALPUFF Control File Inputs - Input Group 1
General Run Control Parameters

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| METRUN | integer | Control parameter for running all periods in met. file (0=no; 1=yes) | 0 |
| IBYR | integer | Starting year of the CALPUFF run (four digits) | - |
| IBMO | integer | Starting month | - |
| IBDY | integer | Starting day | - |
| IBHR | integer | Starting hour (time at end of hour: 00-23) | - |
| IRLG | integer | Length of the run (hours) | - |
| NSPEC | integer | Total number of species modeled | 5 |
| NSE | integer | Number of species emitted | 3 |
| ITEST | integer | Flag to stop run after the setup phase (1 = stops the program, 2 = continues with execution after setup) | 2 |
| MRESTART | integer | Restart control may direct model to read and/or write a file of puff data which allows a run to be segmented<br>0 = Do not read or write a restart file<br>1 = Read a restart file at the beginning of the run<br>2 = Write a restart file during run<br>3 = Read a restart file at beginning of run and write a restart file during run | 0 |
| NRESPD | integer | Number of periods in restart output cycle; a restart file that is written during the run is refreshed at the end of every cycle<br>  0 = File written only at last period<br>>0 = File updated every NRESPD periods | 0 |
| METFM | integer | Meteorological data format<br>1 = CALMET unformatted file (CALMET.DAT)<br>2 = ISC3 ASCII file (ISCMET.DAT)<br>3 = AUSPLUME ASCII file (PLMMET.DAT)<br>4 = CTDMPLUS tower file (PROFILE.DAT) and surface parameters file (SURFACE.DAT) | 1 |
| AVET | real | Averaging time (minutes)<br>PG - $\sigma_y$ is adjusted by the equation $(AVET/PGTIME)^{0.2}$ | 60.0 |
| PGTIME | real | Averaging time (minutes) for PG - $\sigma_y$ | 60.0 |

| Variable | Type | Description | Default Value |
|---|---|---|---|
| MGAUSS | integer | Control variable determining the vertical distribution used in the near field (0 = uniform, 1 = Gaussian) | 1 |
| MCTADJ | integer | Terrain adjustment method 0 = no adjustment 1 = ISC-type of terrain adjustment 2 = simple, CALPUFF-type of terrain adjustment 3 = partial plume path adjustment | 3 |
| MCTSG | integer | CALPUFF subgrid scale complex terrain module (CTSG) flag (0 = CTSG not modeled, 1 = CTSG modeled) | 0 |
| MSLUG | integer | Near-field puffs are modeled as elongated "slugs" ? (0 = no, 1 = yes) | 0 |
| MTRANS | integer | Transitional plume rise modeled ? (0 = only final rise computed, 1 = transitional rise computed)  Note:  Transitional plume rise is always computed for sources subject to building downwash effects. | 1 |
| MTIP | integer | Stack tip downwash modeled ? 0 = no (i.e., no stack tip downwash) 1 = yes (i.e., use stack tip downwash) | 1 |
| MSHEAR | integer | Vertical wind shear above stack top modeled in plume rise? (0 = no, 1 = yes) | 0 |
| MSPLIT | integer | Puff splitting allowed ? (0 = no, 1 = yes) | 0 |
| MCHEM | integer | Chemical mechanism flag. 0 = chemical transformation not modeled 1 = transformation rates computed internally (MESOPUFF II scheme) 2 = user specified transformation rates used (If MCHEM = 2, the user must prepare a file (CHEM.DAT) with a diurnal cycle of transformation rates) 3 = transformation rates computed internally (RIVAD/ARM3 scheme) | 1 |
| MWET | integer | Wet removal modeled ? (0 = no, 1 = yes) | 1 |

| Variable | Type | Description | Default Value |
|---|---|---|---|
| MDRY | integer | Dry deposition modeled ?<br>(0 = no, 1 = yes)<br>Note:  The method used to determine dry deposition velocities is specified by the user on a species-by-species basis in Input Group 3. | 1 |
| MDISP | integer | Method used to compute the horizontal and vertical dispersion coefficients<br>1 = computed from values of $\sigma_v$ and $\sigma_w$ from the PROFILE.DAT file<br>2 = computed from $\sigma_v$ and $\sigma_w$ which are calculated internally from the micrometeorological variables ($u_*$, $w_*$, L, etc.)<br>3 = PG dispersion coefficients used in RURAL areas (computed using the ISCST multi-segment approximation) and MP coefficients used in URBAN areas<br>4 = same as 3 except PG coefficients computed using the MESOPUFF II equations<br>5 = CTDM sigmas used for stable and neutral conditions for unstable conditions, sigmas are computed as in MDISP = 1.  MDISP = 5 assumes that $\sigma_v$ and $\sigma_w$ are read from PROFILE.DAT file. | 3 |
| MTURBV W | integer | Sigma-v/sigma-theta, sigma-w measurements used? (Used only if MDISP = 1 or 5)<br>1 = use sigma-v or sigma-theta measurements from PROFILE.DAT to compute sigma-y (valid for METFM = 1, 2, 3, 4)<br>2 = use sigma-w measurements from PROFILE.DAT to compute sigma-z (valid for METFM = 1, 2, 3, 4)<br>3 = use both sigma-(v/theta) and sigma-w from PROFILE.DAT to compute sigma-y and sigma-z (valid for METFM = 1, 2, 3, 4)<br>4 = use sigma-theta measurements from PLMMET.DAT to compute sigma-y (valid only if METFM = 3) | 3 |

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| MDISP2 | integer | Back-up method used to compute dispersion when measured turbulence data are missing (used only if MDISP = 1 or 5)<br>2 = computed from $\sigma_v$ and $\sigma_w$ which are calculated internally from the micrometeorological variables ($u_*$, $w_*$, L, etc.)<br>3 = PG dispersion coefficients used in RURAL areas (computed using the ISCST multi-segment approximation) and MP coefficients used in URBAN areas<br>4 = same as 3 except PG coefficients computed using the MESOPUFF II equations | 3 |
| MROUGH | integer | PG $\sigma_y$ and $\sigma_z$ adjusted for surface roughness ?<br>(0 = no, 1 = yes) | 0 |
| MPARTL | integer | Partial plume penetration of elevated inversion?<br>(0 = no, 1 = yes) | 1 |
| MTINV | integer | Strength of temperature inversion provided in PROFILE.DAT extended records?<br>(0 = no, computed from gradients; 1= yes) | 0 |
| MPDF | integer | Probability Distribution Function method used for dispersion in the convective boundary layer?<br>(0 = no, 1 = yes) | 0 |
| MSGTIBL | integer | Subgrid scale TIBL module used for shoreline?<br>(0 = no, 1 = yes) | 0 |

Table 4-3 (Continued)
CALPUFF Control File Inputs - Input Group 2
Technical Options

| Variable | Type | Description | Default Value |
|---|---|---|---|
| MREG | integer | Check options for Regulatory values? | 1 |
| | | 0 = NO checks are made | |
| | | 1 = Technical options must conform to USEPA values | |
| | |     METFM    1 | |
| | |     AVET    60. (Min) | |
| | |     MGAUSS    1 | |
| | |     MCTADJ    3 | |
| | |     MTRANS    1 | |
| | |     MTIP    1 | |
| | |     MCHEM    1 (if modeling SOx, NOx) | |
| | |     MWET    1 | |
| | |     MDRY    1 | |
| | |     MDISP    3 | |
| | |     MROUGH    0 | |
| | |     MPARTL    1 | |
| | |     SYTDEP    550. (m) | |
| | |     MHFTSZ    0 | |

Table 4-3 (Continued)
Control File Inputs - Input Group 3
Species List

Input Group 3 consists of two parts. The first part contains a list of species names and a table with four integer flags for each species. These flags indicate if a pollutant is modeled (0=no, 1=yes), emitted (0=no, 1=yes), dry deposited (0=no, 1=yes, treated as a gas with the resistance model, 2=yes, treated as a particle with the resistance model, or 3=yes, user-specified deposition velocities used), and if the species is to be added to group for output by specifying a group number greater than zero. The second part allows one to name the output species groups, if any are identified in the table.

However, the user must first specify the species names to be modeled. Each species is entered on a separate line with ! CSPEC = XXX ! !END!, where XXX is a species name (up to 12 characters in length), and the variable delimiter and group delimiter (!END!) appears on the line. For example, a five-species $SO_x$, $NO_x$ run with MCHEM=1 would be:

```
INPUT GROUP: 3a, 3b  --  Species list
------------------


-------------
Subgroup (3a)
-------------


        ! CSPEC = SO2  !        !END!
        ! CSPEC = SO4  !        !END!
        ! CSPEC = NOX  !        !END!
        ! CSPEC = HNO3 !        !END!
        ! CSPEC = NO3  !        !END!
```

The MESOPUFF II chemical transformation option (MCHEM=1) in CALPUFF is designed to simulate the conversion of $SO_2 \rightarrow SO_4^=$ and $NO_x \rightarrow HNO_3 \leftrightarrow NO_3^-$. For this option, five pollutants in CALPUFF are labeled as $SO_2$, $SO_4^=$, $NO_x$, $HNO_3$, and $NO_3^-$. If the RIVAD/ARM3 transformation option (MCHEM=3) is selected, NO and $NO_2$ are explicitly treated, and six pollutants are labeled as $SO_2$, $SO_4^=$, NO, $NO_2$, $HNO_3$, and $NO_3^-$. However, by setting the appropriate flags controlling the various technical options (chemical transformation, deposition, etc.), other reactive or non-reactive pollutants can be simulated.

The user has control over which species are to be emitted and dry deposited in a particular run. If the dry deposition flag is set equal to 3 for any pollutant, a file called VD.DAT must be made available to the model. This file contains a diurnal cycle of 24 user-specified deposition velocities for each pollutant flagged.

Table 4-3 (Continued)
Control File Inputs - Input Group 3
Species List

Species-groups can be used to allow mass distributions of particles to be source-specific.  In the example provided in Table 4-2, we have defined six particle-sizes as individual species:

```
! CSPEC =          SO2 !          !END!
! CSPEC =          NOX !          !END!
! CSPEC =      PMSIZE1 !          !END!
! CSPEC =      PMSIZE2 !          !END!
! CSPEC =      PMSIZE3 !          !END!
! CSPEC =      PMSIZE4 !          !END!
! CSPEC =      PMSIZE5 !          !END!
! CSPEC =      PMSIZE6 !          !END!

                                           Dry              OUTPUT GROUP
     SPECIES        MODELED        EMITTED        DEPOSITED          NUMBER
      NAME       (0=NO, 1=YES)  (0=NO, 1=YES)  (0=NO,             (0=NONE,
     (Limit: 12                                 1=COMPUTED-GAS    1=1st CGRUP,
     Characters                                 2=COMPUTED-PARTICLE  2=2nd CGRUP,
     in length)                                 3=USER-SPECIFIED)  3= etc.)

!          SO2 =          1,            1,            1,             0   !
!          NOX =          1,            0,            2,             0   !
!      PMSIZE1 =          1,            1,            2,             1   !
!      PMSIZE2 =          1,            1,            2,             1   !
!      PMSIZE3 =          1,            1,            2,             1   !
!      PMSIZE4 =          1,            1,            2,             1   !
!      PMSIZE5 =          1,            1,            2,             1   !
!      PMSIZE6 =          1,            1,            2,             1   !

!END!
```

This allows each size to be modeled separately, each with its own mass emission rate and deposition velocity.  Several sources in the run could have been given different emission rates for these "species", thereby producing unique mass distributions for their particulate emissions.  Prior to reporting any concentrations or deposition fluxes for these individual "species", however, they must be summed to provide the total particulate concentration or deposition flux.  This is done through "grouping":

```
-------------
Subgroup (3b)
-------------

! CGRUP =          PM10 !      !END!
```

Table 4-3 (Continued)
Control File Inputs - Input Group 3
Species List

In this case, the species-group name provided to characterize the total concentration is "PM10".  Only one group name is required because only one non-zero group number was given in Input Group 3a.  This group name must be used later in Input Group 5 when selecting output options for the particulates, and this is the name that will be written to the output files (the list file as well as the concentration/flux files used by the postprocessor).  Note that any species not assigned to a non-zero species-group retain the initial species name in the output.  Also, the order of names provided in Input Group 3b must be consistent with the group numbers provided in Input Group 3a.

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| NX | integer | Number of grid cells in the X direction of the meteorological grid | - |
| NY | integer | Number of grid cells in the Y direction of the meteorological grid | - |
| DGRIDKM | real | Grid spacing (km) of the meteorological grid | - |
| XORIGKM | real | Reference X coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid | - |
| YORIGKM | real | Reference Y coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid | - |
| IUTMZN | integer | UTM zone of coordinates | - |
| XLAT | real | Reference latitude (deg.) of the center of the modeling domain (used in solar elevation angle calculations). Positive for the northern hemisphere, negative for the southern hemisphere. | - |
| XLONG | real | Reference longitude (deg.) of the center of the modeling domain. Positive for west longitude, negative for east longitude. | - |
| XTZ | real | Reference time zone of the center of the modeling domain (PST=8., MST=7., CST=6., EST=5.) | - |
| NZ | integer | Number of vertical layers | - |
| ZFACE | real array | Cell face heights (m) for the meteorological grid (NX + 1 values must be entered). Note: Cell center (grid point) height of layer "i" is ((ZFACE(i+1) + (ZFACE(i))/2). | - |
| IBCOMP | integer | X index of lower left corner of the computational grid ($1 \le$ IBCOMP $\le$ NX) | - |
| JBCOMP | integer | Y index of lower left corner of the computational grid ($1 \le$ JBCOMP $\le$ NY) | - |

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| IECOMP | integer | X index of upper right corner of the computational grid (IBCOMP ≤ IECOMP ≤ NX) | - |
| JECOMP | integer | Y index of upper right corner of computational grid (JBCOMP ≤ JECOMP ≤ NY) | - |
| LSAMP | integer | Flag indicating if an array of gridded receptors (i.e., sampling grid) is used (T = yes, F = no) | T |
| IBSAMP | integer | X index of lower left corner of the sampling grid (IBCOMP ≤ IBSAMP ≤ IECOMP) | - |
| JBSAMP | integer | Y index of lower left corner of the sampling grid (JBCOMP ≤ JBSAMP ≤ JECOMP) | - |
| IESAMP | integer | X index of upper right corner of the sampling grid (IBCOMP ≤ IESAMP ≤ IECOMP) | - |
| JESAMP | integer | Y index of upper right corner of the sampling gird (JBCOMP ≤ JESAMP ≤ JECOMP) | - |
| MESHDN | integer | Nesting factor of the sampling grid (MESHDN ≥ 1). The grid spacing of the sampling grid is DGRIDKM/MESHDN. The number of sampling grid points is NXSAM * NYSAM, where NXSAM = MESHDN * (IESAMP - IBSAMP) + 1 NYSAM = MESHDN * (JESAMP - JBSAMP) + 1 | 1 |

| Variable | Type | Description | Default Value |
|---|---|---|---|
| ICON | integer | Control variable for creation of an output disk file (CONC.DAT) containing concentration fields (species stored in this file are controlled by the output species table described below).<br>(0 = do not create CONC.DAT,<br> 1 = create CONC.DAT) | 1 |
| IDRY | integer | Control variable for creation of an output disk file (DFLX.DAT) containing dry flux fields.  (The species stored in this file are controlled by the output species table in Input Group 5 described below.)<br>(0 = do not create DFLX.DAT,<br> 1 = create DFLX.DAT) | 1 |
| IWET | integer | Control variable for creation of an output disk file (WFLX.DAT) containing wet flux fields.  (The species stored in this file are controlled by the output species table in Input Group 5 described below.)<br>(0 = do not create WFLX.DAT,<br> 1 = create WFLX.DAT) | 1 |
| IVIS | integer | Control variable for creation of an output disk file containing relative humidity data required for visibility applications | 1 |
| LCOMPRS | logical | Control for data compression in the output files (should usually be TRUE) | T |
| IMFLX | integer | Control variable for creating output disc file (MASSFLX.DAT) for mass flux across user-specified boundaries<br>(0 = do not create MASSFLX.DAT,<br> 1 = create MASSFLX. DAT) | 0 |
| IMBAL | integer | Control variable for creating output disk file (MASSBAL.DAT) for mass balance results<br>(0 = do not create MASSBAL.DAT,<br> 1 = create MASSBAL. DAT) | 0 |
| ICPRT | integer | Control variable for printing of concentration fields to the output list file (CALPUFF.LST).<br>(0 = do not print any dry fluxes,<br> 1 = print dry fluxes indicated in output table) | 0 |
| IDPRT | integer | Control variable for printing of dry flux fields to the output list file (CALPUFF.LST).<br>(0 = do not print any dry fluxes,<br> 1 = print dry fluxes indicated in output table) | 0 |

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| IWPRT | integer | Control variable for printing of wet flux fields to the output list file (CALPUFF.LST). (0 = do not print any wet fluxes, 1 = print wet fluxes indicated in output table)     0 | 0 |
| ICFRQ | integer | Printing interval for the concentration fields. Concentrations are printed every "ICFRQ" hours. (Used only if ICPRT = 1.) | 1 |
| IDFRQ | integer | Printing interval for the dry flux fields. Dry fluxes are printed every "IDFRQ" hours. (Used only if IDPRT = 1.) | 1 |
| IWFRQ | integer | Printing interval for the wet flux fields. Wet fluxes are printed every "IWFRQ" hours. (Used only if IWPRT = 1.) | 1 |
| IMESG | integer | Control variable determining if messages tracking the progress of the run are written to the screen (0 = not written, 1 = written). | 1 |
| IPRTU | integer | Control variable for selecting units used for concentrations and deposition fluxes reported in the list file | 1 |
| LDEBUG | logical | Control variable for activation of "debug" write statements | F |
| IPFDEB | integer | Puff ID number to start tracking in debug option (used only if LDEBUG = T) | 1 |
| NPFDEB | integer | Number of puffs to track in debug option (used only if LDEBUG = T) | 1 |
| NN1 | integer | Time period (hour) to begin debug output (used only if LDEBUG = T) | 1 |
| NN2 | integer | Time period (hour) to stop debug output (used only if LDEBUG = T) | 10 |

For IPRTU:

|  | Concentration | Deposition |
|--|---------------|------------|
| 1 = | g/m**3 | g/m**2/s |
| 2 = | mg/m**3 | mg/m**2/s |
| 3 = | ug/m**3 | ug/m**2/s |
| 4 = | ng/m**3 | ng/m**2/s |
| 5 = | Odour Units | |

In addition to the variables described above, Input Group 5 also contains a table of species with a series of flags indicating if the pollutant's concentration and wet/dry flux fields are to be printed to the output list file (CALPUFF.LST) and/or stored in the output disk files (CONC.DAT, DFLX.DAT, WFLX.DAT, and MASSFLX.DAT).

The format of the species output table is shown below. A value of 0 indicates "no", and a value of 1 indicates "yes". Note that the names provided here must be the ouput species names, which would be the species-group names if any species were grouped in Input Group 4.

```
     SPECIES (or GROUP for combined species) LIST FOR OUTPUT OPTIONS

              ---- CONCENTRATIONS ----  ------ DRY FLUXES ------  ------ WET FLUXES ------  -- MASS FLUX --
    SPECIES
    /GROUP     PRINTED?  SAVED ON DISK?  PRINTED?  SAVED ON DISK?  PRINTED?  SAVED ON DISK?  SAVED ON DISK?
    -------    ----------------------    ----------------------    ----------------------    ---------------
!       SO2 =    1,          1,            0,          1,            0,          0,              0   !
!       NOX =    1,          1,            0,          1,            0,          0,              0   !
!      PM10 =    1,          1,            0,          1,            0,          0,              0   !
```

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| **(Input Group 6a - General CTSG Parameters)** | | | |
| NHILL | integer | Number of subgrid scale terrain features | 0 |
| NCTREC | integer | Number of special subgrid scale complex terrain receptors | 0 |
| MHILL | integer | Terrain and receptor data for CTSG hills input in CTDM format ? (1 = data created by CTDM processors and read from HILL.DAT and HILLRCT.DAT files;  2 = hill data created by OPTHILL & input below in Subgroup (6b)). | - |
| XHILL2M | real | Factor to convert horizontal dimensions to meters (used only if MHILL = 1) | 1.0 |
| ZHILL2M | real | Factor to convert vertical dimensions to meters (used only if MHILL = 1) | 1.0 |
| XCTDMKM | real | X-origin of CTDM system relative to CALPUFF coordinate system, in Kilometers (MHILL = 1) | - |
| YCTDMKM | real | Y-origin of CTDM system relative to CALPUFF coordinate system, in Kilometers (MHILL = 1) | - |
| **(Input Group 6b - Hill Information)** | | | |
| XC | real | UTM X coordinate (km) of the center of the hill on the meteorological grid | - |
| YC | real | UTM Y coordinate (km) of the center of the hill on the meteorological grid | - |
| THETAH | real | Orientation of the major axis of the hill (in degrees) clockwise from north | - |
| ZGRID | real | Height (m) of the "zero-plane" of the grid above mean sea level | - |
| RELIEF | real | Height (m) of the crest of the hill above the grid elevation | - |
| EXPO1 | real | Hill shape exponent for the major axis of the hill | - |
| EXPO2 | real | Hill shape exponent for the minor axis of the hill | - |
| SCALE1 | real | Horizontal length scale of the hill along the major axis | - |
| SCALE2 | real | Horizontal length scale of the hill along the minor axis | - |
| AMAX1 | real | Maximum allowed axis length of the major axis of the hill | - |
| AMAX2 | real | Maximum allowed axis length of the minor axis of the hill | - |

The variables in Input Group 6b are entered for each of the "NHILL" subgrid scale hills treated in the model run.  <u>The data for each hill is treated as a separate input subgroup, and therefore must end with an input group terminator (i.e., !END!)</u>.  The format of Input Group 6b is shown below.

```
------------------
Subgroup (6b)
------------------

                      1 **
     HILL INFORMATION
```

| HILL NO. | XC (km) | YC (km) | THETAH (deg.) | ZGRID (m) | RELIEF (m) | EXPO 1 (m) | EXPO 2 (m) | SCALE 1 (m) | SCALE 2 (m) | AMAX1 (m) | AMAX2 (m) | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 ! HILL = | 170.5, | 3841.0 , | 69. , | 1310. , | 300. , | 1.91 , | 1.24 , | 1523. , | 2896. , | 2000., | 1500. ! | !END! | |
| 2 ! HILL = | 173.0, | 3839.0 , | 49. , | 1310. , | 230. , | 1.50 , | 1.50 , | 3000. , | 1000. , | 4000., | 2000. ! | !END! | |

Note that the hill number is an optional user comment which is outside of the delimiters containing the required data.  The data for each hill must follow the opening delimiter and "HILL=".  The data for each hill is followed by a closing delimiter and an input group terminator (i.e., !END!).

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| | | **(Input Group 6c - CTSG Receptor Data)** | |
| XRCT | real | UTM X coordinate (km) on the meteorological grid system of a CTSG receptor | - |
| YRCT | real | UTM Y coordinate (km) on the meteorological grid system of a CTSG receptor | - |
| ZRCT | real | Height (m) of the ground above mean sea level at the CTSG receptor | - |
| XHH | real | Hill number associated with this CTSG receptor | - |

The variables in Input Group 6c are entered for each of the "NCTREC" complex terrain receptors in the model run. <u>The data for each receptor is treated as a separate input subgroup, and therefore must end with an input group terminator (i.e., !END!)</u>. The format of Input Group 6c is shown below.

```
-----------------
Subgroup (6c)
-----------------

                                              1  **
      COMPLEX TERRAIN RECEPTOR INFORMATION

              XRCT     YRCT     ZRCT      XHH
              (km)     (km)     (m)
              ------   ------   --------   ------
! CTREC =    170.5,   3840.0 ,   1430. ,    1. !  !END!
! CTREC =    169.0,   3840.5 ,   1430. ,    1. !  !END!
! CTREC =    170.5,   3841.0 ,   1580. ,    1. !  !END!
! CTREC =    173.5,   3840.0 ,   1525. ,    2. !  !END!
! CTREC =    172.5,   3840.0 ,   1430. ,    2. !  !END!


------------------
```

** The data for each CTSG receptor must follow an opening delimiter and "CTREC=". The data for each receptor is followed by a closing delimiter and an input group terminator (i.e., !END!).

Table 4-3 (Continued)
CALPUFF Control File Inputs - Input Group 7
Dry Deposition Parameters - Gases

Input Group 7 consists of a table containing the following five parameters which are required by the resistance deposition model for computing deposition velocities for gases:

- Pollutant diffusivity ($cm^2/s$)
- Aqueous phase dissociation constant, $\alpha_*$
- Pollutant reactivity
- Mesophyll resistance, $r_m$ (s/cm)
- Henry's Law coefficient, H (dimensionless)

These parameters must be specified for each pollutant with a dry deposition flag of "1" in the species list (Input Group 3) indicating the use of the resistance model for a gas.

The format of the input table is shown below:

```
-------------------------------------------------------------------------------------------------------------------------------

INPUT GROUP: 7 -- Chemical parameters for dry deposition of gases
-------------------------

SPECIES     DIFFUSIVITY    ALPHA STAR    REACTIVITY    MESOPHYLL RESISTANCE    HENRY'S LAW COEFFICIENT
 NAME       (cm**2/s)                                         (s/cm)                (dimensionless)

----------  ----------------  ------------------  ------------------  ------------------------------------  ----------------------------------------

! SO2  =      0.1509    ,     1.00E3   ,      8.0   ,           0.0      ,                 4.e-2     !
! NOX  =      0.1656    ,     1.00     ,      8.0   ,           5.0      ,                 3.5       !
! HNO3 =      0.1628    ,     1.00     ,     18.0   ,           0.0      ,                 8.e-8     !

!END!
```

Input Group 8 consists of a table containing the geometric mass mean diameter (microns) and the geometric standard deviation (microns) required by the resistance deposition model for computing deposition velocities for particulate matter.

These parameters must be specified for each pollutant with a dry deposition flag of "2" in the species list (Input Group 3) indicating the use of the resistance model for a pollutant deposited as particulate matter.

The format of the input table is shown below:

```
--------------------------------------------------------------------------------------------------------------------------------------------------------

INPUT GROUP: 8 -- Size parameters for dry deposition of particles
------------------

SPECIES        GEOMETRIC MASS MEAN          GEOMETRIC STANDARD
 NAME               DIAMETER                    DEVIATION
                    (microns)                    (microns)

-----------    ---------------------------    -------------------------------
! SO4   =            0.48          ,               2.00   !
! NO3   =            0.48          ,               2.00   !


!END!
```

| Variable | Type | Description | Default Value |
|---|---|---|---|
| RCUTR | real | Reference cuticle resistance (s/cm) | 30. |
| RGR | real | Reference ground resistance (s/cm) | 10. |
| REACTR | real | Reference pollutant reactivity | 8. |
| NINT | integer | Number of particle-size intervals used to evaluate effective particle deposition velocity | 9 |
| IVEG | integer | Flag specifying the state of vegetation in unirrigated areas<br>1 = vegetation is active and unstressed<br>2 = vegetation is active and stressed<br>3 = vegetation is inactive | 1 |

Input Group 10 consists of a table containing pollutant-dependent values of the scavenging coefficient, $\lambda$, for both liquid and frozen precipitation types.  The format of the input table is shown below.

```
--------------------------------------------------------------------------------------------

INPUT GROUP: 10 -- Wet Deposition Parameters
--------------------------

                           Scavenging Coefficient -- Units: (sec)⁻¹

        Pollutant        Liquid Precip.        Frozen Precip.
        ------------     ----------------      -----------------
        !  SO2    =        3.0e-5          ,       0.0           !
        !  SO4    =        10.0e-5         ,       3.0e-5        !
        !  NOX    =        0.0             ,       0.0           !
        !  HNO3   =        6.0e-5          ,       0.0           !
        !  NO3    =        10.0e-5         ,       3.0e-5        !

    !END!
```

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| MOZ | integer | Control variable for the input of hourly ozone data used in the chemical transformation module<br>(Used only if MCHEM = 1,3)<br>　0 = use a constant background ozone value<br>　　in chemistry calculation<br>　1 = use hourly ozone concentrations from<br>　　the OZONE.DAT data file | 1 |
| BCKO3 | real | Background ozone concentration in ppb<br>(Used only if MCHEM=1,3 and MOZ = 0 or if (MOZ=1 and all hourly ozone data are missing)) | 80. |
| BCKNH3 | real | Background ammonia concentration in ppb | 10. |
| RNITE1 | real | Nighttime $SO_2$ loss rate in percent/hour | 0.2 |
| RNITE2 | real | Nighttime $NO_x$ loss rate in percent/hour | 2.0 |
| RNITE3 | real | Nighttime $HNO_3$ formation rate in percent/hour | 2.0 |

| Variable | Type | Description | Default Value |
|---|---|---|---|
| SYTDEP | real | Horizontal size of a puff (m) beyond which the time-dependent dispersion equation of Heffter (1965) | 550. |
| MHFTRZ | integer | Use Heffter formulas for $\sigma_z$ ? (0 = no; 1 = yes). If yes, the distance at which the Heffter formula will be applied for $\sigma_z$ is determined by when $\sigma_y$ switches to Heffter's eqn. (see SYTDEP). | 0 |
| JSUP | integer | Stability class used to determine dispersion rates for puffs above the boundary layer (e.g., 6 = F stability) | 5 |
| CONK1 | real | Vertical dispersion constant for stable conditions | 0.01 |
| CONK2 | real | Vertical dispersion constant for neutral/unstable conditions | 0.10 |
| TBD | real | Factor for determining transition-point from Schulman-Scire to Huber-Snyder Building Downwash scheme (SS used for Hs < Hb + TBD * HL)<br>TBD < 0    always use Huber-Snyder<br>TBD = 1.5   always use Schulman-Scire<br>TBD = 0.5   ISC transition-point | 0.5 |
| IURB1, IURB2 | integer | Land use categories associated with urban areas. If MDISP = 3 or 4, MP dispersion coefficients are used when puff is over land use type IURB1 through IURB2 | 10,19 |
| **(Site characterization parameters for single-point met. data files*)** | | | |
| *ILANDUIN | integer | Land use category for modeling domain | 20 |
| *Z0IN | real | Roughness length (m) for modeling domain | 0.25 |
| *XLAIIN | real | Leaf area index for modeling domain | 3.0 |
| *ELEVIN | real | Elevation (m) above sea level | 0.0 |
| *XLATIN | real | North Latitude (deg) of station; positive for the northern hemisphere, negative for the southern hemisphere (used for solar angle in RIVAD/ARM3 chem. transformation) | -999. |
| *XLONIN | real | West Longitude (deg) of station; positive west of 0.0, negative east of 0.0 (used for solar angle in RIVAD/ARM3 chem. transformation) | -999. |
| *ANEMHT | real | Anemometer height (m) (used only if METFM = 2,3) | 10.0 |

## Table 4-3 (Continued)
## CALPUFF Control File Inputs - Input Group 12
## Dispersion and Computational Parameters

| Variable | Type | Description | Default Value |
|---|---|---|---|
| *ISIGMAV | integer | Form of lateral turbulence data in PROFILE.DAT file (used only if METFM = 4 or MTURBVW = 1 or 3)<br>0 = read sigma-theta<br>1 = read sigma-v | 1 |
| *IMIXCTDM | integer | Choice of mixing heights (used only if METFM = 4)<br>0 = read PREDICTED mixing heights<br>1 = read OBSERVED mixing heights | 0 |
| XMXLEN | real | Maximum length of an emitted slug (in met. grid units) | 1.0 |
| XSAMLEN | real | Maximum travel distance of a slug or puff (in met. grid units) during one sampling step | 1.0 |
| MXNEW | integer | Maximum number of puffs or slugs released from one source during one time step (serves as a cap if XMXLEN is specified too small) | 99 |
| MXSAM | integer | Maximum number of sampling steps during one time step for a puff or slug (serves as a cap if XSAMLEN is specified too small) | 99 |
| NCOUNT | integer | Number of iterations used when computing the transport wind for a sampling step that includes transitional plume rise (used when METFM=1 or 4) | 2 |
| SYMIN | real | Minimum $\sigma_y$ (m) a new puff or slug | 1.0 |
| SZMIN | real | Minimum $\sigma_z$ (m) a new puff or slug | 1.0 |
| SVMIN | real | Minimum turbulence $\sigma_v$ (m/s) | 6*0.50 |
| SWMIN | real | Minimum turbulence $\sigma_w$ (m/s) | 0.20, 0.12, 0.08, 0.06, 0.03, 0.016 |
| CDIV(2) | real | Divergence criterion for dw/dz in met cell used to initiate adjustment for horizontal convergence (l/s). Partial adjustment starts at CDIV(1), and full adjustment is reached at CDIV(2) | 0.0, 0.0 |
| WSCALM | real | Minimum wind speed allowed for non-calm conditions. Wind speeds less than WSCALM will be considered as "calm" by the model. WSCALM is also used as the minimum speed returned from the power law extrapolation of the wind speed toward the surface. | 0.5 |
| XMAXZI | real | Maximum mixing height (m) | 3000. |
| XMINZI | real | Minimum mixing height (m) | 50. |

| Variable | Type | Description | Default Value |
|---|---|---|---|
| SL2PF | real | Slug-to-puff transition criterion factor (max. $\sigma_y$/slug length before transition to puff) | 10. |
| WSCAT(5) | real array | Upper bounds on the first 5 wind speed classes (m/s); The last class has no upper limit | 1.54, 3.09, 5.14, 8.23, 10.8 |
| PLX0(6) | real array | Wind speed profile power-law exponents for stabilities A-F | 0.07, 0.07, 0.10, 0.15, 0.35, 0.55 |
| PTG0(2) | real array | Potential temperature gradient (deg. k/m) for stability classes E and F | .020, .035 |
| PPC(6) | real array | Default plume path coefficients for each stability class (used when option for partial plume height terrain adjustment is selected, MCTADJ = 3) | 0.50, 0.50, 0.50, 0.50, 0.35, 0.35 |
| | | **(Puff-Spliting Control Variables \*)** | |
| *NSPLIT | integer | Number of puffs that result every time a puff is split; nsplit=2 means that 1 puff splits into 2 | 3 |
| *IRESPLIT (24) | integer array | Time(s) of a day when split puffs are eligible to be split once again; this is typically set once per day, around sunset before nocturnal shear develops. 24 values: 0 is midnight (00:00) and 23 is 11 PM (23:00) 0=do not re-split; 1=eligible for re-split | 17*0, 1, 6*0 |
| *ZISPLIT | real | Split is allowed only if last hour's mixing height (m) exceeds this minimum value | 100 |
| *ROLDMAX | real | Split is allowed only if ratio of last hour's mixing ht to the maximum mixing ht experienced by the puff is less than this maximum value (this postpones a split until a nocturnal layer develops) | 0.25 |
| | | **(Integration Control Variables \*)** | |
| *EPSSLUG | real | Fractional convergence criterion for numerical slug sampling integration | 1.0e-04 |
| *EPSAREA | real | Fractional convergence criterion for numerical area source integration | 1.0e-06 |
| *DSRISE | real | Trajectory step length (m) for numerical rise integration. | 1.0 |

| Variable | Type | Description | Default Value |
|---|---|---|---|
| **(Input Group 13a - General Data)** | | | |
| NPT1 | integer | Number of point sources with constant stack parameters or variable emission rate scale factors | - |
| IPTU | integer | Units choice for emission rates from point sources<br>1 = g/s<br>2 = kg/hr<br>3 = lb/hr<br>4 = tons/yr<br>5 = Odour Unit * m**3/s (vol. flux of compound)<br>6 = Odour Unit * m**3/min<br>7 = metric tons/yr | 1 |
| NSPT1 | integer | Number of source-species with variable emission rate scaling factors provided in 13d | 0 |
| NPT2 | integer | Number of point sources with arbitrarily-varying emission parameters (If NPT2 > 0, the point source emissions file PTEMARB.DAT must be provided) | - |
| **(Input Group 13b - Point Source Data for Sources with Constant Stack Parameters or Variable Emission Rate Scale Factors)** | | | - |
| SRCNAM | character*12 | Source name, used to coordinate inputs in Subgroups b,c,d | - |
| XUTM | real | X coordinate (km) of the stack on the meteorological grid | - |
| YUTM | real | Y coordinate (km) of the stack on the meteorological grid | - |
| HSTAK | real | Stack height (m) | - |
| SELEV | real | Stack base elevation (m) above mean sea level | - |
| DIAM | real | Stack diameter (m) | - |
| EXITW | real | Stack gas exit velocity (m/s) | - |
| EXITT | real | Stack gas exit temperature (deg. K) | - |
| BDOWN | real | Building downwash flag<br>0. = building downwash not modeled,<br>1. = building downwash modeled | - |
| EMS | real array | Emission rate (g/s) of each modeled species<br>Note: "NSPEC" values must be entered | - |

| Variable | Type | Description | Default Value |
|---|---|---|---|
| **(Optional Variables for Input Group 13b)** | | | |
| SIGMAYI | real | Initial sigma-y (m) associated with the release from this source | 0.0 - |
| SIGMAZI | real | Initial sigma-z (m) associated with the release from this source | 0.0 |

The variables in Input Group 13b are entered for each of the "NPT1" point sources. <u>The data for each source is treated as a separate input subgroup, and therefore, must end with an input group terminator (i.e., !END!).</u> Note that the source number is an optional user comment which is outside of the delimiter containing the required source data. The data for each source must follow an opening delimiter and "X=". The data for each source is followed by a closing delimiter and an input group terminator.

The two optional variables may be provided for point sources that have a characteristic distribution much like volume sources. The values are entered in order between delimiters, following "SIGYZI=". This record must be placed before the input group terminates (i.e., !END!) for the point source.

The format of Input Group 13b for a simulation with eight species is shown below.

```
---------------
Subgroup (13b)
---------------
                                   a
          POINT SOURCE: CONSTANT DATA
          ----------------------------
                                                       b          c
  Source     X UTM      Y UTM     Stack  Base     Stack   Exit  Exit   Bldg.  Emission
   No.    Coordinate Coordinate Height Elevation Diameter Vel.  Temp.  Dwash  Rates
            (km)       (km)       (m)    (m)       (m)   (m/s) (deg. K)
  ------  ---------- ---------- ------ ------   -------- ----- -------- ----- --------
   1 ! SRCNAM = BLR1 !
   1 ! X =      0.1,     -3.,    40.,   25.,      2.2,   10.,   450.,   1., 1.7E00, 1.0E00,
      1.0E-02, 1.0E-01, 2.0E-01, 2.4E-01, 2.5E-01, 2.0E-01 !
   1 ! SIGYZI =      3.,     1.5   !
     !END!
--------
   a
    Data for each source are treated as a separate input subgroup
    and therefore must end with an input group terminator.

   b
    0. = No building downwash modeled, 1. = downwash modeled
    NOTE: must be entered as a REAL number (i.e., with decimal point)

   c
    An emission rate must be entered for every pollutant modeled.
    Enter emission rate of zero for secondary pollutants that are
    modeled, but not emitted.  Units are specified by IPTU
    (e.g. 1 for g/s).
```

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| **(Input Group 13c - Building Dimension Data)** | | | |
| SRCNAM | character*12 | Source name, used to coordinate inputs in Subgroups b,c,d | - |
| HEIGHT | real array | Array of 36-direction-specific building heights (m) for flow vectors from 10°-360° in 10° increments | - |
| WIDTH | real array | Array of 36 direction-specific building widths (m) for flow vectors from 10°-360° in 10° increments | - |

The variables in Input Group 13c are entered for each point source for which IDOWN=1 in Input Group 13b. The data for each point source (i.e., source name, 36 widths and 36 heights) is treated as a separate input subgroup and therefore must end with an input group terminator (i.e., !END!). Once again, the source number is an optional user comment which is outside of the delimiters. The source name is used to place the building information with the correct source. The data for each source must follow an opening delimiter and either "WIDTH=" or "HEIGHT=". The data for each source is followed by a closing delimiter and an input group terminator (i.e., !END!). The format of Input Group 13c is shown below.

```
--------------
Subgroup (13c)
--------------

          BUILDING DIMENSION DATA FOR SOURCES SUBJECT TO DOWNWASH
          ------------------------------------------------------
Source                                                               a
 No.      Effective building width and height (in meters) every 10 degrees
------    -------------------------------------------------------------

 1    ! SRCNAM  =   BLR1 !
 1    ! HEIGHT  =  45., 45., 45., 45., 45., 45., 45., 45., 45.,  0.,  0.,  0.,
       0.,  0.,  0.,  0.,  0.,  0., 45., 45., 45., 45., 45., 45.,
                 45., 45., 45.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0. !
 1    ! WIDTH   =   12.5, 12.5, 12.5, 12.5, 12.5, 12.5, 12.5, 12.5, 12.5,  0.,   0.,   0.,
                   0.,   0.,   0.,   0.,   0.,   0.,  12.5, 12.5, 12.5, 12.5, 12.5, 12.5,
                  12.5, 12.5, 12.5,  0.,   0.,   0.,   0.,   0.,   0.,   0.,   0.,   0. !
!END!
--------
    a
    Each pair of width and height values is treated as a separate input
    subgroup and therefore must end with an input group terminator.
```

Table 4-3 (Continued)
CALPUFF Control File Inputs - Input Group 13
Point Source Parameters

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| **(Input Group 13d - Variable Emissions Scale Factors)** | | | |
| SRCNAM | character*12 | Source name, used to coordinate inputs in Subgroups b,c,d | - |
| IVARY | integer | Type of scale factor variation (diurnal, monthly, etc.)<br>0 = Constant<br>1 = Diurnal cycle<br>(24 scaling factors: hours 1-24)<br>2 = Monthly cycle<br>(12 scaling factors: months 1-12)<br>3 = Hour & Season<br>(4 groups of 24 hourly scaling factors, where first group is DEC-JAN-FEB)<br>4 = Speed & Stab.<br>(6 groups of 6 scaling factors, where first group is Stability Class A, and the 6 speed classes have upper bounds (m/s) defined in Group 12)<br>5 = Temperature<br>(12 scaling factors, where temperature classes have upper bounds (C) of: 0, 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 50+) | 0 |
| QFAC | real array | Array of emissions scaling factors for this source and the species indicated | - |

The variables in Input Group 13d are entered for each point source - species combination indicated by NSPT1 in Input Group 13a (e.g., only NSPT1 combinations are entered). The data for each point source-species combination (i.e., source name, type of variation, and the QFAC array ) are treated as a separate input subgroup and therefore must end with an input group terminator (i.e., !END!). Once again, the source number is an optional user comment which is outside of the delimiters. The source name is used to place the scaling factors with the correct source. The data for each source-species combination must follow an opening delimiter and "(cspec)=", where (cspec) is a species name defined in Group 3. The data for each source-species combination is followed by a closing delimiter and an input group terminator (i.e., !END!). If NSPT1=0, no scaling factors should be defined here.

The format for Input Group 13d is shown below.

```
---------------
Subgroup (13d)
---------------
                                            a
          POINT SOURCE: VARIABLE EMISSIONS DATA
          -------------------------------------

 1  ! SRCNAM = BLR1 !
 1  ! IVARY  =  2  !   (12 Months)
 1  ! SO2          = 0.1,0.1,0.5,0.9,2,2.2,
                     2.5,1.5,1.1,0.9,0.5,0.1      !
!END!

--------
    a
    Data for each species are treated as a separate input subgroup
    and therefore must end with an input group terminator.
```

| Variable | Type | Description | Default Value |
|---|---|---|---|
| **(Input Group 14a - General Area Source Data)** | | | |
| NAR1 | integer | Number of area sources with constant parameters or variable emission rate scale factors | - |
| IARU | integer | Units choice for emission rates from area sources<br>1 = g/m**2/s<br>2 = kg/m**2/hr<br>3 = lb/m**2/hr<br>4 = tons/m**2/yr<br>5 = Odour Unit * m/s (vol. flux/m**2 of compound)<br>6 = Odour Unit * m/min<br>7 = metric tons/m**2/yr | 1 |
| NSAR1 | integer | Number of source-species with variable emission rate scaling factors provided in 14d | 0 |
| NAR2 | integer | Number of buoyant area sources with arbitrary varying emission parameters | - |
| **(Input Group 14b - Area Source Data for Sources with Constant Parameters or Emissions Scale Factors)** | | | |
| SRCNAM | character*12 | Source name, used to coordinate inputs in Subgroups b,c,d | - |
| HTEFF | real | Effective height (m) of the area source | - |
| AELEV | real | Base elevation (m) above mean sea level | - |
| SIGZI | real | Initial vertical dispersion coefficient ($\sigma_z$), in meters, of the area source | - |
| EMIS | real array | Emission rate ($g/s/m^2$) of each modeled species<br>Note: "NSPEC" values must be entered | - |

The variables in Input Group 14b are entered for each of the "NAR1" area sources. The data for each source is treated as a separate input subgroup, and therefore, must end with an input group terminator (i.e., !END!). Note that the source number is an optional user comment which is outside of the delimiter containing the required source data. The data for each source must follow an opening delimiter and "X=". The data for each source is followed by a closing delimiter and an input group terminator.

The format of Input Group 14b for a simulation with eight species is shown below.

```
---------------
Subgroup (14b)
---------------
                                         a
          AREA SOURCE: CONSTANT DATA
          ---------------------------
                                                  b
Source            Effect.   Base     Initial   Emission
 No.              Height  Elevation  Sigma z    Rates
                   (m)      (m)        (m)
-------           ------   ------    --------   ---------

   1! SRCNAM = AREA1 !
   1! X =           1.,        0.,       2.5,   8.5E-01,  0.5E00,  0.0E00,
                                  0.0E00,  0.0E00,  0.0E00,  0.0E00,  0.0E00 !
    !END!
   2! SRCNAM = AREA2 !
   2! X =           1.5,       0.,       3.,    0.0E00,  0.0E00, 1.0E-01,
                                  0.0E00,  0.0E00, 5.0E-01,  1.0E00,  1.3E00 !
    !END!

--------
   a
    Data for each source are treated as a separate input subgroup
    and therefore must end with an input group terminator.
   b
    An emission rate must be entered for every pollutant modeled.
    Enter emission rate of zero for secondary pollutants that are
    modeled, but not emitted.  Units are specified by IARU
    (e.g. 1 for g/m**2/s).
```

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| **(Input Group 14c - Vertex Data for Area Sources with Constant Parameters or Emissions Scale Factors)** | | | |
| SRCNAM | character*12 | Source name, used to coordinate inputs in Subgroups b,c,d | - |
| XVERT | real | X coordinates (km) of each vertex of the area source on the meteorological grid | - |
| YVERT | real | Y coordinate (km) of each vertex of the area source on the meteorological grid | - |

The variables in Input Group 14c are entered for each of the "NAR1" area sources.  <u>The data for each source is treated as a separate input subgroup, and therefore, must end with an input group terminator (i.e., !END!)</u>.  Note that the source number is an optional user comment which is outside of the delimiter containing the required source data.  The data for each source must follow an opening delimiter and "X=".  The data for each source is followed by a closing delimiter and an input group terminator.

The format of Input Group 14c is shown below.

```
--------------
Subgroup (14c)
--------------

          COORDINATES (UTM-km) FOR EACH VERTEX(4) OF EACH POLYGON
          -----------------------------------------------------
Source                                                           a
 No.      Ordered list of X followed by list of Y, grouped by source
------    ----------------------------------------------------------

 1    ! SRCNAM  =   AREA1 !
 1      !  XVERT = 0.5,    0.51,    0.51,    0.5!
 1      !  YVERT = 1.61,   1.61,    1.6,    1.6!
      !END!
 2    ! SRCNAM  =   AREA2 !
 2      !  XVERT = 0.75,    0.76,    0.76,   0.75!
 2      !  YVERT = 1.81,    1.81,    1.8,    1.8!
      !END!

--------
    a
    Data for each source are treated as a separate input subgroup
    and therefore must end with an input group terminator.
```

| Variable | Type | Description | Default Value |
|---|---|---|---|
| **(Input Group 14d - Variable Emissions Scale Factors)** | | | |
| SRCNAM | character*12 | Source name, used to coordinate inputs in Subgroups b,c,d | - |
| IVARY | integer | Type of scale factor variation (diurnal, monthly, etc.)<br>0 =    Constant<br>1 =    Diurnal cycle<br>    (24 scaling factors: hours 1-24)<br>2 =    Monthly cycle<br>    (12 scaling factors: months 1-12)<br>3 =    Hour & Season<br>    (4 groups of 24 hourly scaling factors,<br>    where first group is DEC-JAN-FEB)<br>4 =    Speed & Stab.<br>    (6 groups of 6 scaling factors, where<br>    first group is Stability Class A,<br>    and the 6 speed classes have upper<br>    bounds (m/s) defined in Group 12)<br>5 =    Temperature<br>    (12 scaling factors, where temperature<br>    classes have upper bounds (C) of:<br>    0, 5, 10, 15, 20, 25, 30, 35, 40,<br>    45, 50, 50+) | 0 |
| QFAC | real array | Array of emissions scaling factors for this source and the species indicated | - |

The variables in Input Group 14d are entered for each area source - species combination indicated by NSAR1 in Input Group 14a (e.g., only NSAR1 combinations are entered). <u>The data for each area source-species combination (i.e., source name, type of variation, and the QFAC array ) are treated as a separate input subgroup and therefore must end with an input group terminator (i.e., !END!)</u>. Once again, the source number is an optional user comment which is outside of the delimiters. The source name is used to place the scaling factors with the correct source. The data for each source-species combination must follow an opening delimiter and "(cspec)=", where (cspec) is a species name defined in Group 3. The data for each source-species combination is followed by a closing delimiter and an input group terminator (i.e., !END!). If NSAR1=0, no scaling factors should be defined here.

The format of Input Group 14d is shown below.

```
---------------
Subgroup (14d)
---------------
                                                  a
          AREA SOURCE: VARIABLE EMISSIONS DATA
          -------------------------------------

 2  ! SRCNAM = AREA2 !
 2  ! IVARY  =  4  !    (6 speed classes for each stability)
 2  ! PMSIZE1       = 0.1,0.1,0.5,0.9,1,1.5,
                      0.1,0.1,0.5,0.9,1,1.5,
                      0.1,0.1,0.5,0.9,1,1.5,
                      0.1,0.1,0.5,0.9,1,1.5,
                      0.1,0.1,0.5,0.9,1,1.5,
                      0.1,0.1,0.5,0.9,1,1.5      !
!END!

--------
    a
    Data for each species are treated as a separate input subgroup
    and therefore must end with an input group terminator.
```

| Variable | Type | Description | Default Value |
|---|---|---|---|
| **(Input Group 15a - General Line Source Data)** | | | |
| NLN2 | integer | Number of buoyant line sources with variable location and emission parameters (all data provided in file LNEMARB.DAT) | 0 |
| NLINES | integer | Number of buoyant line sources | - |
| ILNU | integer | Units choice for line source emissions<br>1 = g/s<br>2 = kg/hr<br>3 = lb/hr<br>4 = tons/yr<br>5 = Odour Unit * m**3/s (vol. flux of compound)<br>6 = Odour Unit * m**3/min<br>7 = metric tons/yr | 1 |
| NSLN1 | integer | Number of source-species with variable emission rate scaling factors provided in 15c | 0 |
| MXNSEG | integer | Maximum number of line segments into which each line may be divided (if MSLUG=1); Actual number of virtual points which will be used to represent each line (if MSLUG=0) | 7 |
| NLRISE | integer | Number of distances at which transitional rise is computed | 6 |
| XL | real | Average building length (m) | - |
| HBL | real | Average building height (m) | - |
| WBL | real | Average building width (m) | - |
| WML | real | Average line source width (m) | - |
| DXL | real | Average separation between buildings (m) | - |
| FPRIMEL | real | Average buoyancy parameter ($m^4/s^3$) | - |
| **(Input Group 15b - Buoyant Line Source Data) - repeated for each line source** | | | |
| SRCNAM | character*12 | Source name, used to coordinate inputs in Subgroups b,c | - |
| XBEGL | real | Beginning X coordinate of line source (km) | - |
| YBEGL | real | Beginning Y coordinate of line source (km) | - |
| XENDL | real | Ending X coordinate of line source (km) | - |
| YENDL | real | Ending Y coordinate of line source(km) | - |
| HTL | real | Release height (m) | - |

## Table 4-3 (Continued)
## CALPUFF Control File Inputs - Input Group 15
## Line Source Parameters

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| ELEVL | real | Base elevation (m) | - |
| QL | real | Emissions rate (g/s) of each pollutant | - |

The variables in Input Group 15b are entered for each of the "NLINES" line sources.  <u>The data for each line is treated as a separate input subgroup, and therefore, must end with an input group terminator (i.e., !END!)</u>.  Note that the line number is an optional user comment which is outside of the delimiter containing the required source data.  The data for each line must follow an opening delimiter and "X=".  The data for each line is followed by a closing delimiter and an input group terminator.

The format of Input Group 15b for a simulation with eight species is shown below.

```
---------------
Subgroup (15b)
---------------

         BUOYANT LINE SOURCE: CONSTANT DATA
         ----------------------------------
                                                                a
Source    Beg. X       Beg. Y      End. X      End. Y    Release   Base       Emission
No.      Coordinate  Coordinate  Coordinate  Coordinate  Height    Elevation    Rates
          (km)         (km)        (km)        (km)        (m)       (m)
------    ----------  ----------  ---------   ----------  -------   ---------    ---------
   1! SRCNAM = LINE1 !
   1! X =       12.,        35.,       12.5,        35.,    22.000,    0.000, 2.3E00, 1.1E00,
                        0.0E00, 0.0E00, 0.0E00, 0.0E00, 0.0E00, 0.0E00 !
    !END!
   2! SRCNAM = LINE2 !
   2! X =       12.,     35.022,       12.5,     35.022,    22.000,    0.000, 2.3E00, 1.1E00,
                        0.0E00, 0.0E00, 0.0E00, 0.0E00, 0.0E00, 0.0E00 !
    !END!

--------

   a
    Data for each source are treated as a separate input subgroup
    and therefore must end with an input group terminator.

   b
    An emission rate must be entered for every pollutant modeled.
    Enter emission rate of zero for secondary pollutants that are
    modeled, but not emitted.  Units are specified by ILNTU
    (e.g. 1 for g/s).
```

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| **(Input Group 15c - Variable Emissions Scale Factors)** | | | |
| SRCNAM | character*12 | Source name, used to coordinate inputs in Subgroups b,c | - |
| IVARY | integer | Type of scale factor variation (diurnal, monthly, etc.) | 0 |
| | | 0 = Constant | |
| | | 1 = Diurnal cycle | |
| | | (24 scaling factors: hours 1-24) | |
| | | 2 = Monthly cycle | |
| | | (12 scaling factors: months 1-12) | |
| | | 3 = Hour & Season | |
| | | (4 groups of 24 hourly scaling factors, where first group is DEC-JAN-FEB) | |
| | | 4 = Speed & Stab. | |
| | | (6 groups of 6 scaling factors, where first group is Stability Class A, and the 6 speed classes have upper bounds (m/s) defined in Group 12) | |
| | | 5 = Temperature | |
| | | (12 scaling factors, where temperature classes have upper bounds (C) of: 0, 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 50+) | |
| QFAC | real array | Array of emissions scaling factors for this source and the species indicated | - |

The variables in Input Group 15c are entered for each line source - species combination indicated by NSLN1 in Input Group 15a (e.g., only NSLN1 combinations are entered). <u>The data for each line source-species combination (i.e., source name, type of variation, and the QFAC array ) are treated as a separate input subgroup and therefore must end with an input group terminator (i.e., !END!)</u>. Once again, the source number is an optional user comment which is outside of the delimiters. The source name is used to place the scaling factors with the correct source. The data for each source-species combination must follow an opening delimiter and "(cspec)=", where (cspec) is a species name defined in Group 3. The data for each source-species combination is followed by a closing delimiter and an input group terminator (i.e., !END!). If NSLN1=0, no scaling factors should be defined here.

The format of Input Group 15c is shown below.

```
--------------
Subgroup (15c)
--------------
                                              a
           BUOYANT LINE SOURCE: VARIABLE EMISSIONS DATA
           --------------------------------------------

 1  ! SRCNAM = LINE1 !
 1  ! IVARY  = 1  !    (24 Hours)
 1  ! SO2         = 0.1,0.1,0.1,0.2,0.2,0.3,
                    0.3,0.4,0.4,0.5,0.6,1,
                    1,1,1,1,1,1,
                    0.6,0.4,0.3,0.2,0.1,0.1      !
!END!

--------
    a
     Data for each species are treated as a separate input subgroup
     and therefore must end with an input group terminator.
```

# Table 4-3 (Continued)
## CALPUFF Control File Inputs - Input Group 16
## Volume Source Parameters

| Variable | Type | Description | Default Value |
|---|---|---|---|
| **(Input Group 16a - General Volume Source Data)** | | | |
| NVL1 | integer | Number of volume sources with constant parameters or variable emission scale factors | - |
| IVLU | integer | Units choice for volume source emissions<br>1 = g/s<br>2 = kg/hr<br>3 = lb/hr<br>4 = tons/yr<br>5 = Odour Unit * m**3/s (vol. flux of compound)<br>6 = Odour Unit * m**3/min<br>7 = metric tons/yr | 1 |
| NSVL1 | integer | Number of source-species with variable emission rate scaling factors provided in 16c | 0 |
| IGRDVL | integer | Gridded volume source data used?<br>(0 = no, 1 = yes - read from file VOLEM.DAT) | - |
| VEFFHT | real | Effective height (m) of emissions in gridded volume source file | - |
| VSIGYI | real | Initial $\sigma_y$ (m) of emissions in gridded volume source file | - |
| VSIGZI | real | Initial $\sigma_z$ (m) of emissions in gridded volume source file | - |
| **(Input Group 16b - Volume Source Data for Sources with Constant Parameters or Variable Emission Scaling Factors (repeated for each volume source (NVL1))** | | | |
| SRCNAM | character*12 | Source name, used to coordinate inputs in Subgroups b,c | - |
| XVOL | real | X coordinate (km) of center of volume source | - |
| YVOL | real | Y coordinate (km) of center of volume source | - |
| HTVOL | real | Effective height (m) of volume source | - |
| ELEVOL | real | Base elevation (m) of volume source | - |
| SYVOL | real | Initial $\sigma_y$ (m) of volume source | - |
| SZVOL | real | Initial $\sigma_z$ (m) of volume source | - |
| QVOL | real | Emission rates (g/s) of each pollutant from volume source | - |

Table 4-3 (Continued)
CALPUFF Control File Inputs - Input Group 16
Volume Source Parameters

The variables in Input Group 16b are entered for each of the "NVL1" volume sources. <u>The data for each source is treated as a separate input subgroup, and therefore, must end with an input group terminator (i.e., !END!)</u>. Note that the source number is an optional user comment which is outside of the delimiter containing the required source data. The data for each source must follow an opening delimiter and "X=". The data for each source is followed by a closing delimiter and an input group terminator.

The format of Input Group 16b for a simulation with eight species is shown below.

```
---------------
Subgroup (16b)
---------------
                                          a
            VOLUME SOURCE: CONSTANT DATA
            ----------------------------
                                                          b
         X UTM      Y UTM    Effect.    Base    Initial   Initial   Emission
       Coordinate Coordinate  Height  Elevation Sigma y   Sigma z    Rates
         (km)       (km)       (m)      (m)       (m)       (m)
       ---------- ---------- ------   ------   --------  --------  --------

  1! SRCNAM = VOLS1 !
! X =     -5.6,      -1.2,    10.,      0.,       6.2,      6.2, 2.2E00, 4.0E00, 0.0E00,
                                                  0.0E00, 0.0E00, 0.0E00, 0.0E00, 0.0E00 !
!END!

--------
    a
     Data for each source are treated as a separate input subgroup
     and therefore must end with an input group terminator.

    b
     An emission rate must be entered for every pollutant modeled.
     Enter emission rate of zero for secondary pollutants that are
     modeled, but not emitted.  Units are specified by IVLU
     (e.g. 1 for g/s).
```

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| **(Input Group 16c - Variable Emissions Scale Factors)** | | | |
| SRCNAM | character*12 | Source name, used to coordinate inputs in Subgroups b,c | - |
| IVARY | integer | Type of scale factor variation (diurnal, monthly, etc.)<br>0 =    Constant<br>1 =    Diurnal cycle<br>    (24 scaling factors: hours 1-24)<br>2 =    Monthly cycle<br>    (12 scaling factors: months 1-12)<br>3 =    Hour & Season<br>    (4 groups of 24 hourly scaling factors,<br>    where first group is DEC-JAN-FEB)<br>4 =    Speed & Stab.<br>    (6 groups of 6 scaling factors, where<br>    first group is Stability Class A,<br>    and the 6 speed classes have upper<br>    bounds (m/s) defined in Group 12)<br>5 =    Temperature<br>    (12 scaling factors, where temperature<br>    classes have upper bounds (C) of:<br>    0, 5, 10, 15, 20, 25, 30, 35, 40,<br>    45, 50, 50+) | 0 |
| QFAC | real array | Array of emissions scaling factors for this source and the species indicated | - |

The variables in Input Group 16c are entered for each volume source - species combination indicated by NSVL1 in Input Group 16a (e.g., only NSVL1 combinations are entered). The data for each volume source-species combination (i.e., source name, type of variation, and the QFAC array ) are treated as a separate input subgroup and therefore must end with an input group terminator (i.e., !END!). Once again, the source number is an optional user comment which is outside of the delimiters. The source name is used to place the scaling factors with the correct source. The data for each source-species combination must follow an opening delimiter and "(cspec)=", where (cspec) is a species name defined in Group 3. The data for each source-species combination is followed by a closing delimiter and an input group terminator (i.e., !END!). If NSVL1=0, no scaling factors should be defined here.

The format of Input Group 16c is shown below.

```
---------------
Subgroup (16c)
---------------
                                               a
            VOLUME SOURCE: VARIABLE EMISSIONS DATA
            --------------------------------------

 1  ! SRCNAM = VOLS1 !
 1  ! IVARY  = 1  !    (24 Hours)
 1  ! SO2         = 0.1, 0.1, 0.1, 0.2, 0.2, 0.3,
                    0.3, 0.4, 0.4, 0.5, 0.6,   1,
                      1,   1,   1,   1,   1,   1,
                    0.6, 0.4, 0.3, 0.2, 0.1, 0.1  !
!END!

--------
   a
    Data for each species are treated as a separate input subgroup
    and therefore must end with an input group terminator.
```

Table 4-3 (Concluded)
CALPUFF Control File Inputs - Input Group 17
Non-Gridded (Discrete) Receptor Data

| Variable | Type | Description | Default Value |
|----------|------|-------------|---------------|
| **(Input Group 17a - General Discrete Receptor Data)** | | | |
| NREC | integer | Number of non-gridded receptors | - |
| **(Input Group 17b - Discrete Receptor Data)** | | | |
| XUTM | real | X coordinate (km) of the discrete receptor on the meteorological grid | - |
| YUTM | real | Y coordinate (km) of the discrete receptor on the meteorological grid | - |
| ELEV | real | Ground elevation (m) above mean sea level of the receptor | - |
| ZREC | real | Height (m) of discrete receptor above the ground | 0.0 |

The variables in Input Group 17b are entered for each of the "NREC" discrete receptors. The data for each receptor is treated as a separate input subgroup, and therefore, must end with an input group terminator (i.e., !END!). The format of Input Group 17b is shown below.

```
--------------
Subgroup (17b)
--------------
                                            a
           NON-GRIDDED (DISCRETE) RECEPTOR DATA
           -----------------------------------

                 X UTM       Y UTM      Ground      Height   b
Receptor      Coordinate  Coordinate  Elevation  Above Ground
  No.            (km)        (km)        (m)         (m)
--------      ----------  ----------  ---------  ------------
    1 ! X =          1.,         1.,    12.500,       0.000!   !END!
    2 ! X =         2.5,        4.2,    28.100,       0.000!   !END!
    3 ! X =        2.89,        3.2,    39.600,       0.000!   !END!


-------------
   a
    Data for each receptor are treated as a separate input subgroup
    and therefore must end with an input group terminator.

   b
    Receptor height above ground is optional.  If no value is entered,
    the receptor is placed on the ground.
```

Note that the receptor number is an optional user comment which is outside of the delimiter. The data for each receptor must follow an opening delimiter and "X=". The data for each receptor is followed by a closing delimiter and an input group terminator (i.e., !END!).

4.2     Meteorological Data Files

Four types of meteorological data files can be used to drive the CALPUFF model.  In order to take full advantage of the capabilities of the model to simulate the effects spatially-varying meteorological fields, gridded fields of winds, temperatures, mixing heights, and other meteorological variables should be input to CALPUFF through the CALMET.DAT file.  The format and contents of this file are described in Section 4.2.1.

Alternatively, CALPUFF will accept single station meteorological data in the ISC3 format, CTDMPLUS format, or AUSPLUME format.  The ISC3 meteorological data file (ISCMET.DAT) is described in Section 4.2.2, the AUSPLUME file (PLMMET.DAT) is described in Section 4.2.3, and the CTDMPLUS meteorological data files SURFACE.DAT and PROFILE.DAT are described in Section 4.2.4.

4.2.1   CALMET.DAT

The CALMET.DAT file contains gridded meteorological data fields required to drive the CALPUFF model.  It also contains certain geophysical fields, such as terrain elevations, surface roughness lengths, and land use types, used by both the CALMET meteorological model and CALPUFF.  Although the input requirements of CALPUFF are designed to be directly compatible with CALMET, meteorological fields produced by other meteorological models can be substituted for the CALMET output as long as the required variables are produced and the output is reformatted to be consistent with the CALMET.DAT file specifications described in this section.

**CALMET.DAT File - Header Records**

The CALMET.DAT file consists of a set of up to fifteen header records, followed by a set of hourly data records.  The header records contain a descriptive title of the meteorological run, information including the horizontal and vertical grid systems of the meteorological grid, the number, type, and coordinates of the meteorological stations included in the CALMET run, gridded fields of surface roughness lengths, land use, terrain elevations, leaf area indexes, and a pre-computed field of the closest surface meteorological station number to each grid point.

The actual number of header records may vary because, as explained below, records containing surface, upper air, and precipitation station coordinates are not included if these stations were not included in the run.  A description of each variable in the header records is provided in Table 4-4.

The following variables stored in the CALMET.DAT header records are checked in the setup phase of the CALPUFF model run to ensure compatibility with variables specified in the CALPUFF control file:

number of grid cells in the X and Y directions, grid size, reference UTM or Lambert conformal coordinates of the grid origin, and UTM zone of the grid origin.

Sample FORTRAN write statements for the CALMET.DAT header records are:

```
c ---       Header record 1 -- Run title
            write(iunit)TITLE

c ---       Header records 2 and 3 -- General run and grid information
            write(iunit)VER,LEVEL,IBYR,IBMO,IBDY,IBHR,IBTZ,IRLG,IRTYPE,
           1          NX,NY,NZ,DGRID,XORIGR,YORIGR,IUTMZN,IWFCOD,NSSTA,
           2          NUSTA,NPSTA,NOWSTA,NLU,IWAT1,IWAT2,LCALGRD
            write(iunit)XLAT0,XLON0,LLCONF,CONEC,XLAT1,XLAT2,RLAT0,RLAT0

c ---       Header record 4 -- Vertical cell face heights (nz+1 values)
            write(iunit)CLAB1,IDUM,ZFACEM

c ---       Header records 5 and 6 -- Surface station coordinates
            if(nssta.ge.1)then
                  write(iunit)CLAB2,IDUM,XSSTA
                  write(iunit)CLAB3,IDUM,YSSTA
            endif

c ---       Header records 7 and 8 -- Upper air station coordinates
            if(nusta.ge.1)then
                  write(iunit)CLAB4,IDUM,XUSTA
                  write(iunit)CLAB5,IDUM,YUSTA
            endif

c ---          Header records 9 and 10 -- Precipitation station coordinates
            if(npsta.ge.1)then
                  write(iunit)CLAB6,IDUM,XPSTA
                  write(iunit)CLAB7,IDUM,YPSTA
            endif

c ---       Header record 11 -- Surface roughness lengths
            write(iunit)CLAB8,IDUM,Z0

c ---       Header record 12 -- Land use categories
            write(iunit)CLAB9,IDUM,ILANDU

c ---       Header record 13 -- Terrain elevations
            write(iunit)CLAB10,IDUM,ELEV

c ---       Header record 14 - Leaf area indexes
            write(iunit)CLAB11,IDUM,XLAI

c ---       Header record 15 - Nearest surface station to each grid point
            write(iunit)CLAB12,IDUM,NEARS
```

where the following declarations apply:

```
      real ZFACEM(nz+1),XSSTA(nssta),YSSTA(nssta),XUSTA(nusta),YUSTA(nusta)
      real XPSTA(npsta),YPSTA(npsta)
      real Z0(nx,ny),ELEV(nx,ny),XLAI(nx,ny)
      integer ILANDU(nx,ny),NEARS(nx,ny)
      character*80 TITLE(3)
      character*8 VER,LEVEL,CLAB1,CLAB2,CLAB3,CLAB4,CLAB5,CLAB6
      character*8 CLAB7,CLAB8,CLAB9,CLAB10,CLAB11,CLAB12
      logical LCALGRD,LLCONF
```

Table 4-4

CALMET.DAT file - Header Records

| Header Record No. | Variable No. | Variable | Type[a] | Description |
|---|---|---|---|---|
| 1 | 1 | TITLE | char*80 array | Array with three 80-character lines of the user's title of the CALMET run |
| 2 | 1 | VER | char*8 | CALMET model version number |
| 2 | 2 | LEVEL | char*8 | CALMET model level number |
| 2 | 3 | IBYR | integer | Starting year of CALMET run |
| 2 | 4 | IBMO | integer | Starting month |
| 2 | 5 | IBDY | integer | Starting day |
| 2 | 6 | IBHR | integer | Starting hour (time at end of hour) |
| 2 | 7 | IBTZ | integer | Base time zone (e.g., 05=EST, 06=CST, 07=MST, 08=PST) |
| 2 | 8 | IRLG | integer | Run length (hours) |
| 2 | 9 | IRTYPE | integer | Run type (0=wind fields only, 1=wind and micrometeorological fields).  IRTYPE must be run type 1 to drive CALGRID or options in CALPUFF that use boundary layer parameters |
| 2 | 10 | NX | integer | Number of grid cells in the X direction |
| 2 | 11 | NY | integer | Number of grid cells in the Y direction |
| 2 | 12 | NZ | integer | Number of vertical layers |
| 2 | 13 | DGRID | real | Grid spacing (m) |
| 2 | 14 | XORIGR | real | X coordinate (m) of southwest corner of grid cell (1,1) |
| 2 | 15 | YORIGR | real | Y coordinate (m) of southwest corner of grid cell (1,1) |
| 2 | 16 | IUTMZN | integer | UTM zone of coordinates (0 if using a Lambert conformal projection) |
| 2 | 17 | IWFCOD | integer | Wind field module used (0=objective analysis, 1=diagnostic model) |
| 2 | 18 | NSSTA | integer | Number of surface meteorological stations |
| 2 | 19 | NUSTA | integer | Number of upper air stations |

[a]char*80 = Character*80
 char*8 = Character*8

Table 4-4 (Continued)

CALMET.DAT file - Header Records

| Header Record No. | Variable No. | Variable | Type[a] | Description |
|---|---|---|---|---|
| 2 | 20 | NPSTA | integer | Number of precipitation stations |
| 2 | 21 | NOWSTA | integer | Number of over water stations |
| 2 | 22 | NLU | integer | Number of land use categories |
| 2 | 23 | IWAT1 | integer | Range of land use categories |
| 2 | 24 | IWAT2 | integer | Corresponding to water surfaces (IWAT1 or IWAT2, inclusive) |
| 2 | 25 | LCALGRD | logical | Flag indicating if the full set of meteorological parameters required by CALGRID are contained in the file (LCALGRD is normally set to TRUE for CALPUFF applications) |
| 3 | 1 | XLAT0 | real | N. Latitude of southwest corner of MET grid |
| 3 | 2 | XLON0 | real | W. Longitude of southwest corner of MET grid |
| 3 | 3 | LLCONF | logical | Lambert conformal (LC) projection if TRUE |
| 3 | 4 | CONEC | real | Cone constant for LC map |
| 3 | 5 | XLAT1 | real | Standard parallel #1 for LC map |
| 3 | 6 | XLAT2 | real | Standard parallel #2 for LC map |
| 3 | 7 | RLAT0 | real | North latitude for origin of LC map |
| 3 | 8 | RLON0 | real | Reference west longitude for LC map |
| 4 | 1 | CLAB1 | char*8 | Variable label ('ZFACE') |
| 4 | 2 | IDUM | integer | Variable not used |
| 4 | 3 | ZFACEM | real array | Heights (m) of cell faces (NZ + 1 values) |
| 5[b] | 1 | CLAB2 | char*8 | Variable label ('XSSTA') |
| 5[b] | 2 | IDUM | integer | Variable not used |
| 5[b] | 3 | XSSTA | real array | X coordinates (m) of each surface met. station |

[a] char*8 = Character*8
[b] Included only if NSSTA > 0

Table 4-4 (Continued)
CALMET.DAT file - Header Records

| Header Record No. | Variable No. | Variable | Type[a] | Description |
|---|---|---|---|---|
| 6[b] | 1 | CLAB3 | char*8 | Variable label (‹YSSTA') |
| 6[b] | 2 | IDUM | integer | Variable not used |
| 6[b] | 3 | YSSTA | real array | Y coordinates (m) of each surface met. station |
| 7[c] | 1 | CLAB4 | char*8 | Variable label (‹XUSTA') |
| 7[c] | 2 | IDUM | integer | Variable not used |
| 7[c] | 3 | XUSTA | real array | X coordinates (m) of each upper air met. station |
| 8[c] | 1 | CLAB5 | char*8 | Variable label (‹YUSTA') |
| 8[c] | 2 | IDUM | integer | Variable not used |
| 8[c] | 3 | YUSTA | real array | Y coordinate (m) of each upper air met. station |
| 9[d] | 1 | CLAB6 | char*8 | Variable label (‹XPSTA') |
| 9[d] | 2 | IDUM | integer | Variable not used |
| 9[d] | 3 | XPSTA | real array | X coordinate (m) of each precipitation station |
| 10[d] | 1 | CLAB7 | char*8 | Variable label (‹YPSTA') |
| 10[d] | 2 | IDUM | integer | Variable not used |
| 10[d] | 3 | YPSTA | real array | Y coordinate (m) of each precipitation station |
| 11 | 1 | CLAB8 | char*8 | Variable label (‹Z0') |
| 11 | 2 | IDUM | integer | Variable not used |
| 11 | 3 | Z0 | real array | Gridded field of surface roughness lengths (m) for each grid cell |

[a] char*8 = Character*8
[b] Included only if NSSTA > 0
[c] Included only if NUSTA > 0
[d] Included only if NPSTA > 0

Table 4-4 (Concluded)
CALMET.DAT file - Header Records

| Header Record No. | Variable No. | Variable | Type[a] | Description |
|---|---|---|---|---|
| 12 | 1 | CLAB9 | char*8 | Variable label ('ILANDU') |
| 12 | 2 | IDUM | integer | Variable not used |
| 12 | 3 | ILANDU | integer array | Gridded field of land use category for each grid cell |
| 13 | 1 | CLAB10 | char*8 | Variable label ('ELEV') |
| 13 | 2 | IDUM | integer | Variable not used |
| 13 | 3 | ELEV | real array | Gridded field of terrain elevations for each grid cell |
| 14 | 1 | CLAB11 | char*8 | Variable label ('XLAI') |
| 14 | 2 | IDUM | integer | Variable not used |
| 14 | 3 | XLAI | real array | Gridded field of leaf area index for each grid cell |
| 15 | 1 | CLAB12 | char*8 | Variable label ('NEARS') |
| 15 | 2 | IDUM | integer | Variable not used |
| 15 | 3 | NEARS | integer array | Nearest surface meteorological station to each grid point |

[a]char*8 = Character*8

## CALMET.DAT File - Data Records

The CALMET.DAT data records include hourly fields of winds and meteorological variables.  In addition to the regular CALMET output variables, both CALGRID and CALPUFF require additional three-dimensional fields of air temperature and vertical velocity.  The presence of these fields in the CALMET output file is flagged by the header record logical variable, LCALGRD, having a value of TRUE.

The data records contain three-dimensional gridded fields of U, V, and W wind components and air temperature, two-dimensional fields of PGT stability class, surface friction velocity, mixing height, Monin-Obukhov length, convective velocity scale, and precipitation rate (not used by CALGRID), and values of the temperature, air density, short-wave solar radiation, relative humidity, and precipitation type codes (not used by CALGRID) defined at the surface meteorological stations.  A description of each variable in the data records is provided in Table 4-5.

Sample FORTRAN write statements for the CALMET.DAT data records are:

```
c ---       Write U, V, W wind components
                        ┌─         Loop over vertical layers, k

                        │            write(iunit)CLABU,NDATHR,((U(i,j,k),i=1,nx),j=1,ny)
                        │            write(iunit)CLABV,NDATHR,((V(i,j,k),i=1,nx),j=1,ny)
                        │            if(LCALGRD)write(iunit)CLABW,NDATHR((W(i,j,k+1),i=1,nx),j=1,ny)

                        └─         End loop over vertical layers

c ---       Write 3-D temperature field
            if(LCALGRD.and.irtype.eq.1) then
                        ┌─         Loop over vertical layers, k

                        │            write(iunit)CLABT,NDATHR,((ZTEMP(i,j,k),i=1,nxm),j=1,nym)

                        └─         End loop over vertical layers
            endif

c ---       Write 2-D meteorological fields
            if(irtype.eq.1) then

                        write(iunit)CLABSC,NDATHR,IPGT
                        write(iunit)CLABUS,NDATHR,USTAR
                        write(iunit)CLABZI,NDATHR,ZI
                        write(iunit)CLABL,NDATHR,EL
                        write(iunit)CLABWS,NDATHR,WSTAR
                        write(iunit)CLABRMM,NDATHR,RMM

            endif
```

```
c ---      Write 1-D variables defined at surface met. stations
           if(irtype.eq.1) then

                   write(iunit)CLABTK,NDATHR,TEMPK
                   write(iunit)CLABD,NDATHR,RHO
                   write(iunit)CLABQ,NDATHR,QSW
                   write(iunit)CLABRH,NDATHR,IRH
                   write(iunit)CLABPC,NDATHR,IPCODE

           endif
```

where the following declarations apply:

```
           real U(nx,ny,nz),V(nx,ny,nz),W(nx,ny,nz)
           real ZTEMP(nx,ny,nz)
           real USTAR(nx,ny),ZI(nx,ny),EL(nx,ny)
           real WSTAR(nx,ny),RMM(nx,ny)
           real TEMPK(nssta),RHO(nssta),QSW(nssta)
           integer IPGT(nx,ny)
           integer IRH(nssta),IPCODE(nssta)
           character*8 CLABU, CLABV, CLABW, CLABT, CLABSC, CLABUS, CLABZI
           character*8 CLABL, CLABWS, CLABRMM, CLABTK, CLABD, CLABQ, CLABRH
           character*8 CLABPC
```

Table 4-5

CALMET.DAT file - Data Records

| Record Type | Variable No. | Variable Name | Type[a] | Description |
|---|---|---|---|---|
| 1 | 1 | CLABU | char*8 | Variable label (‹U-LEVxxx', where xxx indicates the layer number) |
| 1 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 1 | 3 | U | real array | U-component (m/s) of the winds at each grid point |
| 2 | 1 | CLABV | char*8 | Variable label (‹V-LEVxxx', where xxx indicates the layer number) |
| 2 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 2 | 3 | V | real array | V-component (m/s) of the winds at each grid point |
| 3[b] | 1 | CLABW | char*8 | Variable label (‹WFACExxx"), where xxx indicates the layer number) |
| 3[b] | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 3[b] | 3 | W | real array | W-component (m/s) of the winds at each grid point |

(Record types 1,2,3 repeated NZ times (once per layer) as a set)

| Record Type | Variable No. | Variable Name | Type[a] | Description |
|---|---|---|---|---|
| 4[b] | 1 | CLABT | char*8 | Variable label (‹T-LEVxxx', where xxx indicates the layer number) |
| 4[b] | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 4[b] | 3 | ZTEMP | real array | Air temperature (deg. K) at each grid point |

(Record type 4 repeated NZM times (once per layer))

---

[a] char*8 = Character*8
[b] Record types 3 and 4 are included only if LCALGRD is TRUE

Table 4-5 (Continued)
CALMET.DAT file - Data Records

| Record Type | Variable No. | Variable Name | Type[a] | Description |
|---|---|---|---|---|
| 5 | 1 | CLABSC | char*8 | Variable label ('IPGT') |
| 5 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 5 | 3 | IPGT | integer array | PGT stability class at each grid point |
| 6 | 1 | CLABUS | char*8 | Variable label ('USTAR') |
| 6 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 6 | 3 | USTAR | real array | Surface friction velocity (m/s) |
| 7 | 1 | CLABZI | char*8 | Variable label ('ZI') |
| 7 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 7 | 3 | ZI | real array | Mixing height (m) |
| 8 | 1 | CLABL | char*8 | Variable label ('EL') |
| 8 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 8 | 3 | EL | real array | Monin-Obukhov length (m) |
| 9 | 1 | CLABWS | char*8 | Variable label ('WSTAR') |
| 9 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 9 | 3 | WSTAR | real array | Convective velocity scale (m/s) |
| 10 | 1 | CLABRMM | char*8 | Variable label ('RMM') |
| 10 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 10 | 3 | RMM | real array | Precipitation rate (mm/hr).  Not used by CALGRID. |

[a] char*8 = Character*8

Table 4-5 (Concluded)
CALMET.DAT file - Data Records

| Record Type | Variable No. | Variable Name | Type[a] | Description |
|---|---|---|---|---|
| 11 | 1 | CLABTK | char*8 | Variable label (⊲TEMPK') |
| 11 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 11 | 3 | TEMPK | real array | Temperature (deg. K) at each surface met. station |
| 12 | 1 | CLABD | char*8 | Variable label (⊲RHO') |
| 12 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 12 | 3 | RHO | real array | Air density ($kg/m^3$) at each surface met. station |
| 13 | 1 | CLABQ | char*8 | Variable label (⊲QSW') |
| 13 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 13 | 3 | QSW | real array | Short-wave solar radiation ($W/m^2$) at each surface met. station |
| 14 | 1 | CLABRH | char*8 | Variable label (⊲IRH') |
| 14 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 14 | 3 | IRH | integer array | Relative humidity (percent) at each surface met. station |
| 15 | 1 | CLABPC | char*8 | Variable label (⊲IPCODE') |
| 15 | 2 | NDATHR | integer | Year, Julian day and hour in the form YYYYJJJHH (or YYJJJHH) |
| 15 | 3 | IPCODE | integer array | Precipitation type code (not used by CALGRID)<br>0      - no precipitation<br>1 to 18    - liquid precipitation<br>19 to 45 - frozen precipitation |

---

[a] char*8 = Character*8

4.2.2    ISCMET.DAT

CALPUFF can be driven by a single-station standard ISC3-type of meteorological file, compatible with the earlier ISC2 version of the model, or the augmented ISC3-type of meteorological file.  In addition, the ISCMET.DAT file used by CALPUFF can accommodate an extended data record that includes the augmented ISC3 data plus variables not found in either a standard ISC3 data record, or the augmented ISC3 data record.  In the description to follow, we refer to the standard ISC3 file as the "base" ISC3 format.

CALPUFF is normally run with a full three-dimensional wind field and temperature field, as well as two-dimensional fields of mixing heights and other meteorological variables (see CALMET.DAT in Section 4.2.1).  However, in some near-field applications, when spatial variability of the meteorological fields may not be significant (e.g., uniform terrain and land use), the single-station data file may be used.  The model uses the data in the ISCMET.DAT file to fill the 2-D or 3-D arrays with the scalar values read from the file.  In single-station mode, CALPUFF assigns the single value of each variable read from the ISCMET.DAT file to all grid points, resulting in a spatially uniform gridded field.  However, the model does <u>not</u> assume that the meteorological conditions are steady-state, which allows the important effects of causality to be simulated even with the single-station meteorological data.  For example, the time required for plume material to reach a receptor is accounted for in the puff formulation, and curved trajectories and variable dispersion and stability conditions over multiple hours of transport will result even when using the single-station meteorological data.  However, in general, the preferred mode for most applications of CALPUFF is to use the spatially variable fields generated by CALMET.

The minimum data required in the ISCMET.DAT file includes hourly values of the vector flow direction, wind speed, temperature, stability class, and mixing height (urban or rural), which are found in the "base" ISC3 format.  In addition, if dry or wet deposition are being modeled, or if turbulence-based dispersion coefficients are to be computed based on micrometeorological parameters, hourly values of the surface friction velocity ($u_*$), Monin-Obukhov length (L), a time-varying surface roughness length ($z_o$), precipitation rate, and precipitation type code are entered on an extended record.  These additional variables are contained in the augmented ISC3 meteorological file.  If chemical transformation is being modeled, hourly values of short-wave solar radiation and relative humidity can also be included in the extended record.  In addition, hourly values of the potential temperature lapse rate ($d\theta/dz$) and power law profile exponent (p) can be entered.  Non-missing values of the basic meteorological variables (i.e., vector wind direction, wind speed, temperature, stability class, and mixing height) must be provided for all applications.  The data fields for the extended record variables ($u_*$, L, etc.) may be left blank if the CALPUFF options are set so that they are not needed (e.g., no wet or dry deposition, no chemical transformation, no computation of turbulence-based dispersion coefficients).  However, if the CALPUFF model options are set to require them, the model assumes that valid values of the extended record variables will be provided for every hour.  The only exceptions are $d\theta/dz$ and p, which can be entered for some hours and not others.  If values of $d\theta/dz$ or p are missing (i.e., blank) for a given hour, the model

will use its default or user-specified stability-dependent values (see the PLX0 and PTG0 variables in Input Group 12 of the control file).

Sample ISCMET.DAT files are shown in Tables 4-6(a) and 4-6(b). Part (a) of the table shows the "base" ISC3 meteorological data record. The fully extended data record is shown in Part (b) of the table. Table 4-7 lists the contents of the ISCMET.DAT header records, and Table 4-8 describes the data records.

Note that other data associated with the meteorological data in ISCMET.DAT are provided in the CALPUFF.INP control file. These data include the anemometer height, surface roughness length, land use type, elevation, and leaf area index of the modeling region. The anemometer height is required in the vertical power law extrapolation of the wind speed. The roughness length is used if turbulence-based dispersion coefficients are selected, and in the calculation of dry deposition velocities, when the hourly value is missing. The land use category is used to determine if urban or rural dispersion coefficients are appropriate when the Pasquill-Gifford/McElroy-Pooler dispersion coefficients are used. Also see the variables IURB1 and IURB2 in Input Group 12 of the control file. They define the range of land use categories that are to be considered urban (i.e., if the value of the land use category in the ISCMET.DAT file is between IURB1 and IURB2, inclusive, the modeling domain will be consider urban). Otherwise, it will be considered rural. The leaf area index is only used by the model if dry deposition velocities are being computed. The elevation is used to fill the 2-D terrain elevation array in CALPUFF that is normally filled from the CALMET file. This array is used to determine, through interpolation, the elevation of the *gridded* receptors generated by the model as an option. Because a single value is available when the ISCMET.DAT file is used, all of the gridded receptors will be assigned this elevation. Receptor-specific elevations are assigned to each *discrete* receptor by the user in the CALPUFF control file (see Input Group 17).

## Table 4-6
## Sample ISCMET.DAT files


### (a) Base Data Records

```
 94728     90  14735     90
90 1 1 1  81.0000   3.0866 280.9 5   881.5    53.0
90 1 1 2  98.0000   1.5433 279.8 6   904.6    53.0
90 1 1 3 114.0000   2.5722 279.8 5   927.8    53.0
90 1 1 4 113.0000   4.1155 280.4 4   951.0   951.0
90 1 1 5 103.0000   3.0866 279.8 5   974.2    53.0
90 1 1 6 102.0000   5.1444 280.4 4   997.4   997.4
90 1 1 7 105.0000   4.6300 280.4 4  1020.6  1020.6
90 1 1 8  73.0000   2.5722 280.4 4  1043.8  1043.8
90 1 1 9 117.0000   4.1155 280.9 4  1067.0  1067.0
90 1 110 141.0000   3.6011 283.7 3  1090.2  1090.2
 ↑ ↑ ↑ ↑      ↑        ↑     ↑   ↑     ↑       ↑
yr  dy   WD vect     WS  Temp    rural   urban
  mo  hr                    stab   zi      zi
```


### (b) Extended Data Records

```
 94728     90  14735     90
90 1 1 1  81.0000   3.0866 280.9 5   881.5    53.0    0.33    355.   0.25  0   0.0    .020  .35     0.  77
90 1 1 2  98.0000   1.5433 279.8 6   904.6    53.0    0.17    122.   0.25  0   0.0    .035  .55     0.  68
90 1 1 3 114.0000   2.5722 279.8 5   927.8    53.0    0.28    259.   0.25  0   0.0          .30     0.  72
90 1 1 4 113.0000   4.1155 280.4 4   951.0   951.0    0.45    655.   0.25  0   0.0          .15     0.  74
90 1 1 5 103.0000   3.0866 279.8 5   974.2    53.0    0.33    355.   0.25  0   0.0    .022          0.  75
90 1 1 6 102.0000   5.1444 280.4 4   997.4   997.4    0.56   1025.   0.25  1   .25          .18     0.  73
90 1 1 7 105.0000   4.6300 280.4 4  1020.6  1020.6    0.50  -1005.   0.25  0   0.0          .17    70.  71
90 1 1 8  73.0000   2.5722 280.4 4  1043.8  1043.8    0.28   -355.   0.25  1   .75                 120.  65
90 1 1 9 117.0000   4.1155 280.9 4  1067.0  1067.0    0.45   -395.   0.25  2  2.64          .22    180.  68
90 1 110 141.0000   3.6011 283.7 3  1090.2  1090.2    0.39   -148.   0.25  0   0.0          .12    240.  62
 ↑ ↑ ↑ ↑      ↑        ↑     ↑   ↑     ↑       ↑       ↑       ↑      ↑    ↑    ↑      ↑     ↑     ↑   ↑
yr  dy   WD vect     WS  Temp    rural   urban       u*       L     zo    p  precip.  dθ/dz  p    SW  rh
  mo  hr                    stab   zi      zi                             code  amt.             rad. %
```

Table 4-7

ISCMET.DAT File - Header Record


Record 1.  Surface and mixing height station numbers, and years.


| Record | Columns | Variable | Type | Description |
|--------|---------|----------|------|-------------|
| 1 | 1-6 | * | integer | Surface station number. |
| 1 | 8-13 | * | integer | Surface station year. |
| 1 | 15-20 | * | integer | Mixing height station number. |
| 1 | 22-27 | * | integer | Mixing height station year. |

\*   These variables are not interpreted in CALPUFF

Table 4-8
ISCMET.DAT File - Data Records
(One record per hour)


Records 2,3,4,...  Hourly meteorological data.


| Columns | Variable | Type | Description |
|---------|----------|------|-------------|
| | | | |
| | Base Data | | |
| 1-2 | IY | integer | Year of data in record |
| 3-4 | IM | integer | Month |
| 5-6 | ID | integer | Day |
| 7-8 | IH | integer | Hour (ISC3 convention (1-24) at end of hour) |
| 9-17 | FVEC | real | Flow vector (deg.) |
| 18-26 | WSPD | real | Wind speed (m/s) |
| 27-32 | TMPK | real | Temperature (deg. K) |
| 33-34 | KST | integer | Stability class (1-6) |
| 35-41 | RMIX | real | Rural mixing height (m) |
| 42-48 | UMIX | real | Urban mixing height (m) |
| | | | |
| | Extended data | | |
| 49-57 | USTR | real | Friction velocity (m/s) |
| 58-67 | XMON | real | Monin-Obukhov length (m) |
| 68-75 | Z0M | real | Surface roughness length (m) |
| 76-79 | IPC | integer | Precipitation type code |
| | | | 0        - no precipitation |
| | | | 1 to 18   - liquid precipitation |
| | | | 19 to 45 - frozen precipitation |
| 80-86 | PMMHR | real | Precipitation rate (mm/hr) |
| 87-96 | DTHTD | real | Potential temperature lapse rate (deg. K/m) |
| 97-101 | PLAW | real | Wind speed power law exponent |
| 102-110 | QSWRAD | real | Short-wave solar radiation ($W/m^2$) |
| 111-113 | IRH | integer | Relative humidity (%) |

4.2.3    PLMMET.DAT

In addition to the capability to use three-dimensional wind fields generated by CALMET, a single-station meteorological file can also be used by CALPUFF as its source of meteorological data.  One form of single station data accepted by CALPUFF is the AUSPLUME (Lorimer, 1976) type of data file.  The standard AUSPLUME data file can be used without modification, although some CALPUFF options require additional meteorological variables that must be added as part of an extended data record.

CALPUFF is normally run with a full three-dimensional wind field and temperature field, as well as two-dimensional fields of mixing heights and other meteorological variables (see CALMET.DAT in Section 4.2.1).  However, in some near-field applications, when spatial variability of the meteorological fields may not be significant (e.g., uniform terrain and land use), the single-station data file may be used.  In single station mode, CALPUFF assigns the single value of each variable read from the PLMMET.DAT file to all grid points, resulting in a spatially uniform gridded field.  However, the model does <u>not</u> assume the meteorological conditions are steady-state, which allows the important effects of causality to be simulated even with the single-station meteorological data.  For example, the time required for plume material to reach a receptor is accounted for in the puff formulation, and curved trajectories and variable dispersion and stability conditions over multiple hours of transport will result even when using the single-station meteorological data.  However, in general, the preferred mode for most applications of CALPUFF is to use the spatially variable fields generated by CALMET.

The PLMMET.DAT file includes the basic hourly data required by CALPUFF, including the wind direction, wind speed, temperature, stability class, and mixing height.  Note that PLMMET.DAT uses *wind direction* in the usual meteorological convention (i.e., winds from the west blowing toward the east has a value of 270°), while ISCMET.DAT uses *flow vector* (i.e., winds from the west toward the east have a vector direction of 90°).  The PLMMET.DAT format also contains data for the horizontal component of turbulence ($\sigma_\theta$).  If both components of turbulence are available, they should be entered through the use of the PROFILE.DAT data file (see Section 4.2.4).  Also, CALPUFF contains several options for modeling chemical transformation that do not involve the use of a decay constant.

The PLMMET.DAT format does not contain micrometeorological variables (the surface friction velocity and Monin-Obukhov length), precipitation data, solar radiation, or relative humidity.  The Monin-Obukhov length is inferred from the stability class and the surface roughness length using the Golder (1972) relations.  The friction velocity can then be estimated from the surface-layer similarity wind profile equation.  The remaining variables must be added to the standard file in an exended data record.  These fields may remain blank if they are not needed for the CALPUFF options selected.  Precipitation is needed for wet deposition modeling, and the solar radiation and humidity data are needed for chemical transformation calculations.

Sample PLMMET.DAT files are shown in Tables 4-9(a) and 4-9(b).  Part (a) of the table shows the

standard AUSPLUME meteorological data record. The extended data record is shown in Part (b) of the table. A description of the contents of the header record is provided in Table 4-10, and the data records are described in Table 4-11. The header record contains an 80-character title of the data set.

Note that other data associated with the PLMMET.DAT are provided in the CALPUFF.INP control file. These data include the anemometer height, surface roughness length, land use type, elevation, and leaf area index of the modeling region. The anemometer height is required in the vertical power law extrapolation of the wind speed. The roughness length is used to estimate the micrometeorological variables, the turbulence-based dispersion coefficients (when selected), and in the calculation of dry deposition velocities. The land use category is used to determine if urban or rural dispersion coefficients are appropriate when the Pasquill-Gifford/McElroy-Pooler dispersion coefficients are used. Also see the variables IURB1 and IURB2 in Input Group 12 of the control file. They define the range of land use categories that are to be considered urban (i.e., if the value of the land use category in the PLMMET.DAT file is between IURB1 and IURB2, inclusive, the modeling domain will be consider urban). Otherwise, it will be considered rural. The leaf area index is only used by the model if dry deposition velocities are being computed. The elevation is used to fill the 2-D terrain elevation array in CALPUFF that is normally filled from the CALMET file. This array is used to determine, through interpolation, the elevation of the *gridded* receptors generated by the model as an option. Because a single value is available here, all of the gridded receptors will be assigned this elevation. Receptor-specific elevations are assigned to each *discrete* receptor by the user in the CALPUFF control file (see Input Group 17).

Table 4-9
Sample PLMMET.DAT file

## (a) Base Data Records

```
Sample PLMMET.DAT data file.   Min. ws=1.0 m/s
94010101 19  1.0 270 F  100  17. 0.55 .035        0.
94010102 19  1.2 270 F  122  22.       .030       0.
94010103 20  1.5 270 F  132  18.                  0.
94010104 19  3.2 270 E  256       0.35            0.
94010105 20  1.8 270 F  103       0.45 .031       0.
94010106 20  3.3 270 E  201       0.32 .024       0.
94010107 21  5.0 270 D  284       0.25            0.
94010108 21  4.6 270 D  301  12.                  0.
94010109 22  3.5 270 D  525  11.                  0.
94010110 22  3.9 270 C  658  16. 0.19             0.
 ↑ ↑ ↑ ↑  ↑    ↑   ↑ ↑   ↑    ↑    ↑    ↑           ↑
yr  dy  Temp WS  WD    zi   σ_θ   p  dθ/dz  decay
  mo   hr            stab
```

## (b) Extended Data Records

```
Sample PLMMET.DAT data file.   Min. ws=1.0 m/s
94010101 19  1.0 270 F  100  17. 0.55 .035        0.  0       0.0       0. 65
94010102 19  1.2 270 F  122  22.       .030       0.  0       0.0       0. 69
94010103 20  1.5 270 F  132  18.                  0.  0       0.0       0. 65
94010104 19  3.2 270 E  256       0.35            0.  0       0.0       0. 66
94010105 20  1.8 270 F  103       0.45 .031       0.  0       0.0       0. 69
94010106 20  3.3 270 E  201       0.32 .024       0.  0       0.0       0. 73
94010107 21  5.0 270 D  284       0.25            0.  1       1.80      11. 78
94010108 21  4.6 270 D  301  12.                  0.  1        .95      82. 76
94010109 22  3.5 270 D  525  11.                  0.  0       0.0      116. 58
94010110 22  3.9 270 C  658  16. 0.19             0.  0       0.0      250. 55
 ↑ ↑ ↑ ↑  ↑    ↑   ↑ ↑   ↑    ↑    ↑    ↑           ↑  ↑        ↑         ↑  ↑
yr  dy  Temp WS  WD    zi   σ_θ   p  dθ/dz  decay  p    precip.     SW rh
  mo   hr            stab                        code   amount      rad. %
```

Table 4-10
PLMMET.DAT File - Header Record

Record 1.  Title.

| Record | Columns | Variable | Type | Description |
|--------|---------|----------|------|-------------|
| 1 | 1-80 | TITLE | character*80 | Title of file. |

# Table 4-11
## PLMMET.DAT File - Data Records
### (One record per hour)

Records 2,3,4,...  Hourly meteorological data.

| Columns | Variable | Type | Description |
|---|---|---|---|
| | **Base Data** | | |
| 1-2 | IY | integer | Year of data in record |
| 3-4 | IM | integer | Month |
| 5-6 | ID | integer | Day |
| 7-8 | IH | integer | Hour (1-24) time at end of hour |
| 9-11 | TMPC | real | Temperature (deg. C) |
| 12-16 | WSPD | real | Wind speed (m/s) |
| 17-20 | IWD | integer | Wind direction (deg.) |
| 21-22 | KST  * | character | Stability class (A-F) |
| 23-27 | ZMIX | real | Mixing height (m) |
| 28-32 | SIGTHA | real | $\sigma_\theta$ (deg.).  Or use PROFILE.DAT file for turbulence measurements. |
| 33-37 | PLEXP | real | Wind speed power law exponent |
| 38-42 | PTGDF | real | Potential temperature gradient (deg. K/m) |
| 43-52 | DECAY | real | Decay constant ($s^{-1}$).  Not used by CALPUFF. |
| | **Extended Data** | | |
| 53-55 | IPC | integer | Precipitation type code |
| | | | 0        - no precipitation |
| | | | 1 to 18   - liquid precipitation |
| | | | 19 to 45 - frozen precipitation |
| 56-64 | PMMHR | real | Precipitation rate (mm/hr) |
| 65-73 | QSWRAD | real | Short-wave solar radiation ($W/m^2$) |
| 74-76 | IRELHUM | integer | Relative humidity (%) |

\* KST is converted from character (A-F) to integer (1-6)

### 4.2.4   SURFACE.DAT and PROFILE.DAT

In addition to the capability to use three-dimensional wind fields generated by CALMET, a single-station meteorological file can also be used by CALPUFF as its source of meteorological data.  One form of single station data accepted by CALPUFF is the CTDMPLUS (Perry et al., 1989) form.  The standard meteorological data files SURFACE.DAT and PROFILE.DAT can be used without modification, although some CALPUFF options require additional meteorological variables that must be added as part of an extended data record to SURFACE.DAT.  Unlike the other two types of single-station data described above, the PROFILE.DAT file contains a vertical profile of data each hour, rather than measurements made at a single height above ground.  In this way, more detailed data from an on-site tower with supporting remote measurement platforms (e.g., SODAR) can be used to define the vertical structure of the flow.  SURFACE.DAT contains calculated micrometeorological variables and the mixing height.

CALPUFF is normally run with a full three-dimensional wind field and temperature field, as well as two-dimensional fields of mixing heights and other meteorological variables (see CALMET.DAT in Section 4.2.1).  However, in some near-field applications, when spatial variability of the meteorological fields may not be significant (e.g., uniform terrain and land use), the single-station data file may be used.  In single station mode, CALPUFF assigns the single value of each variable read from the file to all grid points, resulting in a spatially uniform gridded field.  However, the model does <u>not</u> assume the meteorological conditions are steady-state, which allows the important effects of causality to be simulated even with the single-station meteorological data.  For example, the time required for plume material to reach a receptor is accounted for in the puff formulation, and curved trajectories and variable dispersion and stability conditions over multiple hours of transport will result even when using the single-station meteorological data.  However, in general, the preferred mode for most applications of CALPUFF is to use the spatially variable fields generated by CALMET.

SURFACE.DAT is created by the CTDMPLUS meteorological preprocessor, and the user should consult the CTDMPLUS documentation to learn of its use and requirements.  SURFACE.DAT includes hourly mixing height, surface friction velocity, Monin-Obukhov length, and surface roughness.  PROFILE.DAT is created directly by the user.  In standard form, it includes the hourly wind direction, wind speed (vector and scalar), temperature, and turbulence ($\sigma_w$, and either $\sigma_v$ or $\sigma_\theta$) at each measurement level.  Note that PROFILE.DAT uses *wind direction* in the usual meteorological convention (i.e., winds from the west blowing toward the east has a value of $270°$).

As an option, a non-standard, or extended version of PROFILE.DAT can also be used to provide the temperature jump across an inversion above a mixed layer.  This jump is used as a measure of the strength of the temperature inversion when assessing the ability of a buoyant plume to penetrate the top of the mixed layer (for the partial penetration option: MPARTL = 1).  When a positive temperature difference is provided at the end of the <u>first</u> record for the hour, CALPUFF will recognize it and use it.

Otherwise, available temperature gradient data are used to estimate the inversion strength.

Precipitation data, solar radiation, and relative humidity are not required in CTDMPLUS. They may be added to SURFACE.DAT in an exended data record. These fields may remain blank if they are not needed for the CALPUFF options selected. Precipitation is needed for wet deposition modeling, and the solar radiation and humidity data are needed for chemical transformation calculations.

Other data associated with the SURFACE.DAT and PROFILE.DAT are provided in the CALPUFF.INP control file. These data include the land use type, elevation, and leaf area index of the modeling region, and two control variables (ISIGMAV and IMIXCTDM). The land use category is used to determine if urban or rural dispersion coefficients are appropriate when the Pasquill-Gifford/McElroy-Pooler dispersion coefficients are used during convective regimes. Also see the variables IURB1 and IURB2 in Input Group 12 of the control file. They define the range of land use categories that are to be considered urban (i.e., if the value of the land use category is between IURB1 and IURB2, inclusive, the modeling domain will be consider urban). Otherwise, it will be considered rural. The leaf area index is only used by the model if dry deposition velocities are being computed. The elevation is used to fill the 2-D terrain elevation array in CALPUFF that is normally filled from the CALMET file. This array is used to determine, through interpolation, the elevation of the *gridded* receptors generated by the model as an option. Because a single value is available here, all of the gridded receptors will be assigned this elevation. Receptor-specific elevations are assigned to each *discrete* receptor by the user in the CALPUFF control file (see Input Group 17). ISIGMAV indicates the form of the lateral turbulence data, and IMIXCTDM indicates which mixing height field (observed or calculated) is to be used.

Sample SURFACE.DAT files are shown in Tables 4-12(a) and 4-12(b). Part (a) of the table shows the standard SURFACE.DAT data record. The extended data record is shown in Part (b) of the table. A sample PROFILE.DAT file is shown in Table 4-13. Data records for SURFACE.DAT are described in Table 4-14, and data records for PROFILE.DAT are described in Table 4-15. Note that the year may be specified in either a YY (e.g., 94) or YYYY (e.g., 1994) format. The YY format is the original CTDM PLUS format.

The PROFILE.DAT file may also be used in conjunction with the other meteorological data options in CALPUFF to provide measured turbulence data, or to provide the strength of the temperature inversion. When turbulence data are supplied, wind speeds should be provided in the file as well as the turbulence, so that conversions between $\sigma_v$ and $\sigma_\theta$ can be made.

## Table 4-12
## Sample SURFACE.DAT file


### (a) Base Data Records


```
94  1  1   1   1        658.       30.      0.047       15.7  0.500E+00
94  1  1   1   2        658.       37.      0.067       15.7  0.500E+00
94  1  1   1   3        658.       35.      0.060       15.7  0.500E+00
94  1  1   1   4        658.       33.      0.053       15.7  0.500E+00
94  1  1   1   5        658.       30.      0.047       15.7  0.500E+00
94  1  1   1   6        658.       35.      0.060       15.7  0.500E+00
94  1  1   1   7        658.      125.      0.202       61.1  0.500E+00
94  1  1   1   8         61.       44.      0.093       15.7  0.500E+00
94  1  1   1   9        160.       44.      0.093       15.7  0.500E+00
94  1  1   1  10        260.      858.      0.285     -143.0  0.500E+00
 ↑  ↑  ↑   ↑   ↑          ↑         ↑         ↑          ↑          ↑
Yr    Dy Jul Hr        Ziobs     Zipre     Ustar      Monin       Zo
    Mo     Dy                                         Obukhov
```


### (b) Extended Data Records


```
94  1  1   1   1        658.       30.      0.047       15.7  0.500E+00   0      0.0      0. 65
94  1  1   1   2        658.       37.      0.067       15.7  0.500E+00   0      0.0      0. 69
94  1  1   1   3        658.       35.      0.060       15.7  0.500E+00   0      0.0      0. 65
94  1  1   1   4        658.       33.      0.053       15.7  0.500E+00   0      0.0      0. 66
94  1  1   1   5        658.       30.      0.047       15.7  0.500E+00   0      0.0      0. 69
94  1  1   1   6        658.       35.      0.060       15.7  0.500E+00   0      0.0      0. 73
94  1  1   1   7        658.      125.      0.202       61.1  0.500E+00   1     1.80      0. 78
94  1  1   1   8         61.       44.      0.093       15.7  0.500E+00   1      .95      0. 76
94  1  1   1   9        160.       44.      0.093       15.7  0.500E+00   0      0.0      6. 58
94  1  1   1  10        260.      858.      0.285     -143.0  0.500E+00   0      0.0    250. 55
 ↑  ↑  ↑   ↑   ↑          ↑         ↑         ↑          ↑         ↑      ↑  ↑      ↑     ↑  ↑
Yr    Dy Jul Hr        Ziobs     Zipre     Ustar      Monin       Zo   p  precip.   SW rh
    Mo     Dy                                         Obukhov        code amount    rad. %
```

## Table 4-13
## Sample PROFILE.DAT file

### (a) Base Data Records

```
94  1  1  1    2. 0 -999.9   -9.9  259.6  -99.9 -9.90 -999.9
94  1  1  1   10. 0  156.4    0.7  263.2   42.5  0.01 -999.9
94  1  1  1   40. 0 -999.9   -9.9  265.4  -99.9 -9.90 -999.9
94  1  1  1   70. 0  177.9    2.4  266.0   18.3  0.16 -999.9
94  1  1  1  100. 0  207.1    3.0  266.3   23.9  0.20 -999.9
94  1  1  1  120. 0  218.0    2.8 -999.9  -99.9 -9.90 -999.9
94  1  1  1  150. 0  233.0    4.3 -999.9  -99.9 -9.90 -999.9
94  1  1  1  180. 0  238.0    6.0 -999.9  -99.9 -9.90 -999.9
94  1  1  1  210. 1  242.0    7.2 -999.9  -99.9 -9.90 -999.9
94  1  1  2    2. 0 -999.9   -9.9  258.9  -99.9 -9.90 -999.9
94  1  1  2   10. 0  162.9    1.0  262.1   28.8  0.01 -999.9
94  1  1  2   40. 0 -999.9   -9.9  263.9  -99.9 -9.90 -999.9
94  1  1  2   70. 0  155.6    2.2  265.4    8.9  0.09 -999.9
94  1  1  2  100. 0  179.1    1.8  266.0   10.5  0.10 -999.9
94  1  1  2  120. 0  191.0    1.8 -999.9  -99.9 -9.90 -999.9
94  1  1  2  150. 0  224.0    2.2 -999.9  -99.9 -9.90 -999.9
94  1  1  2  180. 0  246.0    3.2 -999.9  -99.9 -9.90 -999.9
94  1  1  2  210. 0  259.0    4.7 -999.9  -99.9 -9.90 -999.9
94  1  1  2  240. 0  265.0    6.1 -999.9  -99.9 -9.90 -999.9
94  1  1  2  270. 0  268.0    7.3 -999.9  -99.9 -9.90 -999.9
 ↑  ↑  ↑  ↑    ↑ ↑     ↑       ↑     ↑       ↑     ↑      ↑
Yr Mo Dy Hr    Z Ilast WD     WS   Temp    σ_v   σ_w     WS
                            Scalar                      Vector
```

### (b) Extended Data Records

```
94  1  1 13    2. 0 -999.9   -9.9  275.8  -99.9 -9.90 -999.9   .18
94  1  1 13   10. 0  162.9    0.9  275.6   51.6  0.03 -999.9
94  1  1 13   40. 0 -999.9   -9.9  274.6  -99.9 -9.90 -999.9
94  1  1 13   70. 0  176.5    2.6  274.4    8.9  0.11 -999.9
94  1  1 13  100. 0  185.3    2.7  274.1   14.0  0.10 -999.9
94  1  1 13  120. 0  194.0    2.0 -999.9  -99.9 -9.90 -999.9
94  1  1 13  150. 0  225.0    1.8 -999.9  -99.9 -9.90 -999.9
94  1  1 13  180. 0  259.0    2.3 -999.9  -99.9 -9.90 -999.9
94  1  1 13  210. 1  269.0    3.5 -999.9  -99.9 -9.90 -999.9
94  1  1 14    2. 0 -999.9   -9.9  275.8  -99.9 -9.90 -999.9
94  1  1 14   10. 0  162.9    0.9  275.6   51.6  0.03 -999.9
94  1  1 14   40. 0 -999.9   -9.9  274.6  -99.9 -9.90 -999.9
94  1  1 14   70. 0  176.5    2.6  274.4    8.9  0.11 -999.9
94  1  1 14  100. 0  185.3    2.7  274.1   14.0  0.10 -999.9
94  1  1 14  120. 0  194.0    2.0 -999.9  -99.9 -9.90 -999.9
94  1  1 14  150. 0  225.0    1.8 -999.9  -99.9 -9.90 -999.9
94  1  1 14  180. 0  259.0    2.3 -999.9  -99.9 -9.90 -999.9
94  1  1 14  210. 1  269.0    3.5 -999.9  -99.9 -9.90 -999.9
94  1  1 15    2. 0 -999.9   -9.9  275.8  -99.9 -9.90 -999.9   .5
94  1  1 15   10. 0  162.9    0.9  275.6   51.6  0.03 -999.9
94  1  1 15   40. 0 -999.9   -9.9  274.6  -99.9 -9.90 -999.9
94  1  1 15   70. 0  176.5    2.6  274.4    8.9  0.11 -999.9
94  1  1 15  100. 0  185.3    2.7  274.1   14.0  0.10 -999.9
 ↑  ↑  ↑  ↑    ↑ ↑     ↑       ↑     ↑       ↑     ↑      ↑       ↑
Yr Mo Dy Hr    Z Ilast WD     WS   Temp    σ_v   σ_w     WS     ΔT at
                            Scalar                      Vector Inversion
```

Table 4-14
SURFACE.DAT File - Data Records
(One record per hour)


Records 1,2,3,... Hourly meteorological data.


| Columns | Variable | Type | Description |
|---------|----------|------|-------------|
| | | | |
| | Base Data | | |
| * | IY | integer | Year of data in record (YY or YYYY format) |
| * | IM | integer | Month |
| * | ID | integer | Day |
| * | IJUL | integer | Julian day (1-366) |
| * | IH | integer | Hour (1-24) at end of hour |
| * | ZIOBS | real | Observed mixing height (m) |
| * | ZIPRE | real | Calculated mixing height (m) |
| * | USTR | real | Surface friction velocity (m/s) |
| * | XMON | real | Monin-Obukhov length (m) |
| * | Z0M | real | Hourly surface roughness length (m) |
| | | | |
| | Extended Data | | |
| * | IPC | integer | Precipitation type code |
| | | | 0 - no precipitation |
| | | | 1 to 18 - liquid precipitation |
| | | | 19 to 45 - frozen precipitation |
| * | PMMHR | real | Precipitation rate (mm/hr) |
| * | QSWRAD | real | Short-wave solar radiation ($W/m^2$) |
| * | IRELHUM | integer | Relative humidity (%) |

* Free format

Table 4-15
PROFILE.DAT File - Data Records
(One or more records per hour)


Records 1,2,3,...  Hourly meteorological data.


| Columns | Variable | Type | Description |
|---|---|---|---|
| | Base Data | | |
| * | IY | integer | Year of data in record (YY or YYYY format) |
| * | IM | integer | Month |
| * | ID | integer | Day |
| * | IH | integer | Hour (1-24) time at end of hour |
| * | ZPRF | real | Height of measurement above ground (m) |
| * | ILAST | integer | 0 if not the highest (last) level; otherwise 1 |
| * | WDPRF | real | Wind direction (deg.) |
| * | SSPRF | real | Scalar wind speed (m/s) |
| * | TPRF | real | Ambient dry bulb temperature (K) |
| * | SVPRF | real | $\sigma_\theta$ (deg.) or $\sigma_v$ (m/s) |
| * | SWPRF | real | $\sigma_w$ (m/s) |
| * | WSPRF | real | Vector wind speed (m/s) |
| | Extended Data | | |
| * | DPTINV | real | Increase in potential temperature across the inversion at the top of the mixed layer (K); only on first record each hour |

* Free format, one record per height in ascending order

4.3     Point Source Emissions File With Arbitrarily Varying Emissions (PTEMARB.DAT)

The PTEMARB.DAT file contains point source emissions data for sources with detailed, arbitrarily varying emissions parameters. In the PTEMARB.DAT file, values for the stack parameters and emission rates can be specified for each time step in the run. Plume rise is computed within the CALPUFF model for each source.

PTEMARB.DAT may be provided as either a sequential unformatted data file, or as a free-formatted ASCII data file (see Table 4-16 for an example). Both of these use the same record structure consisting of three header records, followed by a set of data records containing time-invariant source information, and a set of records for the time-varying data. The time-invariant records contain the stack height, diameter, coordinates, building downwash flag, one user-defined optional descriptive code for each source, and controlling building heights and widths (36 values for every 10°) for each source identified by the building downwash flag. The time varying emissions and stack parameter data follow in subsequent records. One data record per source is required for each time period (e.g.,usually at hourly intervals).

The data in the PTEMARB.DAT file are independent of the horizontal and vertical grid systems being used in the model. The horizontal coordinates are specified in terms of the meteorological grid projection (UTM or Lambert conformal coordinates). The vertical layers receiving the emissions of the source are based on the plume rise of the source computed internally by the model. However, the PTEMARB.DAT file does contain time-dependent data specifying the emission parameters for a particular time period.

**NOTE**: There are structural differences between the PTEMARB.DAT file accepted by CALPUFF (Version 5.0) and that accepted by earlier versions, so anyone familiar with the previous versions must be certain to review the contents of the next few pages! CALPUFF (5.0) will test the variable VRS2 contained in the header of PTEMARB.DAT to see that it identifies the correct version. If the file uses an older format, changing VRS2 to the correct value will disable this check, and the results of the CALPUFF application may be in error. Do not use an "old" version of this data file unless you are certain that the format is correct.

Table 4-16

Sample PTEMARB.DAT file

```
'PTEMARB'      3     2    16   1988011      1   1988012      0  '5'     'EXAMPLE'
'POL1'    'POL2'
       30.000      30.000
'Source 1'      0.13489    0.00360 18.600   9.754   88.70   1.00    0.00
   18.590   18.590   18.590   27.430   28.960   14.330
   18.590   18.590   18.590   18.590   28.960   18.590
   18.590   18.590   18.590   18.590   18.590   18.590
   18.590   18.590   18.590   27.430   28.960   28.960
   28.960   28.960   28.960   28.960   28.960   18.590
   18.590   18.590   18.590   18.590   18.590   18.590
   19.010   26.080   22.550   96.020   88.200   14.330
   14.200   18.480   22.160   25.660   85.390   20.820
   21.590   21.690   22.250   22.320   21.720   20.450
   19.010   26.080   22.550   53.360   88.200   87.590
   84.330   85.190   87.930   88.000   85.390   20.820
   21.590   21.690   22.250   22.320   21.720   20.450
'Source 2'      0.07380   -0.00280 50.100   4.251   88.70   0.00    0.00
'Source 3'      0.01272   -0.00919 35.850   3.100   88.70   0.00    0.00
   1988011      1  1988011      1
'Source 1'   280.55      8.66  0.468814E+01  0.202236E+02
'Source 2'   380.4       8.66  610.          120.
'Source 3'   280.55      2.66  0.468814E+01  0.202236E+02
   1988011      2  1988011      2
'Source 1'   279.27      8.50  0.449538E+01  0.204942E+02
'Source 2'   380.4       8.66  0.0           0.0
'Source 3'   279.27      2.66  0.449538E+01  0.204942E+02
   1988011      3  1988011      3
'Source 1'   279.26      8.50  0.449753E+01  0.204895E+02
'Source 2'   380.4       8.66  0.0           0.0
'Source 3'   279.26      2.66  0.449753E+01  0.204895E+02
   1988011      4  1988011     23
'Source 1'   277.97      8.41  0.430570E+01  0.207542E+02
'Source 2'   380.4       8.66  0.0           0.0
'Source 3'   277.97      2.66  0.430570E+01  0.207542E+02
   1988012      0  1988012      0
'Source 1'   285.82      8.90  0.553510E+01  0.189712E+02
'Source 2'   380.4       8.66  610.          120.
'Source 3'   285.82      2.66  0.553510E+01  0.189712E+02
```

**PTEMARB.DAT File - Header Records**

The header records of the PTEMARB.DAT file (see Table 4-17) contain the number of sources, starting and ending time periods of data in the file, and a list of the emitted species. Sample Fortran read statements for the unformatted file are:

```
      READ(iunit)FNAME2,NSRC2,NSE2,IUTMZ2,IBDAT2,IBTIM2,IEDAT2,
    1 IETIM2,VRS2,LABEL2

      READ(iunit)CSLST2
      READ(iunit)XMWEM2
```

where the following declarations apply:

```
      CHARACTER*12 FNAME2,VRS2,LABEL2,CSLST2(nse2)
      REAL XMWEM2(nse2)
```

Table 4-17

PTEMARB.DAT - Header Record 1 - General Data

| No. | Variable | Typeᵃ | Description | Sample Values |
|-----|----------|-------|-------------|---------------|
| 1 | FNAME2 | C*12 | Data set name | PTEMARB |
| 2 | NSRC2 | integer | Number of sources in the file | 10 |
| 3 | NSE2 | integer | Number of species emitted | 3 |
| 4 | IUTMZ2 | integer | UTM zone in which source coordinates are specified (enter 0 if using Lambert conformal coordinates) | 11 |
| 5 | IBDAT2 | integer | Date of beginning of data in the file (YYYYJJJ, where YYYY=year, JJJ=Julian day) | 1984220 |
| 6 | IBTIM2 | integer | Hour of beginning of data in the file (00-23, LST; end of hour) | 00 |
| 7 | IEDAT2 | integer | Date of end of data in the file (YYYYJJJ, where YYYY=year, JJJ=Julian day) | 1984224 |
| 8 | IETIM2 | integer | Hour of end of data in the file (00-23, LST; end of hour) | 23 |
| 9 | VRS2 | C*12 | Data set version = CALPUFF version | 5 |
| 10 | LABEL2 | C*12 | Data set label | Major pts. |

ᵃ C*12 = Character*12

(Note: YYJJJ date format formerly used is also accepted.)

Table 4-17 (Continued)
PTEMARB.DAT - Header Record 2 - Species List

| No.[*] | Type[a] | Description | Sample Values |
|------|------|-------------|---------------|
| 1 | C*12 | Species identifier for species 1 | SO2 |
| 2 | C*12 | Species identifier for species 2 | SO4 |
| . | . | . | . |
| . | . | . | . |
| . | . | . | . |
| NSE2 | C*12 | Species identifier for species "NSE2" | NOX |

[*] "NSE2" elements of CSLST2 array

[a] C*12 = Character*12

Table 4-17 (Concluded)

PTEMARB.DAT - Header Record 3 - Molecular Weights

| No.[*] | Type[a] | Description | Sample Values |
|---|---|---|---|
| 1 | real | Molecular weight for species 1 | 64. (SO2) |
| 2 | real | Molecular weight for species 2 | 96. (SO4) |
| . | . | . | . |
| . | . | . | . |
| . | . | . | . |
| NSE2 | real | Molecular weight for species "NSE2" | 30. (NOX as NO) |

[*] "NSE2" elements of XMWEM2 array

## PTEMARB.DAT File - Data Records

The PTEMARB.DAT file contains two types of data records.  A set of time-invariant records (see Table 4-18) are read after the header records.  These records specify the time-invariant source parameters, including the source coordinates, stack height, diameter, and building data for sources subject to building downwash.  A set of time-varying data follows (see Table 4-19).  The time-varying records contain the stack temperature, exit velocity, and emission rate for each species.

Sample Fortran read statements for time-invariant data records in the unformatted file are:

```
┌── Loop over sources
│
│       READ(iunit)CID,TIDATA
│       READ(iunit)BHT (only if TIDATA(6) = 1)
│       READ(iunit)BWD (only if TIDATA(6) = 1)
│
└── End loop over sources
```

where the following declarations apply:

```
        CHARACTER*16 CID

        REAL TIDATA(7), BHT(36), BWD(36)
```

Sample Fortran read statements for time-varying data records in the unformatted file are:

```
    ┌── Loop over time periods
    │
    │   READ(iunit)IBDAT,IBTIM,IEDAT,IETIM
    │
    │       ┌── Loop over sources
    │       │
    │       │   READ(iunit)CID,TEMPK,VEXIT,QEMIT
    │       │
    │       └── End loop over sources
    │
    └── End loop over time periods
```

where the following declarations apply:

```
        CHARACTER*16 CID
        REAL QEMIT(nse2)
```

Table 4-18

PTEMARB.DAT - Time-Invariant Data Record Contents

(Repeated for each source)

| Data Record No. | Variable No. | Variable | Type[a] | Description |
|---|---|---|---|---|
| 1 | 1 | CID | C*16 | Source identifier (16 characters = 4 words) |
| 1 | 2 | TIDATA(1) | real | Easting UTM or Lambert conformal coordinate (km) of the source |
| 1 | 3 | TIDATA(2) | real | Northing UTM or Lambert conformal coordinate (km) of the source |
| 1 | 4 | TIDATA(3) | real | Stack height (m) |
| 1 | 5 | TIDATA(4) | real | Stack diameter (m) |
| 1 | 6 | TIDATA(5) | real | Stack base elevation (m) |
| 1 | 7 | TIDATA(6) | real | Building downwash flag (0 = no, 1 = yes) |
| 1 | 8 | TIDATA(7) | real | User defined flag (e.g., fuel code) |
| 2[b] | 1-36 | BHT | real | Controlling building heights (m) for each 10° flow direction, starting 10° from North |
| 3[b] | 1-36 | BWD | real | Controlling building width (m) for each 10° flow direction, starting 10° from North |

[a]   C*16 = Character*16

[b]   Time-invariant data Records 2 and 3 are provided only for those sources identified as being subject to building downwash

Table 4-19

PTEMARB.DAT - Time-Varying Data Record Contents

(First record of "NSRC2"+1 records required for each time period)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | IBDAT | integer | Beginning date for which data in this set is valid (YYYYJJJ, where YYYY=year, JJJ=Julian day) |
| 2 | IBTIM | integer | Beginning hour for which data in this set is valid (00-23, LST; end of hour) |
| 3 | IEDAT | integer | Ending date for which data in this set is valid (YYYYJJJ, where YYYY=year, JJJ=Julian day) |
| 4 | IETIM | integer | Ending hour for which data in this set is valid (00-23, LST; end of hour) |

Example:
Data on each record is valid for 1 hour:
IBDAT=1989183,IBTIM=00,IEDAT=1989183,IETIM=00
IBDAT=1989183,IBTIM=01,IEDAT=1989183,IETIM=01
IBDAT=1989183,IBTIM=02,IEDAT=1989183,IETIM=02

Data on each record is valid for 3 hours:
IBDAT=1989183,IBTIM=00,IEDAT=1989183,IETIM=02
IBDAT=1989183,IBTIM=03,IEDAT=1989183,IETIM=05
IBDAT=1989183,IBTIM=06,IEDAT=1989183,IETIM=08

(Note: YYJJJ date format formerly used is also accepted.)

Table 4-19 (Concluded)
PTEMARB.DAT - Time-Varying Data Record Contents
(Next "NSRC2" records)

| No. | Variable | Type[a] | Description |
|---|---|---|---|
| 1 | CID | C*16 | Source identifier (must match values in time-invariant records) |
| 2 | TEMPK | real | Exit temperature (deg. K) |
| 3 | VEXIT | real | Exit velocity (m/s) |
| Next NSE2 | QEMIT | real array | Emission rates (g/s) for each species in the order specified in Header Record 2 |

[a]C*16 = Character*16

4.4     Buoyant Area Source Emissions File With Arbitrarily Varying Emissions (BAEMARB.DAT)

The BAEMARB.DAT file contains buoyant area source emissions data for sources with detailed, arbitrarily varying emissions parameters.  This file can be generated from the output of the Forest Service's Emissions Production Model (EPM) using a reformatting and preprocessing program provided with CALPUFF.  In the BAEMARB.DAT file, values for the source parameters and emission rates can be specified for each time step in the run.  Plume rise is computed within the CALPUFF model for each source using the numerical plume rise algorithm.

BAEMARB.DAT is a free-formatted ASCII data file (see Table 4-20 for an example) consisting of three header records, followed by a set of data records containing source information.  The time-invariant data records contain character source identifiers.  The time varying emissions and source parameter data follow in subsequent records.  One data record per source is required for each time period (e.g.,usually at hourly intervals).

The data in the BAEMARB.DAT file are independent of the horizontal and vertical grid systems being used in the model.  The horizontal coordinates are specified in terms of UTM or Lambert conformal coordinates.  The vertical layers receiving the emissions of the source are based on the plume rise of the source computed internally by the model.  However, the BAEMARB.DAT file does contain time-dependent data specifying the emission parameters for a particular time period.

**NOTE**:  There are structural differences between the BAEMARB.DAT file accepted by CALPUFF (Version 5.0) and that accepted by earlier versions, so anyone familiar with the previous versions must be certain to review the contents of the next few pages!  CALPUFF (V5.0) will test the variable VRS3 contained in the header of BAEMARB.DAT to see that it identifies the correct version.  If the file uses an older format, changing VRS3 to the correct value will disable this check, and the results of the CALPUFF application may be in error.  Do not use an "old" version of this data file unless you are certain that the format is correct.

Table 4-20

Sample BAEMARB.DAT file

```
'BAEMARB'    3   3   0   1995001   0    1995142  12  '5'    'NOX_FIRE_RUN'
'SO2'  'NO'   'NO2'
     64.0000       30.0000        46.0000
'Fire_Number_1'
'Fire_Number_2'
'Fire_Number_3'
       1995001          0   1995142         10
'Fire_Number_1'   -84.8600     -84.7423     -84.7423     -84.8600
    -254.620      -254.620     -254.502     -254.502      1.00000
    2259.00       1126.35      5.76000      7.98000      10.0000
    0.000000      0.000000     0.000000
'Fire_Number_2'   -167.190     -167.029     -167.029     -167.190
    29.0900       29.0900      29.2514      29.2514      1.00000
    1545.00       1126.35      2.97000      20.5500      10.0000
    0.000000      0.000000     0.000000
'Fire_Number_3'   -65.0600     -64.9668     -64.9668     -65.0600
    -88.9500      -88.9500     -88.8568     -88.8568      1.00000
    1527.00       1126.35      19.1300      3.92000      10.0000
    0.000000      0.000000     0.000000
       1995142         11   1995142         11
'Fire_Number_1'   -84.8600     -84.7423     -84.7423     -84.8600
    -254.620      -254.620     -254.502     -254.502      1.00000
    2259.00       1126.35      5.76000      7.98000      10.0000
    0.000000      3.94435      0.672000
'Fire_Number_2'   -167.190     -167.029     -167.029     -167.190
    29.0900       29.0900      29.2514      29.2514      1.00000
    1545.00       1126.35      2.97000      20.5500      10.0000
    0.000000      155.367      26.4700
'Fire_Number_3'   -65.0600     -64.9668     -64.9668     -65.0600
    -88.9500      -88.9500     -88.8568     -88.8568      1.00000
    1527.00       1126.35      19.1300      3.92000      10.0000
    0.000000      0.000000     0.000000
       1995142         12   1995142         12
'Fire_Number_1'   -84.8600     -84.6562     -84.6562     -84.8600
    -254.620      -254.620     -254.416     -254.416      1.00000
    2259.00       1126.35      5.76000      11.2800      10.0000
    0.000000      11.8389      2.01700
'Fire_Number_2'   -167.190     -166.910     -166.910     -167.190
    29.0900       29.0900      29.3695      29.3695      1.00000
    1545.00       1126.35      2.97000      29.0600      10.0000
    0.000000      466.102      79.4100
'Fire_Number_3'   -65.0600     -64.9668     -64.9668     -65.0600
    -88.9500      -88.9500     -88.8568     -88.8568      1.00000
    1527.00       1126.35      19.1300      3.92000      10.0000
    0.000000      0.000000     0.000000
```

**BAEMARB.DAT File - Header Records**

The header records of the BAEMARB.DAT file (see Table 4-21) contain the number of sources, starting and ending time periods of data in the file, and a list of the emitted species.  Sample Fortran read statements are:

```
    READ(iunit,*)FNAME3,NSRC3,NSE3,IUTMZ3,IBDAT3,IBTIM3,IEDAT3,
1 IETIM3,VRS3,LABEL3

    READ(iunit,*)CSLST3
    READ(iunit,*)XMWEM3
```

where the following declarations apply:

```
    CHARACTER*12 FNAME3,VRS3,LABEL3,CSLST3(nse3)
    REAL XMWEM3(nse3)
```

Table 4-21

BAEMARB.DAT - Header Record 1 - General Data

| No. | Variable | Type[a] | Description | Sample Values |
|-----|----------|---------|-------------|---------------|
| 1 | FNAME3 | C*12 | Data set name | BAEMARB |
| 2 | NSRC3 | integer | Number of sources in the file | 10 |
| 3 | NSE3 | integer | Number of species emitted | 3 |
| 4 | IUTMZ3 | integer | UTM zone in which source coordinates are specified (enter 0 is using Lambert conformal coordinates) | 11 |
| 5 | IBDAT3 | integer | Date of beginning of data in the file (YYYYJJJ, where YYYY=year, JJJ=Julian day) | 1984220 |
| 6 | IBTIM3 | integer | Hour of beginning of data in the file (00-23, LST; end of hour) | 00 |
| 7 | IEDAT3 | integer | Date of end of data in the file (YYYYJJJ, where YYYY=year, JJJ=Julian day) | 1984224 |
| 8 | IETIM3 | integer | Hour of end of data in the file (00-23, LST; end of hour) | 23 |
| 9 | VRS3 | C*12 | Data set version = CALPUFF version | 5 |
| 10 | LABEL3 | C*12 | Data set label | Burn #1 |

[a] C*12 = Character*12

(Note: YYJJJ date format formerly used is also accepted.)

Table 4-21 (Continued)
BAEMARB.DAT - Header Record 2 - Species List

| No.[*] | Type[a] | Description | Sample Values |
|---|---|---|---|
| 1 | C*12 | Species identifier for species 1 | PM |
| 2 | C*12 | Species identifier for species 2 | PM10 |
| . | . | . | . |
| . | . | . | . |
| . | . | . | . |
| NSE3 | C*12 | Species identifier for species "NSE3" | PM25 |

[*] "NSE3" elements of CSLST3 array
[a] C*12 = Character*12

Table 4-21 (Concluded)

BAEMARB.DAT - Header Record 3 - Molecular Weights

| No.[*] | Type[a] | Description | Sample Values |
|------|------|-------------|---------------|
| 1 | real | Molecular weight for species 1 | 200. |
| 2 | real | Molecular weight for species 2 | 200. |
| . | . | . | . |
| . | . | . | . |
| . | . | . | . |
| NSE3 | real | Molecular weight for species "NSE3" | 200. |

[*] "NSE3" elements of XMWEM3 array

# BAEMARB.DAT File - Data Records

The BAEMARB.DAT file contains two types of data records.  A set of time-invariant records (see Table 4-22) are read after the header records.  These records specify the time-invariant source names.  A set of time-varying data follows (see Table 4-23).  The time-varying records contain the coordinates of four vertices that define the perimeter of the source, effective release height, ground elevation, temperature, effective vertical velocity, effective radius, initial vertical spread, and an emission rate for each species.  Note that the four vertices must be centered in sequence around the perimeter; all four "x" coordinates followed by all four "y" coordinates.

Sample Fortran read statements for time-invariant data records are:

```
┌── Loop over sources

     READ(iunit,*)CID

└── End loop over sources
```

where the following declarations apply:

```
        CHARACTER*16 CID
```

Sample Fortran read statements for time-varying data records are:

```
   ┌── Loop over time periods

        READ(iunit,*)IBDAT,IBTIM,IEDAT,IETIM

        ┌── Loop over sources

             READ(iunit,*)CID,VERTX,VERTY,HT,ELEV,TEMPK,WEFF,REFF,SIGZ,QEMIT

        └── End loop over sources

   └── End loop over time periods
```

where the following declarations apply:

```
        CHARACTER*16 CID
        REAL VERTX(4),VERTY(4)
        REAL QEMIT(nse3)
```

Table 4-22

BAEMARB.DAT - Time-Invariant Data Record Contents

(Repeated for each source)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | CID | C*16 | Source identifier (16 characters = 4 words) |

[a] C*16 = Character*16

Table 4-23

BAEMARB.DAT - Time-Varying Data Record Contents

(First record of "NSRC3"+1 records required for each time period)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | IBDAT | integer | Beginning date for which data in this set is valid (YYYYJJJ, where YYYY=year, JJJ=Julian day) |
| 2 | IBTIM | integer | Beginning hour for which data in this set is valid (00-23, LST; end of hour) |
| 3 | IEDAT | integer | Ending date for which data in this set is valid (YYYYJJJ, where YYYY=year, JJJ=Julian day) |
| 4 | IETIM | integer | Ending hour for which data in this set is valid (00-23, LST; end of hour) |

Example:
  Data on each record is valid for 1 hour:
      IBDAT=1989183,IBTIM=00,IEDAT=1989183,IETIM=00
      IBDAT=1989183,IBTIM=01,IEDAT=1989183,IETIM=01
      IBDAT=1989183,IBTIM=02,IEDAT=1989183,IETIM=02

  Data on each record is valid for 3 hours:
      IBDAT=1989183,IBTIM=00,IEDAT=1989183,IETIM=02
      IBDAT=1989183,IBTIM=03,IEDAT=1989183,IETIM=05
      IBDAT=1989183,IBTIM=06,IEDAT=1989183,IETIM=08

(Note: YYJJJ date format formerly used is also accepted.)

Table 4-23 (Concluded)
BAEMARB.DAT - Time-Varying Data Record Contents
(Next "NSRC3" records)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | CID | C*16 | Source identifier (must match values in time-invariant records) |
| 2–5 | VERTX | real array | X-coordinate (km) of each of the four vertices defining the perimeter of the area source |
| 6–9 | VERTY | real array | Y-coordinate (km) of each of the four vertices defining the perimeter of the area source |
| 10 | HT | real | Effective height (m) of the emissions above the ground |
| 11 | ELEV | real | Elevation of ground (m MSL) |
| 12 | TEMPK | real | Temperature (deg. K) |
| 13 | WEFF | real | Effective rise velocity (m/s) |
| 14 | REFF | real | Effective radius (m) for rise calculation |
| 15 | SIGZ | real | Initial vertical spread (m) |
| Next NSE3 | QEMIT | real array | Emission rates (g/s) for each species in the order specified in Header Record 2 |

[a]C*16 = Character*16

4.5     Line Source Emissions File With Arbitrarily Varying Emissions (LNEMARB.DAT)

The LNEMARB.DAT file contains line source emissions data for sources with detailed, arbitrarily varying emissions parameters.  In the LNEMARB.DAT file, values for the source parameters and emission rates can be specified for each time step in the run.  Plume rise is computed within the CALPUFF model for groups of line sources using the buoyant line source algorithm.

LNEMARB.DAT is a free-formatted ASCII data file (see Table 4-24 for an example) consisting of three header records, followed by a set of data records containing source information.  The time-invariant data records contain character source identifiers for each of the individual lines, and parameters that control how all lines are processed.  The time varying emissions and source parameter data follow in subsequent records.  One data record per line source in each group is required for each time period (e.g., usually at hourly intervals).  CALPUFF interprets the times obtained from the LNEMARB.DAT file as marking the end of the hour (e.g., 89104, hour 00 denotes the last hour of Julian day 103 in the year 1989.)

The data in the LNEMARB.DAT file are independent of the horizontal and vertical grid systems being used in the model.  The horizontal coordinates are specified in terms of UTM or Lambert conformal coordinates.  The vertical layers receiving the emissions of the source are based on the plume rise of the source computed internally by the model.  However, the LNEMARB.DAT file does contain time-dependent data specifying the emission parameters for a particular time period.

Table 4-24
Sample LNEMARB.DAT file

```
'LNEMARB'   2    1   12     1988001 01  1989001  00   '5'  'Example'
'SO2'
64.
7  6
'Line_Source_1'  'Line_Source_2'
1988001  01  1988001 07
1
2  500.  22.  18.  3.2  22.  100.
'Line_Source_1'    1.  3.     1.5  3.     22.  0.  1.3
'Line_Source_2'    1.  3.022  1.5  3.022  22.  0.  3.1
1988001  08  1988001 13
1
2  500.  22.  18.  3.2  22.  300.
'Line_Source_1'    1.  3.     1.5  3.     22.  0.  2.3
'Line_Source_2'    1.  3.022  1.5  3.022  22.  0.  2.3
1988001  14  1988001 23
1
2  500.  22.  18.  3.2  22.  150.
'Line_Source_1'    1.  3.     1.5  3.     22.  0.  1.3
'Line_Source_2'    1.  3.022  1.5  3.022  22.  0.  3.1
1988002  00  1989001 00
1
2  500.  22.  18.  3.2  22.  150.
'Line_Source_1'    1.  3.     1.5  3.     22.  0.  1.3
'Line_Source_2'    1.  3.022  1.5  3.022  22.  0.  3.1
```

# LNEMARB.DAT File - Header Records

The header records of the LNEMARB.DAT file (see Table 4-25) contain the maximum number of lines in the group, starting and ending time periods of data in the file, and a list of the emitted species.  Sample Fortran read statements are:

```
    READ(iunit,*)FNAME5,NSRC5,NSE5,IUTMZ5,IBDAT5,IBTIM5,IEDAT5,
  1 IETIM5,VRS5,LABEL5

    READ(iunit,*)CSLST5
    READ(iunit,*)XMWEM5
```

where the following declarations apply:

```
    CHARACTER*12 FNAME5,VRS5,LABEL5,CSLST5(nse5)
    REAL XMWEM5(nse5)
```

Table 4-25

LNEMARB.DAT - Header Record 1 - General Data

| No. | Variable | Type[a] | Description | Sample Values |
|-----|----------|---------|-------------|---------------|
| 1 | FNAME5 | C*12 | Data set name | LNEMARB |
| 2 | NSRC5 | integer | Maximum number of lines in any period | 10 |
| 3 | NSE5 | integer | Number of species emitted | 3 |
| 4 | IUTMZ5 | integer | UTM zone in which source coordinates are specified (enter 0 is using Lambert conformal coordinates) | 11 |
| 5 | IBDAT5 | integer | Date of beginning of data in the file (YYYYJJJ, where YYYY=year, JJJ=Julian day) | 1984220 |
| 6 | IBTIM5 | integer | Hour of beginning of data in the file (00-23, LST; end of hour) | 00 |
| 7 | IEDAT5 | integer | Date of end of data in the file (YYYYJJJ, where YYYY=year, JJJ=Julian day) | 1984224 |
| 8 | IETIM5 | integer | Hour of end of data in the file (00-23, LST; end of hour) | 23 |
| 9 | VRS5 | C*12 | Data set version = CALPUFF version | 5 |
| 10 | LABEL5 | C*12 | Data set label | Daily |

[a] C*12 = Character*12


(Note: YYJJJ date format formerly used is also accepted.)

Table 4-25 (Continued)
LNEMARB.DAT - Header Record 2 - Species List

| No.[*] | Type[a] | Description | Sample Values |
|--------|---------|-------------|---------------|
| 1 | C*12 | Species identifier for species 1 | PM |
| 2 | C*12 | Species identifier for species 2 | PM10 |
| . | . | . | . |
| . | . | . | . |
| . | . | . | . |
| NSE5 | C*12 | Species identifier for species "NSE5" | PM25 |

[*] "NSE5" elements of CSLST5 array
[a] C*12 = Character*12

Table 4-25 (Concluded)

LNEMARB.DAT - Header Record 3 - Molecular Weights

| No.[*] | Type[a] | Description | Sample Values |
|---|---|---|---|
| 1 | real | Molecular weight for species 1 | 200. |
| 2 | real | Molecular weight for species 2 | 200. |
| . | . | . | . |
| . | . | . | . |
| . | . | . | . |
| NSE5 | real | Molecular weight for species "NSE5" | 200. |

[*] "NSE5" elements of XMWEM5 array

# LNEMARB.DAT File - Data Records

The LNEMARB.DAT file contains two types of data records.  A set of time-invariant records (see Table 4-26) are read after the header records, to specify parameters used in modeling all line sources in the file, and the number of time-invariant names used to identify each line source.  A set of time-varying data follows (see Table 4-27).  The first record in this group identifies the time period.  The second identifies the number of groups of active line sources.  Thereafter, a block of records must be supplied for each active group.  The first of these identifies the number of active lines, and the average characteristics of this group of active lines.  The remaining time-varying records in the block complete the description for each active line: the character name given to the line, the coordinates of the end-points, the release height, the elevation of the ground, and an emission rate for each species.

Sample Fortran read statements for time-invariant data records are:

    READ(iunit,*)MXNSEG,NLRISE

┌── Loop over maximum number of lines (NSRC5) comprising all groups

│       READ(iunit,*)CID

└── End loop over lines

where the following declarations apply:

    CHARACTER*16 CID

Sample Fortran read statements for time-varying data records are:

┌── Loop over time periods
│
│       READ(iunit,*)IBDAT,IBTIM,IEDAT,IETIM
│       READ(iunit,*)NGROUPS
│
│       ┌── Loop over groups
│       │
│       │    READ(iunit,*)NLINES,XL,HBL,WBL,WML,DXL,FPRIMEL
│       │
│       │       ┌── Loop over active lines (NLINES)
│       │       │
│       │       │    READ(iunit,*)CID,XBEGL,YBEGL,XENDL,YENDL,HTL,ELEVL,QL
│       │       │
│       │       └── End loop over active lines
│       │
│       └── End loop over groups
│
└── End loop over time periods

where the following declarations apply:
        CHARACTER*16 CID
        REAL QL(nse5)

Table 4-26

LNEMARB.DAT - Time-Invariant Data Record Contents

| No. | Variable | Type[a] | Description |
|---|---|---|---|
| 1 | MXNSEG | integer | Maximum number of segments used to model one line |
| 2 | NLRISE | integer | Number of distances at which transitional rise is tabulated |
| Next NSRC5 | CID | C*16 | Source identifier (16 characters = 4 words) |

[a] C*16 = Character*16

Table 4-27

LNEMARB.DAT - Time-Varying Data Record Contents

(First record required for each time period)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | IBDAT | integer | Beginning date for which data in this set is valid (YYYYJJJ, where YYYY=year, JJJ=Julian day) |
| 2 | IBTIM | integer | Beginning hour for which data in this set is valid (00-23, LST; end of hour) |
| 3 | IEDAT | integer | Ending date for which data in this set is valid (YYYYJJJ, where YYYY=year, JJJ=Julian day) |
| 4 | IETIM | integer | Ending hour for which data in this set is valid (00-23, LST; end of hour) |

Example:
Data on each record is valid for 1 hour:
IBDAT=1989183,IBTIM=00,IEDAT=1989183,IETIM=00
IBDAT=1989183,IBTIM=01,IEDAT=1989183,IETIM=01
IBDAT=1989183,IBTIM=02,IEDAT=1989183,IETIM=02

Data on each record is valid for 3 hours:
IBDAT=1989183,IBTIM=00,IEDAT=1989183,IETIM=02
IBDAT=1989183,IBTIM=03,IEDAT=1989183,IETIM=05
IBDAT=1989183,IBTIM=06,IEDAT=1989183,IETIM=08

(Note: YYJJJ date format formerly used is also accepted.)

Table 4-27 (Continued)
LNEMARB.DAT - Time-Varying Data Record Contents
(Second record required for each time period)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | NGROUPS | integer | Number of groups of line sources active this time period |

Table 4-27 (Continued)
LNEMARB.DAT - Time-Varying Data Record Contents
(First record required for each group, each time period)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | NLINES | integer | Number of active lines |
| 2 | XL | real | Average building length (m) |
| 3 | HBL | real | Average building height (m) |
| 4 | WBL | real | Average building width (m) |
| 5 | WML | real | Average line source width (m) |
| 6 | DXL | real | Average separation between buildings (m) |
| 7 | FPRIMEL | real | Average buoyancy parameter ($m^4/s^3$) |

| No. | Variable | Type[a] | Description |
|---|---|---|---|
| 1 | CID | C*16 | Source identifier (must match one of the values in time-invariant records) |
| 2,3 | XBEGL,YBEGL | real | X,Y-coordinates (km) of beginning of line |
| 4,5 | XENDL,YENDL | real | X,Y-coordinates (km) of end of line |
| 6 | HTL | real | Release height (m) of the emissions above the ground |
| 7 | ELEVL | real | Base elevation (m) |
| Next NSE5 | QL | real array | Emission rates for each species in the order specified in Header Record 2 |

[a]C*16 = Character*16

4.6     Volume Source Emissions File (VOLEM.DAT) with Arbitrarily Varying Emissions

Time independent volume source data are contained in the CALPUFF control file (CALPUFF.INP).  The VOLEM.DAT emissions file contains time-dependent volume source emissions data.  VOLEM.DAT is a sequential, unformatted data file containing one two-dimensional grid for each emitted species modeled by CALPUFF for each time step.  There are three header records with information describing the grid system, dates and time of data in the file, species names, and molecular weights.

The total emission rate for each pollutant is specified for the grid column.  Individual source information is not stored in the file, so plume rise is not computed by CALPUFF for the VOLEM.DAT emissions. The effective height and initial vertical and horizontal plume dimensions ($\sigma_y$, $\sigma_z$) are specified by the user in the control file (CALPUFF.INP) for the gridded area source inventory.

**VOLEM.DAT File - Header Records**

The header records contain information regarding the horizontal grid system, species emitted, molecular weights, and dates of the data contained in the file (see Table 4-28).  These data are checked by CALPUFF in the setup phase of the model run to ensure the parameters are compatible with those specified in the CALPUFF control file.  Any mismatch in the specifications results in an error message and termination of the run.

Sample Fortran read statements for the header records are:

```
        READ(iunit)FNAME4,IGTYP4,NX4,NY4,DELX4,DELY4,XORIG4,YORIG4,IUTMZ4,
       1 NSE4,IBDAT4,IBTIM4,IEDAT4,IETIM4,VRS4,LABEL4

        READ(iunit)CSLST4
        READ(iunit)XMWEM4
```

where the following declarations apply:

```
        CHARACTER*12 FNAME4,VRS4,LABEL4,CSLST4(nse4)
        REAL XMWEM4(nse4)
```

Table 4-28

VOLEM.DAT - Header Record 1 - General Grid, Species, and Date Data

| No. | Variable | Type[a] | Description | Sample Values |
|---|---|---|---|---|
| 1 | FNAME4 | C*12 | Data set name | VOLEM |
| 2 | IGTYP4 | integer | Horizontal grid type (always = 1 for CALPUFF runs) | 1 |
| 3 | NX4 | integer | Number of grid cells in the X direction | 30 |
| 4 | NY4 | integer | Number of grid cells in the Y direction | 30 |
| 5 | DELX4 | real | Grid spacing (km) in the X direction | 5. |
| 6 | DELY4 | real | Grid spacing (km) in the Y direction | 5. |
| 7 | XORIG4 | real | Reference X coordinate (km) of the southwest corner of grid cell (1,1) | 168.000 |
| 8 | YORIG4 | real | Reference Y coordinate (km) of the southwest corner of grid cell (1,1) | 3930.000 |
| 9 | IUTMZ4 | integer | UTM zone of horizontal coordinates (enter 0 if using Lambert conformal coordinates) | 11 |
| 10 | NSE4 | integer | Number of species emitted | 3 |
| 11 | IBDAT4 | integer | Date of beginning of data in file (YYYYJJJ, where YYYY=year, JJJ=Julian day) | 1984220 |
| 12 | IBTIM4 | integer | Hour of beginning of data in file (00-23, LST; end of hour) | 00 |
| 13 | IEDAT4 | integer | Date of end of data in file (YYYYJJJ, where YYYY=year, JJJ=Julian day) | 1984224 |
| 14 | IETIM4 | integer | Hour of end of data in file (00-23, LST; end of hour) | 23 |
| 15 | VRS4 | C*12 | Data set version = CALPUFF version | 5 |
| 16 | LABEL4 | C*12 | Data set label | '84 - KERN |

[a]C*12 = Character*12

(Note: YYJJJ date format formerly used is also accepted.)

Table 4-28 (Continued)
VOLEM.DAT - Header Record 2 - Species List

| No. | Type[a] | Description | Sample Values |
|---|---|---|---|
| 1 | C*12 | Species identifier for species 1 | SO2 |
| 2 | C*12 | Species identifier for species 2 | SO4 |
| . | . | . | . |
| . | . | . | . |
| . | . | . | . |
| NSE4 | C*12 | Species identifier for species "NSE4" | NOX |

* "NSE4" elements of CSLST4 array
[a]C*12 = Character*12

Table 4-28 (Concluded)

VOLEM.DAT - Header Record 3 - Molecular Weights

| No. | Type[a] | Description | Sample Values |
|---|---|---|---|
| 1 | real | Molecular weight for species 1 | 64. (SO2) |
| 2 | real | Molecular weight for species 2 | 96. (SO4) |
| . | . | . | . |
| . | . | . | . |
| . | . | . | . |
| NSE4 | real | Molecular weight for species "NSE4" | 30. (NOX) |

\* "NSE4" elements of XMWEM1 array

**VOLEM.DAT File - Data Records**

The VOLEM.DAT file contains a set of "NSE4"+1 records for each time period (e.g., hour). The first data record of each set defines the time period over which the emissions data in the following records are valid. The next "NSE4" records each contain a species identifier and a two-dimensional gridded field of emissions. See Table 4-29 for a description of the variables in the VOLEM.DAT data records.

Sample Fortran read statements for a set of data records are:

```
Loop over time periods (e.g., Hours)

    READ(iunit)IBDAT,IBTIM,IEDAT,IETIM

        Loop over species

        READ(iunit)CSPEC,QEMIT

        End loop over species

End loop over time periods
```

where the following declarations apply:

```
CHARACTER*12 CSPEC

REAL QEMIT(nx4,ny4)
```

Table 4-29

VOLEM.DAT - Data Record Contents

(Record 1 of each set)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | IBDAT | integer | Beginning date for which data in this set is valid (YYYYJJJ, where YYYY=year, JJJ=Julian day) |
| 2 | IBTIM | integer | Beginning time for which data in this set is valid (00-23, LST; end of hour) |
| 3 | IEDAT | integer | Ending date for which data in this set is valid (YYYYJJJ, where YYYY=year, JJJ=Julian day) |
| 4 | IETIM | integer | Ending time for which data in this set is valid (00-23, LST; end of hour) |

Example:

    Data on each record is valid for 1 hour:
        IBDAT=1989183,IBTIM=00,IEDAT=1989183,IETIM=00
        IBDAT=1989183,IBTIM=01,IEDAT=1989183,IETIM=01
        IBDAT=1989183,IBTIM=02,IEDAT=1989183,IETIM=02

    Data on each record is valid for 3 hours:
        IBDAT=1989183,IBTIM=00,IEDAT=1989183,IETIM=02
        IBDAT=1989183,IBTIM=03,IEDAT=1989183,IETIM=05
        IBDAT=1989183,IBTIM=06,IEDAT=1989183,IETIM=08

(Note: YYJJJ date format formerly used is also accepted.)

Table 4-29 (Concluded)
VOLEM.DAT - Data Record Contents
(Records 2, 3, ... "NSE4"+1 of each set)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | CSPEC | C*12 | Species identifier (up to 12 characters) |
| Next NX4*NY4 | QEMIT | real array | Volume source emission rate (g/s) of species "CSPEC" for each grid column (QEMIT (nx4,ny4)) |

[a]C*12 = Character*12

4.7     User-Specified Deposition Velocity Data File (VD.DAT)

The CALPUFF model requires that the user specify the method for determining dry deposition velocities for each species.  In Input Group 3 of the control file, one of the following flags must be specified <u>for each pollutant</u>.

> 0 =     no dry deposition (deposition velocities set to zero)
> 1 =     resistance model used - pollutant deposited as a gas
> 2 =     resistance model used - pollutant deposited as a particle
> 3 =     user-specified deposition velocities used

Note that different methods can be used for different pollutants in the same CALPUFF run.

If any species are flagged as using "user-specified" deposition velocities, CALPUFF reads a formatted user-prepared data file with a 24-hour diurnal cycle of deposition velocities for each species flagged.  The 24 values correspond to hours 01-24 (LST) of the simulated day.  Twenty-four values must be entered for each flagged pollutant, even if the model run is for less than a full diurnal cycle.  The units of the deposition velocities are m/s.

An example of a user-specified VD.DAT file is shown in Table 4-30.  The VD.DAT file uses a control file format (see Section 4.1).  All text outside the delimiters (!) is considered as user comment information and is echoed back but otherwise ignored by the input module.  Each data line consists of a delimiter followed by the species name, 24 deposition velocities, and a terminating delimiter.  The data may extend over more than one line.  The line being continued must end with a comma.  The control file format allows the use of repetition factors (e.g., 3 * 1.0 instead of 1.0, 1.0, 1.0).  The order in which the species are entered in the file is not important.  However, the file must end with an input group terminator (i.e., !END!).

The model checks that values have been entered for each species flagged as using user-specified deposition velocities.  An error message is printed and execution of the run is terminated if any values are missing.  The run will also terminate with an error message from the input routine if too many values are entered (i.e., more than 24 values for a particular pollutant).  The species names must match those used in the chemical mechanism of the model.

Table 4-30

Sample User-Specified Deposition Velocity File for Two Species

```
              DEPOSITION VELOCITY FILE (VD.DAT)
              ---------------------------------


VD.DAT contains 24-hour diurnal cycle of deposition velocities for each species flagged as using
user-specified values in the control file (CALPUFF.INP).

The first value correspond to the period from 0:00 to 1:00, and the 24th value corresponds to 23:00-
0:00.

NOTE: Units are in m/s.
----------------------


SPECIES
 NAME              Deposition Velocities (m/s)
 -------           ---------------------------


! HNO3      =      5*1.5e-2, 4*1.7e-2, 3*1.8e-2, 3*1.9e-2, 3*1.7e-2, 6*1.5e-2        !
! SO2       =      5*0.8e-2, 13*1.0e-2, 6*0.8e-2                                      !


!END!
```

4.8     Hourly Ozone Data File (OZONE.DAT)

If the MESOPUFF II or RIVAD/ARM3 chemical mechanism is used to simulate the chemical transformation of $SO_2 \rightarrow SO_4^=$ and $NO_x \rightarrow HNO_3 \leftrightarrow NO_3^-$, estimates of background ambient ozone concentration levels are required to compute the hourly conversion rates. CALPUFF provides two options for the user to provide these data: (1) a single, typical background value appropriate for the modeling region, or (2) hourly ozone data from one or more ozone monitoring stations. The selection of Option 2 requires that a file called OZONE.DAT be created with the necessary data.

OZONE.DAT is a sequential, formatted data file containing three types of records:  single header record, time-invariant data records, and hourly ozone data records. A sample OZONE.DAT file is shown in Table 4-31. The header record contains information on the number of stations in the data set, the time period of the data, and descriptive information regarding the file. The time-invariant records contain the coordinates of each of the ozone stations. The time-varying data consists of hourly ozone concentrations at each of the ozone stations.

Table 4-31
Sample Hourly Ozone Data File (OZONE.DAT)

```
'OZONE', 3, 11, 1980001, 0, 1980002, 0, '5', 'Test'
'STATION 1',   168.000,       3840.000
'STATION 2',   200.000,       3880.000
'STATION 3',   180.000,       3860.000
1980,   001,    0,    9999.,    62.,    50.
1980,   001,    1,    9999.,  9999.,  9999.
1980,   001,    2,      68.,    61.,  9999.
1980,   001,    3,      66.,  9999.,  9999.
1980,   001,    4,    9999.,  9999.,    53.
1980,   001,    5,    9999.,  9999.,  9999.
1980,   001,    6,    9999.,  9999.,  9999.
1980,   001,    7,    9999.,  9999.,  9999.
1980,   001,    8,      69.,    68.,    60.
1980,   001,    9,      72.,    75.,    65.
1980,   001,   10,      74.,    78.,    69.
1980,   001,   11,      87.,    85.,    74.
1980,   001,   12,     102.,    99.,    84.
1980,   001,   13,     109.,   105.,    92.
1980,   001,   14,     120.,   118.,   102.
1980,   001,   15,     116.,   116.,    95.
1980,   001,   16,     103.,   100.,    97.
1980,   001,   17,      98.,    90.,    88.
1980,   001,   18,      89.,    82.,    83.
1980,   001,   19,    9999.,  9999.,    80.
1980,   001,   20,    9999.,  9999.,    78.
1980,   001,   21,    9999.,  9999.,    74.
1980,   001,   22,    9999.,  9999.,    69.
1980,   001,   23,    9999.,  9999.,    69.
1980,   002,   00,    9999.,  9999.,    68.
```

**OZONE.DAT File - Header Record**

The header records of the OZONE.DAT file contain the name, version, and label of the data set, the number of ozone stations, and starting and ending time periods of data in the file (see Table 4-32).  A sample Fortran read statement for the header record is:

```
 READ(iunit,*)FNAMEO,NOZSTA,IUTMOZ,IBDATO,IBTIMO,IEDATO,
1 IETIMO,VRSOZ,LABOZ
```

where the following declaration applies:

```
CHARACTER*12 FNAMEO,VRSOZ,LABOZ.
```

Table 4-32

OZONE.DAT - Header Record - General Data

| No. | Variable | Type[a] | Description | Sample Values |
|---|---|---|---|---|
| 1 | FNAMEO | C*12 | Data set name | OZONE |
| 2 | NOZSTA | integer | Number of ozone stations in the file | 3 |
| 3 | ITUMOZ | integer | UTM zone in which ozone station coordinates are specified (enter 0 if using Lambert conformal coordinates) | 11 |
| 4 | IBDATO | integer | Date of beginning of data in the file (YYYYJJJ, where YYYY=year, JJJ=Julian day) | 1980001 |
| 5 | IBTIMO | integer | Hour of beginning of data in the file (00-23, LST; end of hour) | 00 |
| 6 | IEDATO | integer | Date of end of data in the file (YYYYJJJ, where YYYY=year, JJJ=Julian day) | 1980002 |
| 7 | IETIMO | integer | Hour of end of data in the file (00-23, LST; end of hour) | 00 |
| 8 | VRSOZ | C*12 | Data set version = CALPUFF version | 5 |
| 9 | LABOZ | C*12 | Data set label | Test |

[a]C*12 = Character*12

(Note: YYJJJ date format formerly used is also accepted.)

**OZONE.DAT File - Data Records**


The OZONE.DAT file contains two types of data records.  A set of time-invariant records are read after the header records.  These records specify the coordinates of each ozone station (see Table 4-33).  A set of time-varying data follows, which contain the hourly ozone concentration (in ppb) for each station (see Table 4-34).

Sample Fortran read statements for time-invariant data records are:

> ┌── Loop over stations
> │
> │   READ(iunit,*)CID,XOZ,YOZ
> │
> └── End loop over stations


where the following declaration applies:

    CHARACTER*16 CID


Sample Fortran read statements for time-varying data records are:

> ┌── Loop over hours
> │
> │   READ(iunit,*)IYR,IJUL,IHR,OZCONC
> │
> └── End loop over hours


where the following declaration applies:

    REAL OZCONC(nozsta)

Table 4-33

OZONE.DAT - Time-Invariant Data Record Contents

(Repeated for each station)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | CID | C*16 | Station identifier (16 characters = 4 words) |
| 2 | XOZ | real | X coordinate (km) of the ozone station |
| 3 | YOZ | real | Y coordinate (km) of the ozone station |

[a]C*16 = Character*16

Table 4-34

OZONE.DAT - Time-Varying Data Record Contents

(One record per hour)

| No. | Variable | Type | Description |
|---|---|---|---|
| 1 | IYR | integer | Year of data (four digits) |
| 2 | IJUL | integer | Julian day |
| 3 | IRH | integer | Hour of data (00-23 LST; end of hour) |
| Next "NOZSTA" | OZCONC | real array | Ozone concentration (ppb) at each ozone station (in the same order as the station coordinates in the time-invariant records; missing value indicator is 9999.) |

(Note: two-digit year format formerly used is also accepted.)

4.9     User-Specified Chemical Transformation Rate Data File (CHEM.DAT)

If chemical conversion is to be considered by CALPUFF, the user must specify a variable in the control file, MCHEM, which determines how chemical transformation rates are computed.  The options for MCHEM are:

> 0 =    chemical transformation is not modeled
> 1 =    the MESOPUFF II chemical scheme is used to compute transformation rates
> 2 =    user-specified 24-hour cycles of transformation rates are used
> 3 =    the RIVAD/ARM3 chemical scheme is used to compute transformation

If MCHEM is set equal to 2, CALPUFF reads a formatted user-prepared data file with 24-hour diurnal cycles of transformation rates $k_1$, $k_2$, $k_3$.  The nature of the equilibrium relationship assumed between pollutants 4 and 5 (e.g., $HNO_3$ and $NO_3^-$) precludes the use of a user-specified conversion rate between these pollutants.  If $NO_3$ is being modeled, the $NH_4NO_3$ dissociation constant is determined as a function of temperature and relative humidity.

A sample user-specified CHEM.DAT file is shown in Table 4-35.  The CHEM.DAT file uses a control file format (see Section 4.1).  All text outside the delimiters (!) is considered as user comment information and is echoed back but otherwise ignored by the input module.  Each data line consists of a delimiter followed by the species name, 24 conversion rates, and a terminating delimiter.  The data may extend over more than one line.  The line being continued must end with a comma.  The control file format allows the use of repetition factors (e.g., 3 * 1.0 instead of 1.0, 1.0, 1.0).  The order in which the species are entered in the file is not important.  However, the file must end with an input group terminator (i.e., !END).

The model checks that the proper number of values have been entered for each conversion rate.  An error message is printed and execution of the run is terminated if any values are missing.  The run will also terminate with an error message from the input routine if too many values are entered (i.e., more than 24 values).

Table 4-35

Sample User-Specified Chemical Transformation Rate Data File (CHEM.DAT)

```
                   CHEMICAL TRANSFORMATION RATE FILE (CHEM.DAT)
                   --------------------------------------------



CHEM.DAT contains a 24-hour diurnal cycle of chemical transformation
rates for the chemical transformation of SO2 to SO4, and NOx to HNO3/PAN.

          k1 = SO2 to SO4 transformation rate(percent/hour)

          k2 = NOx to HNO3 + PAN transformation rate (percent/hour)

          k3 = NOx to HNO3 (only) transformation rate (percent/hour)

The first value correspond to the period from 0:00 to 1:00, and the 24th value corresponds to
23:00-0:00.



                   TRANSFORMATION RATE (percent/hour)
                   ---------------------------------

! K1           =    7*0.2, 0.4, 0.8, 1.2, 1.6, 3*2.0,   1.6,  1.2, 0.8, 0.4, 6*0.2 !
! K2           =    7*2.0, 4.0, 8.0,12.0,15.0, 3*20.0, 15.0, 12.0, 8.0, 4.0, 6*2.0 !
! K3           =    7*2.0, 3.0, 6.0, 8.0,11.0, 3*15.0, 11.0,  8.0, 6.0, 3.0, 6*2.0 !

!END!
```

## 4.10    Site-Specific Turbulence Data (PROFILE.DAT)

CALPUFF provides several options for computing the dispersion coefficients, $\sigma_y$ and $\sigma_z$.  In Input Group 2 of the control file, the user specifies a value for the dispersion method flag, MDISP:

1 =    dispersion coefficients computed from values of $\sigma_v$ and $\sigma_w$ read from a data file (PROFILE.DAT),

2 =    dispersion coefficients determined from internally computed values of $\sigma_v$ and $\sigma_w$ based on similarity scaling relationships,

3 =    PG coefficients (computed using the ISCST multi-segment approximation) used for rural areas and MP coefficients used in urban areas,

4 =    same as 3 except that the PG coefficients are computed using the MESOPUFF II equations.

5 =    CTDMPLUS dispersion coefficients computed from $\sigma_v$ and $\sigma_w$ for neutral/stable.

If Option 1 or Option 5 is selected, the user must prepare a data file with hourly values of $\sigma_v$ and $\sigma_w$.  This option is intended primarily for application to a single source or facility with onsite measurements of $\sigma_v$ and $\sigma_w$.  Therefore, only one set of observations are allowed in the data base and they are assumed to apply over the entire computational region.

The CTDMPLUS meteorological data file PROFILE provides for measurements of turbulence as well as wind speed, wind direction, and temperature at one or more heights on a tower.  Because the PROFILE.DAT file is one of the meteorological formats accepted by CALPUFF, it may also be used for entering turbulence measurements for use with any of the other options.  Its structure is documented in Section 4.2.4.

4.11     CTDMPLUS Terrain Feature Description and Receptors (HILL.DAT, HILLRCT.DAT)

CALPUFF allows two ways of specifying the characteristics of terrain features modeled by CTSG.  The first is by means of the OPTHILL processor described in Section 4.13, which provides the parameters to be entered in the control file CALPUFF.INP.  The second approach allows the use of the terrain preprocessing programs provided with CTDMPLUS (Mills et al., 1987).  If a user is familiar with the terrain preprocessor, then this may be the preferred option because the standard terrain file used in CTDMPLUS, "TERRAIN", can be read by CALPUFF without modification.  CTDMPLUS subroutines that read and process the terrain data have been incorporated in CALPUFF.  Similarly, CTSG receptors may either be entered directly into the control file, or may be read from the corresponding CTDMPLUS "RECEPTOR" file.  Note however that any CTSG receptors that are not located on one of the hill features (designated by a hill ID of 0) are ignored in CALPUFF.  The default filenames in CALPUFF for TERRAIN and RECEPTOR are HILL.DAT and HILLRCT.DAT, respectively, and they are used together so that both must be used if the CTDMPLUS input option is selected.

Table 4-36 illustrates a typical HILL.DAT file for one hill.  This one is defined by ellipse/polynomial shapes determined for a range of 10 "critical elevations" from 25 m to 115 m  above the base of the hill.  After the header record, the first group of 10 records provides the ellipse parameters at each "critical elevation", and the second group of 10 records provides the parameters for the corresponding inverse polynomial shape profile fit to the portion of the hill above it.  Refer to Mills et al. (1987) for more detailed information.  Table 4-37 shows a typical HILLRCT.DAT file.  Data for each CTSG receptor are placed in one record, and identify the location, hill number (ID), ground elevation, and receptor height above the ground.  Note that CALPUFF places all receptors on the ground.  The structure of the data records is defined in Table 4-38 (HILL.DAT) and 4-39 (HILLRCT.DAT).

Other data associated with the HILL.DAT and HILLRCT.DAT are provided in the CALPUFF.INP control file, in Input Group 6.  These reference the coordinate system used to prepare the CTDMPLUS simulation to the system chosen for the CALPUFF simulation.  XHILL2M and ZHILL2M are the conversion factors that scale the CTDMPLUS "user units" in the horizontal and vertical, respectively, to meters.  XCTDMKM and YCTDMKM define the location of the origin of the CTDMPLUS coordinate system in the CALPUFF coordinate system.  The units used for this are kilometers.  Hence, if UTM coordinates are used for both simulations, the origins of the two system are the same, and XCTDMKM=YCTDMKM=0.

Table 4-36

Sample CTDMPLUS Terrain Feature File (HILL.DAT)

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 1 20 | .5000E+03 | | CTSG Test Hill | | | | |
| .000 | .5000E+04 | .2067E-02 | 180.000 | 2498.000 | 2498.000 | | |
| 24.000 | .5000E+04 | .1071E-02 | 180.000 | 2242.000 | 2242.000 | | |
| 48.000 | .5000E+04 | .8304E-03 | 180.000 | 1986.000 | 1986.000 | | |
| 72.000 | .5000E+04 | .4369E-03 | 180.000 | 1820.000 | 1820.000 | | |
| 96.000 | .5000E+04 | .7918E-03 | 180.000 | 1692.000 | 1692.000 | | |
| 120.000 | .5000E+04 | .3501E-03 | 180.000 | 1493.000 | 1493.000 | | |
| 144.000 | .5000E+04 | -.1282E-03 | 180.000 | 1410.000 | 1410.000 | | |
| 168.000 | .5000E+04 | .1463E-03 | 180.000 | 1334.000 | 1334.000 | | |
| 192.000 | .5000E+04 | .7370E-04 | 180.000 | 1263.000 | 1263.000 | | |
| 216.000 | .5000E+04 | .3210E-03 | 180.000 | 1196.000 | 1196.000 | | |
| 240.000 | .5000E+04 | -.2209E-03 | 180.000 | 1071.000 | 1071.000 | | |
| 264.000 | .5000E+04 | .1904E-03 | 180.000 | 1011.000 | 1011.000 | | |
| 288.000 | .5000E+04 | -.7684E-03 | 180.000 | 951.700 | 951.700 | | |
| 312.000 | .5000E+04 | .7754E-03 | 180.000 | 893.300 | 893.300 | | |
| 336.000 | .5000E+04 | .5356E-04 | 180.000 | 835.000 | 835.000 | | |
| 360.000 | .5000E+04 | .5811E-03 | 180.000 | 716.400 | 716.400 | | |
| 384.000 | .5000E+04 | -.1251E-03 | 180.000 | 654.800 | 654.800 | | |
| 408.000 | .5000E+04 | -.1892E-04 | 180.000 | 590.400 | 590.400 | | |
| 432.000 | .5000E+04 | .2414E-03 | 180.000 | 521.900 | 521.900 | | |
| 456.000 | .5000E+04 | .7710E-04 | 180.000 | 446.900 | 446.900 | | |
| .000 | .5000E+04 | .2430E-03 | 180.000 | 2.859 | 2.859 | 959.101 | 959.101 |
| 24.000 | .5000E+04 | .1997E-03 | 180.000 | 3.039 | 3.039 | 914.047 | 914.047 |
| 48.000 | .5000E+04 | .1903E-03 | 180.000 | 3.232 | 3.232 | 872.399 | 872.399 |
| 72.000 | .5000E+04 | .1296E-03 | 180.000 | 3.472 | 3.472 | 832.424 | 832.424 |
| 96.000 | .5000E+04 | .1485E-03 | 180.000 | 3.853 | 3.853 | 792.979 | 792.979 |
| 120.000 | .5000E+04 | .8714E-04 | 180.000 | 3.281 | 3.281 | 779.560 | 779.560 |
| 144.000 | .5000E+04 | .1015E-03 | 180.000 | 3.439 | 3.439 | 743.594 | 743.594 |
| 168.000 | .5000E+04 | .1086E-03 | 180.000 | 3.639 | 3.639 | 707.754 | 707.754 |
| 192.000 | .5000E+04 | .9029E-04 | 180.000 | 3.920 | 3.920 | 671.777 | 671.777 |
| 216.000 | .5000E+04 | .1062E-03 | 180.000 | 4.416 | 4.416 | 635.301 | 635.301 |
| 240.000 | .5000E+04 | .1061E-03 | 180.000 | 3.541 | 3.541 | 620.841 | 620.841 |
| 264.000 | .5000E+04 | .5922E-04 | 180.000 | 3.727 | 3.727 | 584.737 | 584.737 |
| 288.000 | .5000E+04 | .2187E-03 | 180.000 | 3.981 | 3.981 | 547.935 | 547.935 |
| 312.000 | .5000E+04 | .2005E-03 | 180.000 | 4.371 | 4.371 | 510.250 | 510.250 |
| 336.000 | .5000E+04 | .9593E-04 | 180.000 | 5.127 | 5.127 | 471.649 | 471.649 |
| 360.000 | .5000E+04 | .6310E-04 | 180.000 | 3.752 | 3.752 | 449.211 | 449.211 |
| 384.000 | .5000E+04 | .1081E-03 | 180.000 | 4.012 | 4.012 | 406.554 | 406.554 |
| 408.000 | .5000E+04 | .1295E-03 | 180.000 | 4.418 | 4.418 | 361.177 | 361.177 |
| 432.000 | .5000E+04 | .1997E-03 | 180.000 | 5.163 | 5.163 | 312.371 | 312.371 |
| 456.000 | .5000E+04 | .7139E-04 | 180.000 | 6.957 | 6.957 | 259.205 | 259.205 |

Table 4-37

Sample CTDMPLUS Receptor File (HILLRCT.DAT)

| CTSG | 11 | 5057.00 | 1819.00 | 0.00 | 60.00 | 1 |
| CTSG | 12 | 6110.92 | 1441.86 | 0.00 | 60.00 | 1 |
| CTSG | 13 | 6744.54 | 518.94 | 0.00 | 60.00 | 1 |
| CTSG | 14 | 6718.43 | -600.22 | 0.00 | 60.00 | 1 |
| CTSG | 15 | 6041.93 | -1492.11 | 0.00 | 60.00 | 1 |
| CTSG | 16 | 4971.64 | -1819.50 | 0.00 | 60.00 | 1 |
| CTSG | 17 | 3911.83 | -1459.18 | 0.00 | 60.00 | 1 |
| CTSG | 18 | 3263.93 | -546.19 | 0.00 | 60.00 | 1 |
| CTSG | 19 | 3272.78 | 573.16 | 0.00 | 60.00 | 1 |
| CTSG | 20 | 3934.60 | 1476.13 | 0.00 | 60.00 | 1 |
| CTSG | 31 | 5044.00 | 1410.00 | 0.00 | 140.00 | 1 |
| CTSG | 32 | 5860.32 | 1116.84 | 0.00 | 140.00 | 1 |
| CTSG | 33 | 6351.35 | 402.11 | 0.00 | 140.00 | 1 |
| CTSG | 34 | 6331.27 | -464.92 | 0.00 | 140.00 | 1 |
| CTSG | 35 | 5807.34 | -1156.04 | 0.00 | 140.00 | 1 |
| CTSG | 36 | 4978.05 | -1410.00 | 0.00 | 140.00 | 1 |
| CTSG | 37 | 4157.13 | -1130.30 | 0.00 | 140.00 | 1 |
| CTSG | 38 | 3655.12 | -423.18 | 0.00 | 140.00 | 1 |
| CTSG | 39 | 3661.76 | 444.07 | 0.00 | 140.00 | 1 |
| CTSG | 40 | 4174.62 | 1143.51 | 0.00 | 140.00 | 1 |
| CTSG | 51 | 5036.00 | 1132.00 | 0.00 | 220.00 | 1 |
| CTSG | 52 | 5691.56 | 896.77 | 0.00 | 220.00 | 1 |
| CTSG | 53 | 6085.89 | 322.53 | 0.00 | 220.00 | 1 |
| CTSG | 54 | 6069.21 | -373.86 | 0.00 | 220.00 | 1 |
| CTSG | 55 | 5648.17 | -928.84 | 0.00 | 220.00 | 1 |
| CTSG | 56 | 4982.05 | -132.50 | 0.00 | 220.00 | 1 |
| CTSG | 57 | 4322.81 | -907.74 | 0.00 | 220.00 | 1 |
| CTSG | 58 | 3919.67 | -339.71 | 0.00 | 220.00 | 1 |
| CTSG | 59 | 3925.21 | 356.75 | 0.00 | 220.00 | 1 |
| CTSG | 60 | 4337.13 | 918.50 | 0.00 | 220.00 | 1 |
| CTSG | 71 | 5028.00 | 893.00 | 0.00 | 300.00 | 1 |
| CTSG | 72 | 5856.38 | 254.71 | 0.00 | 300.00 | 1 |
| CTSG | 73 | 5511.36 | -732.35 | 0.00 | 300.00 | 1 |
| CTSG | 74 | 4465.87 | -716.09 | 0.00 | 300.00 | 1 |
| CTSG | 75 | 4151.82 | 281.47 | 0.00 | 300.00 | 1 |
| CTSG | 86 | 5016.00 | 521.70 | 0.00 | 420.00 | 1 |
| CTSG | 87 | 5499.93 | 148.95 | 0.00 | 420.00 | 1 |
| CTSG | 88 | 5299.01 | -427.66 | 0.00 | 420.00 | 1 |
| CTSG | 89 | 4688.11 | -418.57 | 0.00 | 420.00 | 1 |
| CTSG | 90 | 4504.92 | 164.14 | 0.00 | 420.00 | 1 |
| CTSG | 96 | 5000.00 | 0.00 | 0.00 | 500.00 | 1 |

Table 4-38

HILL.DAT File - Record Group Structure

| Record Group * | Columns | Variable | Type | Description |
|---|---|---|---|---|
| 1 | 6-7 | NH | integer | Hill ID number |
| 1 | 9-10 | NZ | integer | Number of critical elevations |
| 1 | 21-30 | HTP | real | Elevation of top of feature (user units) |
| 1 | 31-45 | HNAME | character | Hill name |
| 2 ** | 1-10 | ZH | real | Critical elevation (user units) |
| 2 | 11-20 | XHW | real | X-coordinate of ellipse centroid (user units) |
| 2 | 21-30 | YHW | real | Y-coordinate of ellipse centroid (user units) |
| 2 | 31-40 | MAJORW | real | Orientation (deg) of major axis from North |
| 2 | 41-50 | MAJAXW | real | Semi-major axis length (user units) |
| 2 | 51-60 | MINAXW | real | Semi-minor axis length (user units) |
| 3 ** | 1-10 | ZH | real | Critical elevation (again) |
| 3 | 11-20 | L(1) | real | X-coordinate of cut-off hill (user units) |
| 3 | 21-30 | L(2) | real | Y-coordinate of cut-off hill (user units) |
| 3 | 31-40 | MAJORL | real | Orientation (deg) of major axis of cut-off hill from North |
| 3 | 41-50 | EXPOMA | real | Inverse polynomial exponent for major axis |
| 3 | 51-60 | EXPOMI | real | Inverse polynomial exponent for minor axis |
| 3 | 61-70 | SCALMA | real | Inverse polynomial length scale for major axis |
| 3 | 71-80 | SCALMI | real | Inverse polynomial length scale for minor axis |

\*     Record groups are repeated for each hill in the file

\*\*    There are NZ records for group 2 followed by NZ records for group 3

Table 4-39
HILLRCT.DAT File - Data Records
(One record per CTSG receptor)

| Columns | Variable | Type | Description |
|---------|----------|------|-------------|
| 1-16 | RNAME | character | Receptor name |
| 21-30 | XR | real | X-coordinate (user units) |
| 31-40 | YR | real | Y-coordinate (user units) |
| 41-50 | ZR | real | Height above ground (user units) |
| 51-60 | GE | real | Ground-level elevation (user units) |
| 61-65 | NH * | integer | ID number of hill under this receptor |

\*   Receptors with NH=0 are ignored

4.12    Subgrid Scale Coastal Boundary Data File (COASTLN.DAT)

CALPUFF contains an option to treat subgrid scale coastal effects such as the development of a Thermal Internal Boundary Layer (TIBL) within an individual grid cell.  The subgrid scale coastal module is controlled by the MSGTIBL variable in Input Group 2 of the control file.  If MSGTIBL = 1, CALPUFF will introduce a subgrid scale TIBL along a coastal boundary specified in an external file (COASTLN.DAT) when appropriate meteorological conditions exist.  The COASTLN.DAT file contains a set of points that serve to define the coastline.  Multiple coastlines (up to "MXCOAST", see the PARAMS.PUF file) are allowed within a single file.

The COASTLN.DAT file is a sequential, formatted data file (see Table 4-40 for an example) consisting of two types of records: a single header record and a variable number of sets of data records.  Each set of data records includes a record  indicating the location of the water body relative to the coastline (i.e., left or right of the line as one travels in the direction of the data points in the file) and a variable number of records containing the coordinates of each point defining the coastline.

Table 4-40

Sample Subgrid Scale Coastal Boundary Data File (COASTLN.DAT)

```
'COASTLN', 2, 19, '5', 'test'
'WR','Atlantic'
242., 4568.
264., 4588.
270., 4574.
286., 4584.
298., 4602.
308., 4634.
316., 4646.
340., 4610.
354., 4624.
390., 4630.
370., 4648.
340., 4700.
356., 4738.
346., 4744.
394., 4822.
410., 4860.
454., 4862.
474., 4864.
'WL','Large Lake'
200., 4500.
176., 4588.
```

# COASTLN.DAT File - Header Record

The header record of the COASTLN.DAT file contain the name, version, and label of the data set, the UTM zone of the coordinates, and the number of coastlines defined in the file (see Table 4-41). A sample Fortran read statement for the header record is:

    READ(iunit,*)FNAMEC,NCOAST,IUTMCST,VRSCST,LABCST

where the following declaration applies:

    CHARACTER*12 FNAMEC,VRSCST,LABCST.

Table 4-41

COASTLN.DAT - Header Record - General Data

| No. | Variable | Type[a] | Description | Sample Values |
|-----|----------|---------|-------------|---------------|
| 1 | FNAMEC | C*12 | Data set name | COASTLN |
| 2 | NCOAST | integer | Number of coastlines in the file | 2 |
| 3 | ITUMCST | integer | UTM zone in which coastline coordinates are specified (enter 0 if using Lambert conformal coordinates) | 19 |
| 4 | VRSCST | C*12 | Data set version = CALPUFF version | 5 |
| 5 | LABCST | C*12 | Data set label | Test |

[a]C*12 = Character*12

**COASTLN.DAT File - Data Records**

The COASTLN.DAT file contains "NCOAST" groups of coastal coordinates and related data.  Each group of records consists of a single data header record (see Table 4-42) followed by a variable number of data records (see Table 4-43) containing the X and Y coordinates of each point used to define the coastline.   The number of coastlines (NCOAST) must not exceed the maximum number specified in the parameter file (MXCOAST), and the number of points used to define a coastline must not exceed its maximum (MXPTCST).  See the PARAMS.PUF file for the specification of the MXCOAST and MXPTCST variables.

Sample Fortran read statements for COASTLN.DAT data records are:

```
        ┌──   Loop over "NCOAST" coastlines (i)

             READ(iunit,*)ADIR, ALABEL

                  ┌──   Loop over data points (j)

                       READ(iunit,*)XKM(i,j), YKM(i,j)

                  └──   End loop over data points

        └──   End loop over coastlines
```

where the following declarations apply:

```
        REAL XKM(mxcoast,mxptcst),YKM(mxcoast,mxptcst)
        CHARACTER*2 ADIR
        CHARACTER*12 ALABEL
```

Table 4-42

COASTLN.DAT - Data Header Record Contents

(Data header and data point set repeated for each coastline)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | ADIR | C*2 | Flag indicating which side of the coastline water is located as one moves in the direction of the data points in the file (WR indicates water is on right side, WL indicates water is on left side). |
| 2 | ALABEL | C*16 | Character identifier or name of the water body |

[a]C*2 = Character*2
C*16= Character*16

Table 4-43

COASTLN.DAT - Data Record Contents

(Data header and data point set repeated for each coastline)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | XKM | real array | X coordinate (km) of point defining coastline |
| 2 | YKM | real array | Y coordinate (km) of point defining coastline |

4.13  Mass Flux Boundary Data File (FLUXBDY.DAT)

When the IMFLX variable in Input Group 5 of the control file is 1, CALPUFF will compute the hourly mass that crosses boundaries specified in the external file FLUXBDY.DAT.  This file contains a set of points that serve to define one or more boundaries that separate regions.  The mass is said to either pass into or out of a region depending on how the user defines "in" and "out" for each boundary.  Multiple boundaries (up to "MXBNDRY", see the PARAMS.PUF file) are allowed within a single file.

The FLUXBDY.DAT file is a sequential, formatted data file (see Table 4-44 for an example) consisting of two types of records: a single header record and a variable number of sets of data records.  Each set of data records includes one record that establishes which side of the boundary is considered "in" and provides a name for the boundary, and a variable number of records containing the coordinates (km) of each point defining the boundary.

The side of the boundary that is considered "in" may lie either to the left or the right of the boundary as one travels in the direction of the data points provided in the file.  The choice is made by specifying either IR to indicate that the region to the right is inside, or by specifying IL to indicate that the region to the left is inside.

Table 4-44
Sample Mass Flux Boundary Data File (FLUXBDY.DAT)

```
'FLUXBDY', 4, 19, '  5  ', 'test '
'IR','Square 1KM Box'
298., 4629.
298., 4631.
300., 4631.
300., 4629.
298., 4629.
'IL','Diamond 1KM Box'
299., 4629.
298., 4630.
299., 4631.
300., 4630.
299., 4629.
'IR','Square 5KM Box'
294., 4625.
294., 4635.
304., 4635.
304., 4625.
294., 4625.
'IL','Diamond 5KM Box'
299., 4625.
294., 4630.
299., 4635.
304., 4630.
299., 4625.
```

# FLUXBDY.DAT File - Header Record

The header record of the FLUXBDY.DAT file contains the name, version, and label of the data set, the UTM zone of the coordinates, and the number of boundaries defined in the file (see Table 4-45).  A sample Fortran read statement for the header record is:

    READ(iunit,*)DATATYPE,NBNDRY,IUTMBDY,VRSBDY,LABBDY

where the following declaration applies:

    CHARACTER*12 DATATYPE,VRSBDY,LABBDY.

Table 4-45

FLUXBDY.DAT - Header Record - General Data

| No. | Variable | Type[a] | Description | Sample Values |
|-----|----------|---------|-------------|---------------|
| 1 | DATATYPE | C*12 | Data set name | FLUXBDY |
| 2 | NBNDRY | integer | Number of boundaries in the file | 2 |
| 3 | ITUMBDY | integer | UTM zone in which boundary coordinates are specified (enter 0 if using Lambert conformal coordinates) | 19 |
| 4 | VRSBDY | C*12 | Data set version | "5" |
| 5 | LABBDY | C*12 | Data set label | "Test" |

[a]C*12 = Character*12

**FLUXBDY.DAT File - Data Records**


The FLUXBDY.DAT file contains "NBNDRY" groups of boundary coordinates and related data.  Each group of records consists of a single data header record (see Table 4-46) followed by a variable number of data records (see Table 4-47) containing the X and Y coordinates of each point used to define the boundary.   The number of boundaries (NBNDRY) must not exceed the maximum number specified in the parameter file (MXBNDRY), and the number of points used to define a boundary must not exceed its maximum (MXPTBDY).  See the PARAMS.PUF file for the specification of the MXBNDRY and MXPTBDY variables.


Sample Fortran read statements for FLUXBDY.DAT data records are:


```
Loop over "NBNDRY" boundaries (i)

READ(iunit,*)ADIR, ALABEL

       Loop over data points (j)

       READ(iunit,*)XKM(i,j), YKM(i,j)

       End loop over data points

End loop over boundaries
```


where the following declarations apply:


```
REAL XKM(mxbndry,mxptbdy),YKM(mxbndry,mxptbdy)
CHARACTER*2 ADIR
CHARACTER*12 ALABEL
```

Table 4-46

FLUXBDY.DAT - Data Header Record Contents

(Data header and data point set repeated for each boundary)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | ADIR | C*2 | Flag indicating which side of the boundary is considered "in" as one moves in the direction of the data points in the file (IR indicates "in" is on right side, IL indicates "in" is on left side). |
| 2 | ALABEL | C*16 | Character identifier or name of the boundary |

[a]C*2 = Character*2
 C*16= Character*16

Table 4-47

FLUXBDY.DAT - Data Record Contents

(Data header and data point set repeated for each boundary)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | XKM | real array | X coordinate (km) of point defining boundary |
| 2 | YKM | real array | Y coordinate (km) of point defining boundary |

4.14    CALPUFF Output Files

4.14.1   List File (CALPUFF.LST)

The general list file for your CALPUFF run, CALPUFF.LST, is an ASCII text file that may be viewed by
any standard text editor, or printed to any standard printer.  It provides the primary means of
documenting the CALPUFF application, and it also contains all warning messages that may have been
generated by the application.  Note that some problems detected by CALPUFF result in fatal error
messages (the requested modeling period is not simulated), while other problems are not severe enough
to halt the run, and warning messages are written to the list file.  Warning messages may be located
throughout the file, whereas fatal error messages are at the end (because the run is halted).  Therefore, the
list file should always be reviewed.

The contents of the control file are echoed to the first part of the list file, and header records from each
external data file for the run follow.  In the case of CALMET.DAT, the header records include all of the
time-invariant data fields, so that the file can become quite large when large CALMET grids are used.
The remainder of the list file contains any hourly concentrations and deposition fluxes that are selected
for output to the "printer".  This selection is made in Input Group 5 (see Section 4.1) where ICPRT,
IDPRT, and IWPRT identify the types of data selected; ICFRQ, IDFRQ, and IWFRQ identify the interval
(in hours) between the data written to the list file; and IPRTU identifies the units used for this output.
The species written are also explicitly selected here.  Because the primary data files produced by
CALPUFF are CONC.DAT, DFLX.DAT. and WFLX.DAT, which are processed by CALPOST, any data
sent to the list file are generally for making spot-checks prior to the post-processing step, or for viewing
the results of very short runs.

The debug option, controlled by LDEBUG, IPFDEB, NPFDEB, NN1, and NN2 in Input Group 5, also
places a good deal of information in the list file.  Much of this uses internal parameter names, and is most
useful for those who are tracing the treatment of a few specific puffs through the many CALPUFF
subroutines, or for those who are preparing a run and want to obtain more information during the setup
phase (use ITEST=1 in Input Group 1 to stop the run before going into the computational phase).  If
many puffs are traced (NPFDEB) over many modeling periods (NN1 to NN2), the list file will become
huge.  A limited set of puff information is also written to DEBUG.DAT each sampling step when the
debug option is selected.  This file is described in Section 4.14.7.

4.14.2   Restart File (RESTARTE.DAT)

Information for all puffs that are still within the computational grid at the end of a CALPUFF run can be
saved to disk in RESTARTE.DAT to initialize a continuation run.  This allows CALPUFF to properly
account for "old" material within the modeling domain at the start of the continuation run.  This restart
file may also be refreshed periodically during a run, as configured by NRESPD in Input Group 1 of the

control file (see Section 4.1). RESTARTE.DAT is an unformatted data file that contains information about the modeling grid, the date and time at the end of the period simulated, and all of the internal puff array data at the end of the simulation. Note that this file becomes the RESTARTB.DAT input file for the continuation run, and that all CALPUFF output files for the continuation run are "new". For example, if a full year is simulated in four quarterly CALPUFF runs with three restart files, there will be four concentration files rather than one.

4.14.3   Concentration File (CONC.DAT)

The CONC.DAT file is an unformatted data file containing concentrations of one or more species simulated by CALPUFF at each receptor, for each period in the run. The creation and contents of the CONC.DAT file are controlled by user-specified inputs in Input Group 5 of the control file (see Section 4.1). The control file variable ICON must be set equal to one in order to create the CONC.DAT file, and the file will contain only those species that are specifically "saved on disk".

<p align="center">**CONC.DAT File - Header Records**</p>

The CONC.DAT file consists of five header records followed by a set of data records. The header records contain information describing the version of the model used in the run creating the file, horizontal and vertical grid data, a user-input title, a list of the species combinations stored in the output file, and receptor information (see Table 4-48).

Sample FORTRAN read statements for the header records are:

```
    READ(iunit)CMODEL,VER,LEVEL,IBYR,IBJUL,IBHR,
   1 IRLG,IAVG,NXM,NYM,DXKM,DYKM,IONE,XORIGKM,YORIGKM,NSSTA,IBCOMP,IECOMP,
   2 JBCOMP,JECOMP,IBSAMP,JBSAMP,IESAMP,JESAMP,MESHDN,NPTS,NAREAS,NLINES,
   3 NVOLS,NDREC,NCTREC,LSGRID,NSPOUT,LCOMPR
    READ(iunit)TITLE
    READ(iunit)CSOUT
    READ(iunit)XREC,YREC,ZREC
    READ(iunit)XRCT,YRCT,ZRCT,IHILL
```

where the following declarations apply:

```
    Character*80 TITLE(3)
    Character*15 CSOUT(NSPOUT)
    Character*12 CMODEL,VER,LEVEL

    Real XREC(NDREC),YREC(NDREC),ZREC(NDREC)
    Real XRCT(NCTREC),YRCT(NCTREC),ZRCT(NCTREC)

    Integer IHILL(NCTREC)

    Logical LCOMPR
```

Table 4-48

Unformatted CONC.DAT file - Header Record 1 - General Data

| No. | Variable | Type[a] | Description | Sample Values |
|---|---|---|---|---|
| 1 | CMODEL | C*12 | Model name | CALPUFF |
| 2 | VER | C*12 | Model version number | 5.2 |
| 3 | LEVEL | C*12 | Model level number | 991104 |
| 4 | IBYR | integer | Starting year of the run | 1980 |
| 5 | IBJUL | integer | Starting Julian day | 183 |
| 6 | IBHR | integer | Starting hour (00-23 LST; end of hour) | 8 |
| 7 | IRLG | integer | Length of run (hours) | 5 |
| 8 | IAVG | integer | Averaging time (hours) of output concentrations | 1 |
| 9 | NXM | integer | Number of grid points in meteorological grid (X direction) | 20 |
| 10 | NYM | integer | Number of grid points in meteorological grid (Y direction) | 20 |
| 11 | DXKM | real | Grid spacing (km) in the X direction | 5. |
| 12 | DYKM | real | Grid spacing (km) in the Y direction | 5. |
| 13 | IONE | integer | Number of receptor layers (must be equal to one for CALPUFF runs) | 1 |
| 14 | XORIGKM | real | Reference X coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid | 190. |
| 15 | YORIGKM | real | Reference Y coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid | 440. |
| 16 | NSSTA | integer | Number of surface meteorological stations | 5 |
| 17 | IBCOMP | integer | Start of computational grid in X direction | 1 |
| 18 | IECOMP | integer | End of computational grid in X direction | 20 |
| 19 | JBCOMP | integer | Start of computation grid in the Y direction | 1 |
| 20 | JECOMP | integer | End of computational grid in Y direction | 20 |
| 21 | IBSAMP | integer | Start of sampling grid in X direction | 1 |
| 22 | JBSAMP | integer | Start of sampling grid in Y direction | 1 |

[a]C*12 = Character*12

| No. | Variable | Type[a] | Description | Sample Values |
|-----|----------|---------|-------------|---------------|
| 23 | IESAMP | integer | End of sampling grid in X direction | 20 |
| 24 | JESAMP | integer | End of sampling grid in Y direction | 20 |
| 25 | MESHDN | integer | Sampling grid spacing factor | 1 |
| 26 | NPTS | integer | Number of point sources | 2 |
| 27 | NAREAS | integer | Number of area sources | 0 |
| 28 | NLINES | integer | Number of line sources | 0 |
| 29 | NVOLS | integer | Number of volume sources | 0 |
| 30 | NDREC | integer | number of discrete receptors | 0 |
| 31 | NCTREC | integer | Number of complex terrain receptors | 0 |
| 32 | LSGRID | logical | Sampling grid flag (T = gridded receptors used, F = no gridded receptors) | T |
| 33 | NSPOUT | integer | Number of output species | 5 |
| 34 | LCOMPR | logical | Flag indicating if concentration data are compressed (T=yes, F=no) | T |

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | TITLE (3) | C*80 | User-specified run title (three lines of up to 80 characters/line) |

## Header Record 3 - List of Species in Output File

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1-NSPEC | CSOUT array | C*15 | Species name (characters 1-12) and layer (characters 13-15) of concentrations stored in the output file. For example [b], "SO2...........1" indicates $SO_2$ concentrations in Layer 1; "DIOXINP.......1" indicates dioxin in particulate form in Layer 1. CALPUFF concentrations are always computed at ground-level, so therefore are labeled as Layer 1, but there can be up to NZ layers in CALGRID.). |

[a] C*80 = Character*80
 C*15 = Character*15
[b] Dots (....) indicate spaces.

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | XREC | real array | X-coordinate (km) of each discrete receptor |
| 2 | YREC | real array | Y-coordinate (km) of each discrete receptor |
| 3 | ZREC | real array | Ground level elevation (m) of each discrete receptor |

Header Record 5 - Complex Terrain Receptors
(Included only if NCTREC > 0)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | XRCT | real array | X-coordinate (km) of each complex terrain receptor |
| 2 | YRCT | real array | Y-coordinate (km) of each complex terrain receptor |
| 3 | ZRCT | real array | Ground level elevation (m) of each complex terrain receptor |
| 4 | IHILL | integer array | Hill number associated with this receptor |

**CONC.DAT File - Data Records**

The CONC.DAT data records consist of a set of "NSPOUT+1" records for each hour of the CALPUFF run (NSPOUT is the number of output species in the CALPUFF run). The first record of each set contains the date and hour of the data in the records which follow it. The next "NSPOUT" records contain the predicted concentrations in $g/m^3$, for each species, flagged for output in the control file. See Table 4-49 for a description of the variables.

Sample FORTRAN read statements for the data records (in uncompressed format) are:

```
READ(iunit)nyr,njul,nhr

  ┌─  LOOP OVER OUTPUT SPECIES
  │
  │   GRIDDED RECEPTOR CONCENTRATIONS
  │   IF(LSGRID)READ(iunit)CSPECG,CONCG
  │
  │   DISCRETE RECEPTOR CONCENTRATIONS
  │   IF(NDREC.GT.0)READ(iunit)CSPECD,CONCD
  │
  │   COMPLEX TERRAIN RECEPTOR CONCENTRATIONS
  │   IF(NCTREC.GT.0)READ(iunit)CSPECCT,CONCCT
  │
  └─  END LOOP OVER OUTPUT SPECIES
```

where the following declarations apply:

```
Character*15 CSPECG,CPSECD,CSPECCT
Real CONCG(nxg,nyg),CONCD(NDREC),CONCCT(NCTREC)
```
and
```
nxg = IESAMP - IBSAMP+1
nyg = JESAMP - JBSAMP+1
```

CALPUFF contains an option to compress the data by replacing strings of zeroes with a coded repetition factor. The factor is a negative number whose absolute value indicates the number of consecutive zeroes that have been replaced by the repetition factor. This method is especially useful in reducing the size of the output file when large segments of the receptor arrays lie upwind of the puffs during an hour, thereby producing long strings of zeroes in the output arrays. For example, the following record with data for 20 receptors requires 20 unpacked words:

    0.0, 0.0, 0.0, 0.0, 0.0, 1.2, 3.5, 0.0, 0.0, 0.0,

    0.0, 0.0, 0.0, 0.7, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0

These data in packed form would be represented in six words:

    -5., 1.2, 3.5, -6., 0.7, -6.

Table 4-49
Unformatted CONC.DAT File - Data Records
(Record 1 of each set)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | NYR | integer | Year of concentration data (four digits) |
| 2 | NJUL | integer | Julian day of data |
| 3 | NHR | integer | Hour (00-23 LST; end of hour) of data |

(Next Data Record)
(Included only if LSGRID = TRUE)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | CSPECG | C*15 | Species name (characters 1-12) and layer (characters 13-15) of the concentrations in this record. For example [b], "SO2...........1" indicates $SO_2$ concentrations in Layer 1; "DIOXINP.......1" indicates dioxin in particulate form in Layer 1.  (Note:  Layer is always 1 in CALPUFF output, but can be up to NZ in CALGRID.) |
| Next NXG*NYG | CONCG | real array | "IAVG" - hour averaged concentrations ($g/m^3$) for each sampling grid point. |

[a] C*15 = Character*15
[b] Dots (....) indicate spaces.

Table 4-49 (Concluded)
Unformatted CONC.DAT File - Data Records

(Next Data Record)
(Included only if NDREC > 0)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | CSPECD | C*15 | Species name (characters 1-12) and layer (characters 13-15) of the concentrations in this record. For example [b], "SO2...........1" indicates $SO_2$ concentrations in Layer 1; "DIOXINP.......1" indicates dioxin in particulate form in Layer 1. (Note: Layer is always 1 in CALPUFF output, but can be up to NZ in CALGRID.) |
| Next NDREC | CONCD | real array | "IAVG" - hour averaged concentrations ($g/m^3$) for each discrete receptor |

(Next Data Record)
(Included only if NCTREC > 0)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | CSPECCT | C*15 | Species name (characters 1-12) and layer (characters 13-15) of the concentrations in this record. For example [b], "SO2...........1" indicates $SO_2$ concentrations in Layer 1; "DIOXINP.......1" indicates dioxin in particulate form in Layer 1. (Note: Layer is always 1 in CALPUFF output, but can be up to NZ in CALGRID.) |
| Next NCTREC | CONCCT | real array | "IAVG" - hour averaged concentrations ($g/m^3$) at each complex terrain (CTSG) receptor |

[a] C*15 = Character*15
[b] Dots (....) indicate spaces.

4.14.4        Dry Flux File (DFLX.DAT)

The DFLX.DAT file is an unformatted data file containing dry deposition fluxes of one or more species simulated by CALPUFF at each receptor, for each period in the run.  The creation and contents of the DFLX.DAT file are controlled by user-specified inputs in Input Group 5 of the control file (see Section 4.1).

The control file variable IDRY must be set equal to one in order to create the DFLX.DAT file.  The species saved in the output file are also controlled by the user by setting flags in the output species table in Input Group 5 of the control file.  The model checks that only deposited species are flagged for output into the DFLX.DAT file.  The effects of dry deposition on ambient concentrations can be evaluated without saving the dry fluxes in the output file if the actual values of the deposition fluxes are not of interest.

**DFLX.DAT File - Header Records**

The DFLX.DAT file consists of five header records followed by a set of data records.  The header records contain information describing the version of the model used in the run creating the file, horizontal and vertical grid data, a user-input run title, and a list of the deposited species stored in the output file, and receptor information (see Table 4-50).

Sample FORTRAN read statements for the header records are:

```
   READ(iunit)CMODEL,VER,LEVEL,IBYR,IBJUL,IBHR,IRLG,
  1 IAVG,NXM,NYM,DXKM,DYKM,IONE,XORIGKM,YORIGKM,NSSTA,IBCOMP,IECOMP,
  2 JBCOMP,JECOMP,IBSAMP,JBSAMP,IESAMP,JESAMP,MESHDN,NPTS,NAREAS,NLINES,
  3 NVOLS,NDREC,NCTREC,LSGRID,NDFOUT,LCOMPRS
   READ(iunit)TITLE
   READ(iunit)CDFOUT
   READ(iunit)XREC,YREC,ZREC
   READ(iunit)XRCT,YRCT,ZRCT,IHILL
```

where the following declarations apply:

```
   Character*80 TITLE(3)
   Character*15 CDFOUT(NDFOUT)
   Character*12 CMODEL,VER,LEVEL

   Real XREC(NDREC),YREC(NDREC),ZREC(NDREC)
   Real XRCT(NCTREC),YRCT(NCTREC),ZRCT(NCTREC)
   Integer IHILL(NCTREC)
   Logical LCOMPRS
```

Table 4-50

Unformatted DFLX.DAT file - Header Record 1 - General Data

| No. | Variable | Type[a] | Description | Sample Values |
|---|---|---|---|---|
| 1 | CMODEL | C*12 | Model name | CALPUFF |
| 2 | VER | C*12 | Model version number | 5.2 |
| 3 | LEVEL | C*12 | Model level number | 991104 |
| 4 | IBYR | integer | Starting year of the run | 1980 |
| 5 | IBJUL | integer | Starting Julian day | 183 |
| 6 | IBHR | integer | Starting hour (00-23 LST; end of hour) | 8 |
| 7 | IRLG | integer | Length of run (hours) | 5 |
| 8 | IAVG | integer | Averaging time (hours) of output concentrations | 1 |
| 9 | NXM | integer | Number of grid points in meteorological grid (X direction) | 20 |
| 10 | NYM | integer | Number of grid points in meteorological grid (Y direction) | 20 |
| 11 | DXKM | real | Grid spacing (km) in the X direction | 5. |
| 12 | DYKM | real | Grid spacing (km) in the Y direction | 5. |
| 13 | IONE | integer | Layer number (always 1 for deposition fluxes) | 1 |
| 14 | XORIGKM | real | Reference X coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid | 190. |
| 15 | YORIGKM | real | Reference Y coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid | 440. |
| 16 | NSSTA | integer | Number of surface meteorological stations | 5 |
| 17 | IBCOMP | integer | Start of computational grid in X direction | 1 |
| 18 | IECOMP | integer | End of computational grid in X direction | 20 |
| 19 | JBCOMP | integer | Start of computational grid in Y direction | 1 |
| 20 | JECOMP | integer | End of computational grid in Y direction | 20 |
| 21 | IBSAMP | integer | Start of sampling grid in X direction | 1 |
| 22 | JBSAMP | integer | Start of sampling grid in Y direction | 1 |

[a] C*12 = Character*12

| No. | Variable | Type[a] | Description | Sample Values |
|-----|----------|---------|-------------|---------------|
| 23 | IESAMP | integer | End of sampling grid in X direction | 20 |
| 24 | JESAMP | integer | End of sampling grid in Y direction | 20 |
| 25 | MESHDN | integer | Sampling grid spacing factor | 1 |
| 26 | NPTS | integer | Number of point sources | 2 |
| 27 | NAREAS | integer | Number of area sources | 0 |
| 28 | NLINES | integer | Number of line sources | 0 |
| 29 | NVOLS | integer | Number of volume sources | 0 |
| 30 | NDREC | integer | Number of discrete receptors | 0 |
| 31 | NCTREC | integer | Number of complex terrain receptors | 0 |
| 32 | LSGRID | logical | Sampling grid flag (T = gridded receptors used, F = no gridded receptors) | T |
| 33 | NDFOUT | integer | Number of dry deposited species stored in the output file | 5 |
| 34 | LCOMPR | logical | Flag indicating if dry flux data are compressed (T=yes, F=no) | T |

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | TITLE(3) | C*80 | User-specified run title (three lines of up to 80 characters/line) |

### Header Record 3 - List of Species-Layers in Output File

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1-NDFOUT | CDFOUT array | C*15 | Species name (characters 1-12) and variable flag (characters 13-15) of data stored in the output file. The variable flag for dry fluxes is " DF". For example [b], "SO2..........DF" corresponds to $SO_2$ dry fluxes. |

[a] C*80 = Character*80
   C*15 = Character*15
[b] Dots (....) indicate spaces.

Table 4-50 (Concluded)
Unformatted DFLX.DAT file - Header Record 4 - Discrete Receptors
(Included only if NDREC > 0)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | XREC | real array | X-coordinate (km) of each discrete receptor |
| 2 | YREC | real array | Y-coordinate (km) of each discrete receptor |
| 3 | ZREC | real array | Ground level elevation (m) of each discrete receptor |

Header Record 5 - Complex Terrain Receptors
(Included only if NCTREC > 0)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | XRCT | real array | X-coordinate (km) of each complex terrain receptor |
| 2 | YRCT | real array | Y-coordinate (km) of each complex terrain receptor |
| 3 | ZRCT | real array | Ground level elevation (m) of each complex terrain receptor |
| 4 | IHILL | integer array | Hill number associated with this receptor |

**DFLX.DAT File - Data Records**

The DFLX.DAT data records consist of a set of "NDFOUT+1" records for each hour of the CALPUFF runs (NDFOUT is the number of species flagged as being stored in the output file). The first record of each set contains the date and hour of the data in the records which follow it. The next "NDFOUT" records contain predicted one-hour averaged dry deposition fluxes in $g/m^2/s$ for each relevant species (see Table 4-51).

Sample FORTRAN read statements for the data records (in uncompressed format) are:

> READ(iunit)nyr,njul,nhr
>
> LOOP OVER DRY DEPOSITED SPECIES STORED ON DISK
>
> GRIDDED RECEPTOR DRY FLUXES
>     IF(LSGRID)READ(iunit)CDFG,DFLXG
>
> DISCRETE RECEPTOR DRY FLUXES
>     IF(NDREC.GT.0)READ(iunit)CDFD,DFLXD
>
> END LOOP OVER DRY DEPOSITED SPECIES STORED ON DISK

where the following declarations apply:

> Character*15 CDFG,CDFD
> Real DFLXG(nxg,nyg),DFLXD(NDREC)

and

> nxg = IESAMP - IBSAMP+1
> nyg = JESAMP - JBSAMP+1

CALPUFF contains an option to compress the data by replacing strings of zeroes with a coded repetition factor. The factor is a negative number whose absolute value indicates the number of consecutive zeroes that have been replaced by the repetition factor. This method is especially useful in reducing the size of the output file when large segments of the receptor arrays lie upwind of the puffs during an hour, thereby producing long strings of zeroes in the output arrays. For example, the following record with data for 20 receptors requires 20 unpacked words:

> 0.0, 0.0, 0.0, 0.0, 0.0, 1.2, 3.5, 0.0, 0.0, 0.0,
>
> 0.0, 0.0, 0.0, 0.7, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0

These data in packed form would be represented in six words:

> -5., 1.2, 3.5, -6., 0.7, -6.

Table 4-51
Unformatted DFLX.DAT File - Data Records
(Record 1 of each set)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | NYR | integer | Year of dry flux data (four digits) |
| 2 | NJUL | integer | Julian day of data |
| 3 | NHR | integer | Hour (00-23 LST; end of hour) of data |

(Next Data Record)
(Included only if LSGRID = TRUE)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | CDFG | C*15 | Species name (characters 1-12) and variable flag (characters 13-15) of the data in this record. For example [b], "SO2..........DF" corresponds to $SO_2$ dry flux. |
| Next NXG*NYG | DFLXG | real array | "IAVG" - hour averaged dry deposition fluxes $(g/m^2/s)$ for each gridded receptor |

(Next Data Record)
(Included only if NDREC > 0)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | CDFD | C*15 | Species name (characters 1-12) and dry flux flag (characters 13-15) of the data in this record. For example, "SO2..........DF" corresponds to $SO_2$ dry fluxes. |
| Next NDREC | DFLXD | real array | "IAVG" - hour averaged dry deposition fluxes $(g/m^2/s)$ for each discrete receptor |

[a] C*15 = Character*15
[b] Dots (....) indicate spaces.

4.14.5        Wet Flux File (WFLX.DAT)

The WFLX.DAT file is an unformatted data file containing wet deposition fluxes of one or more species simulated by CALPUFF at each receptor, for each period in the run.  The creation and contents of the WFLX.DAT file are controlled by user-specified inputs in Input Group 5 of the control file (see Section 4.1).

The control file variable IWET must be set equal to one in order to create the WFLX.DAT file.  The species saved in the output file are also controlled by the user by setting flags in the output species table in Input Group 5 of the control file.  The model checks that only deposited species are flagged for output into the WFLX.DAT file.  The effects of wet deposition on ambient concentrations can be evaluated without saving the wet fluxes in the output file if the actual values of the deposition fluxes are not of interest.

**WFLX.DAT File - Header Records**

The WFLX.DAT file consists of five header records followed by a set of data records.  The header records contain information describing the version of the model used in the run creating the file, horizontal and vertical grid data, a user-input run title, and a list of the deposited species stored in the output file, and receptor information (see Table 4-52).

Sample FORTRAN read statements for the header records are:

```
    READ(iunit)CMODEL,VER,LEVEL,IBYR,IBJUL,IBHR,IRLG,
      1 IAVG,NXM,NYM,DXKM,DYKM,IONE,XORIGKM,YORIGKM,NSSTA,IBCOMP,IECOMP,
      2 JBCOMP,JECOMP,IBSAMP,JBSAMP,IESAMP,JESAMP,MESHDN,NPTS,NAREAS,NLINES,
      3 NVOLS,NDREC,NCTREC,LSGRID,NWFOUT,LCOMPR
        READ(iunit)TITLE
        READ(iunit)CWFOUT
        READ(iunit)XREC,YREC,ZREC
        READ(iunit)XRCT,YRCT,ZRCT,IHILL
```

where the following declarations apply:

```
    Character*80 TITLE(3)
    Character*15 CWFOUT(NWFOUT)
    Character*12 CMODEL,VER,LEVEL

    Real XREC(NDREC),YREC(NDREC),ZREC(NDREC)
    Real XRCT(NCTREC),YRCT(NCTREC),ZRCT(NCTREC)
    Integer IHILL(NCTREC)
    Logical LCOMPR
```

Table 4-52

Unformatted WFLX.DAT file - Header Record 1 - General Data

| No. | Variable | Type[a] | Description | Sample Values |
|-----|----------|---------|-------------|---------------|
| 1 | CMODEL | C*12 | Model name | CALPUFF |
| 2 | VER | C*12 | Model version number | 5.2 |
| 3 | LEVEL | C*12 | Model level number | 991104 |
| 4 | IBYR | integer | Starting year of the run | 1980 |
| 5 | IBJUL | integer | Starting Julian day | 183 |
| 6 | IBHR | integer | Starting hour (00-23 LST; end of hour) | 8 |
| 7 | IRLG | integer | Length of run (hours) | 5 |
| 8 | IAVG | integer | Averaging time (hours) of output concentrations | 1 |
| 9 | NXM | integer | Number of grid points in meteorological grid (X direction) | 20 |
| 10 | NYM | integer | Number of grid points in meteorological grid (Y direction) | 20 |
| 11 | DXKM | real | Grid spacing (km) in the X direction | 5. |
| 12 | DYKM | real | Grid spacing (km) in the Y direction | 5. |
| 13 | IONE | integer | Layer number (always 1 for deposition fluxes) | 1 |
| 14 | XORIGKM | real | Reference X coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid | 190. |
| 15 | YORIGKM | real | Reference Y coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid | 440. |
| 16 | NSSTA | integer | Number of surface meteorological stations | 5 |
| 17 | IBCOMP | integer | Start of computational grid in X direction | 1 |
| 18 | IECOMP | integer | End of computational grid in X direction | 20 |
| 19 | JBCOMP | integer | Start of computational grid in Y direction | 1 |
| 20 | JECOMP | integer | End of computational grid in Y direction | 20 |
| 21 | IBSAMP | integer | Start of sampling grid in X direction | 1 |
| 22 | JBSAMP | integer | Start of sampling grid in Y direction | 1 |

[a] C*12 = Character*12

| No. | Variable | Type[a] | Description | Sample Values |
|-----|----------|---------|-------------|---------------|
| 23 | IESAMP | integer | End of sampling grid in X direction | 20 |
| 24 | JESAMP | integer | End of sampling grid in Y direction | 20 |
| 25 | MESHDN | integer | Sampling grid spacing factor | 1 |
| 26 | NPTS | integer | Number of point sources | 2 |
| 27 | NAREAS | integer | Number of area sources | 0 |
| 28 | NLINES | integer | Number of line sources | 0 |
| 29 | NVOLS | integer | Number of volume sources | 0 |
| 30 | NDREC | integer | Number of discrete receptors | 0 |
| 31 | NCTREC | integer | Number of complex terrain receptors | 0 |
| 32 | LSGRID | logical | Sampling grid flag (T = gridded receptors used, F = no gridded receptors) | T |
| 33 | NWFOUT | integer | Number of wet deposited species stored in the output file | 5 |
| 34 | LCOMPR | logical | Flag indicating if wet flux data are compressed (T=yes, F=no) | T |

Table 4-52 (Continued)

Unformatted WFLX.DAT file - Header Record 2 - Run Title

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | TITLE(3) | C*80 | User-specified run title (three lines of up to 80 characters/line) |

Header Record 3 - List of Species-Layers in Output File

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1-NWFOUT | CWFOUT array | C*15 | Species name (characters 1-12) and variable flag (characters 13-15) of data stored in the output file. The variable flag for wet flux is " WF". For example [b], `"SO2..........WF"` corresponds to $SO_2$ wet fluxes. |

---

[a] C*80 = Character*80

  C*15 = Character*15

[b] Dots (....) indicate spaces.

Table 4-52 (Concluded)
Unformatted WFLX.DAT file - Header Record 4 - Discrete Receptors
(Included only if NDREC > 0)

| No. | Variable | Type[a] | Description |
|-----|----------|------|-------------|
| 1 | XREC | real array | X-coordinate (km) of each discrete receptor |
| 2 | YREC | real array | Y-coordinate (km) of each discrete receptor |
| 3 | ZREC | real array | Ground level elevation (m) of each discrete receptor |

Header Record 5 - Complex Terrain Receptors
(Included only if NCTREC > 0)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | XRCT | real array | X-coordinate (km) of each complex terrain receptor |
| 2 | YRCT | real array | Y-coordinate (km) of each complex terrain receptor |
| 3 | ZRCT | real array | Ground level elevation (m) of each complex terrain receptor |
| 4 | IHILL | integer array | Hill number associated with this receptor |

**WFLX.DAT File - Data Records**

The WFLX.DAT data records consist of a set of "NWFOUT+1" records for each hour of the CALPUFF runs (NWFOUT is the number of species flagged as being stored in the output file). The first record of each set contains the date and hour of the data in the records which follow it. The next "NWFOUT" records contain predicted one-hour averaged wet deposition fluxes in $g/m^2/s$ for each relevant species (see Table 4-53).

Sample FORTRAN read statements for the data records (in uncompressed format) are:

READ(iunit)nyr,njul,nhr

```
┌── LOOP OVER WET DEPOSITED SPECIES STORED ON DISK
│
│
│      GRIDDED RECEPTOR WET FLUXES
│           IF(LSGRID)READ(iunit)CWFG,WFLXG
│
│
│      DISCRETE RECEPTOR WET FLUXES
│           IF(NDREC.GT.0)READ(iunit)CWFD,WFLXD
│
│
└── END LOOP OVER WET DEPOSITED SPECIES STORED ON DISK
```

where the following declarations apply:

```
Character*15 CWFG,CWFD
Real WFLXG(nxg,nyg),WFLXD(NDREC)
```

and

```
nxg = IESAMP - IBSAMP+1
nyg = JESAMP - JBSAMP+1
```

CALPUFF contains an option to compress the data by replacing strings of zeroes with a coded repetition factor. The factor is a negative number whose absolute value indicates the number of consecutive zeroes that have been replaced by the repetition factor. This method is especially useful in reducing the size of the output file when large segments of the receptor arrays lie upwind of the puffs during an hour, thereby producing long strings of zeroes in the output arrays. For example, the following record with data for 20 receptors requires 20 unpacked words:

    0.0, 0.0, 0.0, 0.0, 0.0, 1.2, 3.5, 0.0, 0.0, 0.0,

    0.0, 0.0, 0.0, 0.7, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0

These data in packed form would be represented in six words:

    -5., 1.2, 3.5, -6., 0.7, -6.

Table 4-53
Unformatted WFLX.DAT File - Data Records
(Record 1 of each set)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | NYR | integer | Year of wet flux data (four digits) |
| 2 | NJUL | integer | Julian day of data |
| 3 | NHR | integer | Hour (00-23 LST; end of hour) of data |

(Next Data Record)
(Included only if LSGRID = TRUE)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | CWFG | C*15 | Species name (characters 1-12) and wet flux flag (characters 13-15) of the data in this record. For example [b], "SO2..........WF" corresponds to $SO_2$ wet fluxes. |
| Next NXG*NYG | DWLXG | real array | "IAVG" - hour averaged wet deposition fluxes ($g/m^2/s$) for each gridded receptor |

(Next Data Record)
(Included only if NDREC > 0)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | CWFD | C*15 | Species name (characters 1-12) and wet flux flag (characters 13-15) of the data in this record. For example [b], "SO2..........WF" corresponds to $SO_2$ wet fluxes. |
| Next NDREC | WFLXD | real array | "IAVG" - hour averaged wet deposition fluxes ($g/m^2/s$) for each discrete receptor |

[a] C*15 = Character*15
[b] Dots (....) indicate spaces.

## 4.14.6    Relative Humidity File for Visibility Processing in CALPOST (VISB.DAT)

The VISB.DAT file is an unformatted data file containing relative humidity data at each surface meteorological station, for each period in the run.  It is required if CALPOST will be used to assess visibility. The variable IVIS in Input Group 5 of the control file (see Section 4.1) must be set equal to one in order to create the VISB.DAT file.

**VISB.DAT File - Header Records**

The VISB.DAT file consists of eight header records followed by a set of data records.  The header records contain information describing the version of the model used in the run creating the file, horizontal and vertical grid data, a user-input run title, receptor information, and the location of all surface meteorological stations in the run (see Table 4-54).

Sample FORTRAN read statements for the header records are:

```
    READ(iunit)CMODEL,VER,LEVEL,IBYR,IBJUL,IBHR,IRLG,
   1 IAVG,NXM,NYM,DXKM,DYKM,IONE,XORIGKM,YORIGKM,NSSTA,IBCOMP,IECOMP,
   2 JBCOMP,JECOMP,IBSAMP,JBSAMP,IESAMP,JESAMP,MESHDN,NPTS,NAREAS,NLINES,
   3 NVOLS,NDREC,NCTREC,LSGRID,NVSOUT,LCOMPR
    READ(iunit)TITLE
    READ(iunit)CVSOUT
    READ(iunit)XREC,YREC,ZREC
    READ(iunit)XRCT,YRCT,ZRCT,IHILL
    READ(iunit)CNAME,NEARS
    READ(iunit)CNAME,XKMSTA
    READ(iunit)CNAME,YKMSTA
```

where the following declarations apply:

```
    Character*80 TITLE(3)
    Character*15 CVSOUT(NVSOUT), CNAME
    Character*12 CMODEL,VER,LEVEL

    Real XREC(NDREC),YREC(NDREC),ZREC(NDREC)
    Real XRCT(NCTREC),YRCT(NCTREC),ZRCT(NCTREC)
    Real XKMSTA(NSSTA),YKMSTA(NSSTA)
    Integer IHILL(NCTREC),NEARS(nxg,nyg)
    Logical LCOMPR
and

    nxg = IESAMP - IBSAMP+1
    nyg = JESAMP - JBSAMP+1
```

Table 4-54

Unformatted VISB.DAT file - Header Record 1 - General Data

| No. | Variable | Type[a] | Description | Sample Values |
|-----|----------|---------|-------------|---------------|
| 1 | CMODEL | C*12 | Model name | CALPUFF |
| 2 | VER | C*12 | Model version number | 5.2 |
| 3 | LEVEL | C*12 | Model level number | 991104 |
| 4 | IBYR | integer | Starting year of the run | 1980 |
| 5 | IBJUL | integer | Starting Julian day | 183 |
| 6 | IBHR | integer | Starting hour (00-23 LST; end of hour) | 8 |
| 7 | IRLG | integer | Length of run (hours) | 5 |
| 8 | IAVG | integer | Averaging time (hours) of output concentrations | 1 |
| 9 | NXM | integer | Number of grid points in meteorological grid (X direction) | 20 |
| 10 | NYM | integer | Number of grid points in meteorological grid (Y direction) | 20 |
| 11 | DXKM | real | Grid spacing (km) in the X direction | 5. |
| 12 | DYKM | real | Grid spacing (km) in the Y direction | 5. |
| 13 | IONE | integer | Layer number (always 1 for deposition fluxes) | 1 |
| 14 | XORIGKM | real | Reference X coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid | 190. |
| 15 | YORIGKM | real | Reference Y coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid | 440. |
| 16 | NSSTA | integer | Number of surface meteorological stations | 5 |
| 17 | IBCOMP | integer | Start of computational grid in X direction | 1 |
| 18 | IECOMP | integer | End of computational grid in X direction | 20 |
| 19 | JBCOMP | integer | Start of computational grid in Y direction | 1 |
| 20 | JECOMP | integer | End of computational grid in Y direction | 20 |
| 21 | IBSAMP | integer | Start of sampling grid in X direction | 1 |
| 22 | JBSAMP | integer | Start of sampling grid in Y direction | 1 |

[a] C*12 = Character*12

| No. | Variable | Type[a] | Description | Sample Values |
|---|---|---|---|---|
| 23 | IESAMP | integer | End of sampling grid in X direction | 20 |
| 24 | JESAMP | integer | End of sampling grid in Y direction | 20 |
| 25 | MESHDN | integer | Sampling grid spacing factor | 1 |
| 26 | NPTS | integer | Number of point sources | 2 |
| 27 | NAREAS | integer | Number of area sources | 0 |
| 28 | NLINES | integer | Number of line sources | 0 |
| 29 | NVOLS | integer | Number of volume sources | 0 |
| 30 | NDREC | integer | Number of discrete receptors | 0 |
| 31 | NCTREC | integer | Number of complex terrain receptors | 0 |
| 32 | LSGRID | logical | Sampling grid flag (T = gridded receptors used, F = no gridded receptors) | T |
| 33 | NVSOUT | integer | Number of data variables stored in the output file (must be 1) | 1 |
| 34 | LCOMPR | logical | Flag indicating if relative humidity data are compressed (T=yes, F=no) — NOT USED | F |

Table 4-54 (Continued)

Unformatted VISB.DAT file - Header Record 2 - Run Title

| No. | Variable | Type[a] | Description |
|---|---|---|---|
| 1 | TITLE(3) | C*80 | User-specified run title (three lines of up to 80 characters/line) |

Header Record 3 - List of Species-Layers in Output File

| No. | Variable | Type | Description |
|---|---|---|---|
| 1 | CVSOUT array | C*15 | Data name (characters 1-15) for data stored in the output file (always ' REL HUM (%)   '). |

[a] C*80 = Character*80
  C*15 = Character*15

Table 4-54 (Continued)
Unformatted VISB.DAT File

Header Record 4 - Discrete Receptors
(Included only if NDREC > 0)

| No. | Variable | Type[a] | Description |
|---|---|---|---|
| 1 | XREC | real array | X-coordinate (km) of each discrete receptor |
| 2 | YREC | real array | Y-coordinate (km) of each discrete receptor |
| 3 | ZREC | real array | Ground level elevation (m) of each discrete receptor |

Header Record 5 - Complex Terrain Receptors
(Included only if NCTREC > 0)

| No. | Variable | Type | Description |
|---|---|---|---|
| 1 | XRCT | real array | X-coordinate (km) of each complex terrain receptor |
| 2 | YRCT | real array | Y-coordinate (km) of each complex terrain receptor |
| 3 | ZRCT | real array | Ground level elevation (m) of each complex terrain receptor |
| 4 | IHILL | integer array | Hill number associated with this receptor |

Table 4-54 (Concluded)
Unformatted VISB.DAT File

Header Record 6 - Nearest Surface Station Array

| No. | Variable | Type[a] | Description |
|---|---|---|---|
| 1 | CNAME | C*15 | Array name (' NEARS        ') |
| Next NXG*NYG | NEARS | integer array | Surface meteorological station index nearest each cell in the modeling grid |

[a] C*15 = Character*15

Header Record 7 - X-coordinate of Each Surface Station

| No. | Variable | Type[a] | Description |
|---|---|---|---|
| 1 | CNAME | C*15 | ' XSSTA-UTM    ' |
| 2 | XKMSTA | real array | X-coordinate (km) of each surface station |

[a] C*15 = Character*15

Header Record 8 - Y-coordinate of Each Surface Station

| No. | Variable | Type[a] | Description |
|---|---|---|---|
| 1 | CNAME | C*15 | ' YSSTA-UTM    ' |
| 2 | YKMSTA | real array | Y-coordinate (km) of each surface station |

[a] C*15 = Character*15

**VISB.DAT File - Data Records**

The VISB.DAT data records consist of a set of "NVSOUT+1" records for each hour of the CALPUFF runs (where NVSOUT is always one). The first record of each set contains the date and hour of the data in the records which follow it. The next "NVSOUT" records contain the relative humidity reported at each meteorological surface station in % (see Table 4-55).

Sample FORTRAN read statements for the data records are:

        READ(iunit)nyr,njul,nhr
        READ(iunit)CNAME,IRHSS

where the following declarations apply:

        Character*15 CNAME
        Integer IRHSS(NSSTA)

Table 4-55

Unformatted VISB.DAT File - Data Records

(Record 1 of each set)

| No. | Variable | Type | Description |
|-----|----------|------|-------------|
| 1 | NYR | integer | Year of relative humidity data (four digits) |
| 2 | NJUL | integer | Julian day of data |
| 3 | NHR | integer | Hour (00-23 LST; end of hour) of data |

(Record 2 of each set)

| No. | Variable | Type[a] | Description |
|-----|----------|---------|-------------|
| 1 | CNAME | C*15 | ' REL HUM (%)  ' |
| Next NSSTA | IRHSS | integer array | Relative humidity (%) reported as an integer for each surface meteorological station |

---

[a] C*15 = Character*15

4.14.7  Debug Puff-Tracking File (DEBUG.DAT)

CALPUFF contains a debug option to report much information about each selected puff as it is transported and sampled over a number of modeling periods.  Most of this extra information is written to the CALPUFF list file (see Section 4.14.1).  A limited set of puff information is also written to DEBUG.DAT each sampling step when the debug option is selected.  The purpose of this file is to provide puff characteristics at the end of each sampling step so that its location and size can be reviewed to visualize the combined effects of transport and diffusion at specific times.

The DEBUG.DAT file is a sequential, formatted data file (see Table 4-56 for an example) consisting of two types of records: two header records and a variable number of sets of data records.  The header records name the variables that are reported in the data records (see Table 4-57).  Each data record provides information about a single puff at the end of a single sampling step.  While there may be many sampling steps over the course of an hour, the time reported for each is the end-time of the current hour.

A series of nested loops controls the sequence in which the data records are written to the file.  The outermost loop is over the number of modeling periods (hours) for which debug output is selected.  Within this is a loop over the range of puffs that has been selected.  The innermost loop is over the sampling steps for each of these puffs.  Because the puff ID and the date and time are included in each record, this structure is readily discerned.

Records for individual puffs are written during the selected modeling period only while that puff exists on the computational grid.  It is not tracked before it is emitted, and it is not tracked once it leaves the modeling domain.

## Table 4-56
## Sample Debug Puff-Tracking File (DEBUG.DAT)

```
                         ---- PUFF/ Old SLUG end ---------
YYYYJJJHH   ipnum cd   zfnl   x(metG)  y(metG)   sigyB   sigzB       QM         QU      zimax  rflctn   dpbl jdstab  Length
198818922     1 1  119.7   3.0080   2.4482    954.5   190.5  1.8000E+04  0.0000E+00   815.6   815.6   815.6   4
198818922     1 1  119.7   3.3639   3.1576   1854.5   268.9  1.8000E+04  0.0000E+00   790.8   790.8   790.8   4
198818922     2 1  119.7   3.0080   2.4482    954.5   190.5  1.8000E+04  0.0000E+00   815.6   815.6   815.6   4
198818922     3 1  100.9   4.2533   3.7418    950.3   189.6  1.8000E+04  0.0000E+00   685.5   685.5   685.5   4
198818922     3 1  100.9   4.6753   4.3929   1850.3   969.4  1.8000E+04  0.0000E+00   665.6   665.6   665.6   4
198818923     1 1  119.7   3.5188   3.7123   2454.5   862.1  1.8000E+04  0.0000E+00   898.4   898.4   898.4   4
198818923     1 1  119.7   3.7095   3.9935   3054.5  1084.2  1.8000E+04  0.0000E+00   898.4   898.4   898.4   4
198818923     1 1  119.7   3.9002   4.2746   3654.5  1091.4  1.8000E+04  0.0000E+00   898.4   898.4   829.2   4
198818923     2 1  119.7   3.1453   3.0027   1554.5   250.4  1.8000E+04  0.0000E+00   941.2   941.2   941.2   4
198818923     2 1  119.7   3.2974   3.5544   2154.5   851.3  1.8000E+04  0.0000E+00   898.4   898.4   898.4   4
198818923     2 1  119.7   3.4881   3.8355   2754.5  1075.4  1.8000E+04  0.0000E+00   898.4   898.4   898.4   4
198818923     3 1  100.9   5.0467   4.8309   2750.3  1295.1  1.8000E+04  0.0000E+00   798.3   798.3   798.3   4
198818923     3 6  100.9   5.4990   5.2454   3650.3  1295.1  1.5955E+04  2.0452E+03   798.3   707.6   707.6   4
198819000     1 1  119.7   4.2947   4.4464   4554.5  1108.1  1.8000E+04  0.0000E+00   898.4   898.4   466.0   5
198819000     1 1  119.7   4.7226   4.5824   5454.5  1125.2  1.8000E+04  0.0000E+00   898.4   898.4   466.0   5
198819000     2 1  119.7   3.8793   4.0499   3654.5  1092.9  1.8000E+04  0.0000E+00   898.4   898.4   538.1   5
198819000     2 1  119.7   4.2736   4.2213   4554.5  1109.6  1.8000E+04  0.0000E+00   898.4   898.4   466.0   5
198819000     3 6  100.9   6.0656   5.4060   4550.3  1295.1  9.6942E+03  8.3058E+03   798.3   429.9   429.9   5
198819000     3 6  100.9   6.6832   5.5231   5450.3  1295.1  1.0735E+04  7.2646E+03   798.3   476.1   476.1   4
```

Table 4-57

DEBUG.DAT - Data Record

| No. | Variable | Description |
|-----|----------|-------------|
| 1 | YYYYJJJHH | Year-Julian Day-Hour for modeling period |
| 2 | IPNUM | Puff ID number |
| 3 | CD | Puff Code<br>1 = Puff within mixed layer & Gaussian<br>2 = Puff within mixed layer & uniform<br>3 = Puff above mixed layer & Gaussian<br>4 = Puff above mixed layer & uniform<br>5 = Puff currently above mixed layer<br>   (but previously below) & Gaussian<br>6 = Puff currently above mixed layer<br>   (but previously below) & uniform<br>11 = Slug within mixed layer & Gaussian<br>12 = Slug within mixed layer & uniform<br>13 = Slug above mixed layer & Gaussian<br>14 = Slug above mixed layer & uniform<br>15 = Slug currently above mixed layer<br>   (but previously below) & Gaussian<br>16 = Slug currently above mixed layer<br>   (but previously below) & uniform<br>99 = Puff/slug off computational grid |
| 4 | ZFNL | Puff height (m) at final rise |
| 5 | X | X-coordinate of puff or old slug-end (Met Grid Units) |
| 6 | Y | Y-coordinate of puff or old slug-end (Met Grid Units) |
| 7 | SIGYB | Sigma-y of puff or old slug-end (m) |
| 8 | SIGZB | Sigma-z of puff or old slug-end (m) |
| 9 | QM | Puff mass (g) of species 1 below mixing lid |
| 10 | QU | Puff mass (g) of species 1 above mixing lid |
| 11 | ZIMAX | Largest mixing height (m) for this puff (10000 m used for unlimited mixing) |
| 12 | RFLCTN | Reflecting lid height (m) for Gaussian distribution (10000 m used for unlimited mixing) |
| 13 | DPBL | Current surface boundary layer height (m) |
| 14 | JDSTAB | Stability class |
| 15 | Length | Emitted slug length (m) |

4.14.8  Mass Flux List File (MASSFLX.DAT)

Mass flux results for those species selected in the control file are reported to the list file MASSFLX.DAT
for each boundary that is contained in the boundary file FLUXBDY.DAT.  MASSFLX.DAT is a
formatted text file that identifies the CALPUFF version and level, echoes the 3-line title of the
CALPUFF simulation, identifies the output as mass flux (g/s), sets out column headings to label each
variable listed, and then reports the mass fluxes for each hour in the simulation.  The boundaries are
identified by the names provided in FLUXBDY.DAT, and for each boundary, the mass flux in and out
across the boundary is reported.  The date and time of each output record marks the time at the end of the
hour, where midnight is hour zero of the new day (CALPUFF convention).

An example list file is provided in Table 4-58.  The four boundaries are identified using the names
provided in the boundary data file.  Note that these boundaries do not surround a source, and enclose
small regions so that the fluxes produced across each boundary are frequently both in and out as the puffs
in this example pass through the enclosed regions.

Table 4-58
Sample Mass Flux List File (MASSFLX.DAT)

```
                              CALPUFF        Version: 5.2        Level: 991104
***********************************************************************************************************************

CALPUFF test case run - 3 point sources
24-Hour Simulation using CALMET met. data
Gridded receptors on 17x17 20-km met grid


                          ---------------
                            Mass Flux
                              (g/s)
                          ---------------


                         Square 1KM Box       Diamond 1KM Box       Square 5KM Box       Diamond 5KM Box
      Yr Day Hr   Species   In      Out         In      Out          In      Out          In      Out

1988 189  1 SO2     0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
1988 189  2 SO2     0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
1988 189  3 SO2     0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
1988 189  4 SO2     0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.50000E+01 0.00000E+00 0.00000E+00 0.00000E+00
1988 189  5 SO2     0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.50000E+01 0.10000E+02 0.10000E+02 0.10000E+02
1988 189  6 SO2     0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
1988 189  7 SO2     0.25000E+01 0.25000E+01 0.25000E+01 0.25000E+01 0.50000E+01 0.50000E+01 0.50000E+01 0.50000E+01
1988 189  8 SO2     0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.25000E+01 0.25000E+01 0.25000E+01 0.25000E+01
1988 189  9 SO2     0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.50000E+01 0.00000E+00 0.00000E+00 0.50000E+01
1988 189 10 SO2     0.25000E+01 0.25000E+01 0.25000E+01 0.25000E+01 0.50000E+01 0.75000E+01 0.50000E+01 0.00000E+00
1988 189 11 SO2     0.50000E+01 0.50000E+01 0.00000E+00 0.00000E+00 0.50000E+01 0.25000E+01 0.00000E+00 0.50000E+01
1988 189 12 SO2     0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.50000E+01 0.50000E+01 0.00000E+00
```

4.14.9  Mass Balance List File (MASSBAL.DAT)

Mass balance results for all species in the run are reported to the list file MASSBAL.DAT.
MASSBAL.DAT is a formatted text file that identifies the CALPUFF version and level, echoes the 3-line
title of the CALPUFF simulation, identifies the output as hourly mass balance (g), sets out column
headings to label each variable listed, and then reports changes in the mass of each species in the entire
modeling domain for each hour in the simulation.  The date and time of each output record marks the
time at the end of the hour, where midnight is hour zero of the new day (CALPUFF convention).

An example list file is provided in Table 4-59.  The first five columns after the species name identify the
hourly change in mass due to emissions, transport out of the domain, chemical transformation, and
depletion (wet and dry deposition).  The last three columns report the current mass totals at the end of the
hour, and the portion that is in the surface mixed layer, and above the mixed layer.  A single record is
written for each species and each hour of the simulation.

Table 4-59
Sample Mass Balance List File (MASSBAL.DAT)

```
                         CALPUFF        Version: 5.2        Level: 991104
********************************************************************************************************************

CALPUFF test case run - 3 point sources
24-Hour Simulation using CALMET met. data
Gridded receptors on 17x17 20-km met grid


                    ----------------------
                      Hourly Mass Balance
                             (g)
                    ----------------------


                                   Advected                        Wet         Dry        Domain      Domain      Domain
   Yr  Day Hr  Species   Emitted      Out    Transformed       Depletion   Depletion     Total       Surface      Aloft

 1988 189  1 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.08000E+05  1.08000E+05  0.00000E+00
 1988 189  2 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  2.16000E+05  2.16000E+05  0.00000E+00
 1988 189  3 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.24000E+05  3.24000E+05  0.00000E+00
 1988 189  4 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  4.32000E+05  4.32000E+05  0.00000E+00
 1988 189  5 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  5.40000E+05  5.40000E+05  0.00000E+00
 1988 189  6 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  6.48000E+05  6.48000E+05  0.00000E+00
 1988 189  7 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  7.56000E+05  7.55506E+05  4.94406E+02
 1988 189  8 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  8.64000E+05  7.67561E+05  9.64391E+04
 1988 189  9 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  9.72000E+05  9.03347E+05  6.86530E+04
 1988 189 10 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.08000E+06  1.04017E+06  3.98287E+04
 1988 189 11 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.18800E+06  1.13525E+06  5.27460E+04
 1988 189 12 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.29600E+06  1.23078E+06  6.52167E+04
 1988 189 13 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.40400E+06  1.32007E+06  8.39310E+04
 1988 189 14 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.51200E+06  1.42405E+06  8.79461E+04
 1988 189 15 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.62000E+06  1.54313E+06  7.68674E+04
 1988 189 16 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.72800E+06  1.65073E+06  7.72731E+04
 1988 189 17 SO2      1.08000E+05  3.60000E+04  0.00000E+00  0.00000E+00  0.00000E+00  1.80000E+06  1.68879E+06  1.11212E+05
 1988 189 18 SO2      1.08000E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  1.90800E+06  1.76439E+06  1.43614E+05
 1988 189 19 SO2      1.08000E+05  1.80000E+04  0.00000E+00  0.00000E+00  0.00000E+00  1.99800E+06  1.82506E+06  1.72942E+05
 1988 189 20 SO2      1.08000E+05  7.20000E+04  0.00000E+00  0.00000E+00  0.00000E+00  2.03400E+06  1.62398E+06  4.10020E+05
 1988 189 21 SO2      1.08000E+05  3.60000E+04  0.00000E+00  0.00000E+00  0.00000E+00  2.10600E+06  1.64662E+06  4.59384E+05
 1988 189 22 SO2      1.08000E+05  9.00000E+04  0.00000E+00  0.00000E+00  0.00000E+00  2.12400E+06  1.63884E+06  4.85155E+05
 1988 189 23 SO2      1.08000E+05  7.20000E+04  0.00000E+00  0.00000E+00  0.00000E+00  2.16000E+06  1.55585E+06  6.04154E+05
 1988 190  0 SO2      1.08000E+05  1.62000E+05  0.00000E+00  0.00000E+00  0.00000E+00  2.10600E+06  1.42564E+06  6.80359E+05
```

4.15    OPTHILL

When the subgrid scale complex terrain (CTSG) option of the CALPUFF model is invoked, two groups
of additional data must be prepared by the user: CTSG receptor and terrain information.  These data may
be provided in external files in the format used by CTDMPLUS (Section 4.11), or they may be entered
into the CALPUFF control file.  The purpose of the optimizer program OPTHILL is to provide the user
with the means for calculating the set of terrain data that best characterizes each feature when these data
are entered into the control file.

4.15.1   CTSG Terrain Information

CTSG requires information on the location, orientation, size, and shape of each terrain feature being
modeled.  The variables that contain this information are:

| | |
|---|---|
| xc,yc | coordinates (km) of the center of the hill |
| thetah | orientation (deg) of major axis of hill (clockwise from north) |
| zgrid | height (m) of "grid-plane" of grid above mean sea level |
| relief | height (m) of crest of hill above the "grid-plane" elevation |
| expo (1) | hill-shape exponent for major axis |
| expo (2) | hill-shape exponent for minor axis |
| scale(1) | horizontal length scale (m) along major axis |
| scale(2) | horizontal length scale (m) along minor axis |
| axmax(1) | maximum allowed axis length (m) for major axis |
| axmax(2) | maximum allowed axis length (m) for minor axis |

The profile of the terrain along each axis of the feature is prescribed by the following equation:

$$ht(x) \; = \; \left[ \frac{1 \; - \; (x/axmax)^{expo}}{1 \; + \; (x/scale)^{expo}} \right] * \; relief \tag{4-1}$$

where ht(x) is the height of the profile above the base of the feature, at a distance x from the peak (Figure
4-1).

The terrain profile-optimizing program (OPTHILL) computes the hill shape exponent (EXPO) and
horizontal terrain length scale (SCALE) parameters from a user-entered terrain profile along each of two
axes.  This terrain profile defines the height of the surface of the hill at a number of distances from the
center of the hill, along each axis.  The OPTHILL program performs computations for one axis (i.e.,
major or minor axis) of the terrain feature at a time.  Therefore, two runs of OPTHILL are necessary for
each subgrid scale terrain feature.
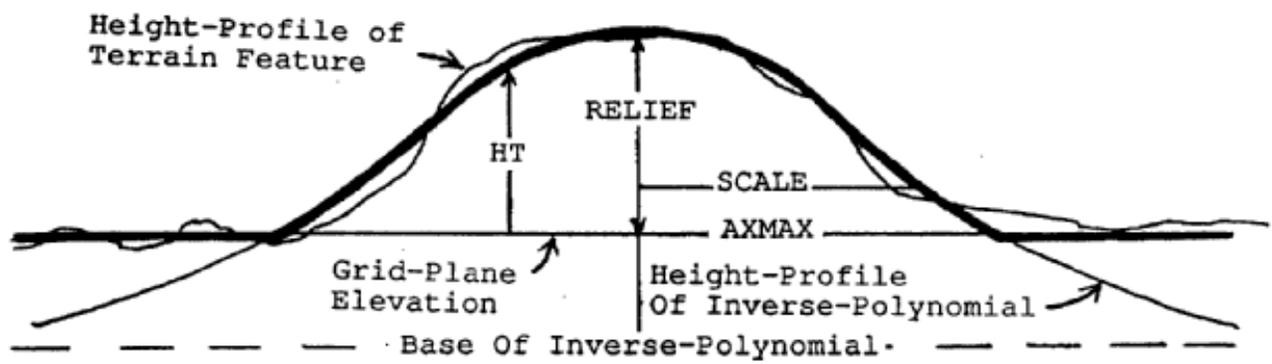
Figure 4-1.    Profile of a terrain feature along one of its two axes.  A best-fit inverse polynomial
               function describes this profile to CTSG.

The following procedure is recommended to determine the terrain inputs for the CALPUFF CTSG algorithm from a topographic map.

a.    **Identify the sub-grid terrain features to be modeled.**

Such features will generally be small enough that they could be contained within one grid-square. This does not mean that they cannot straddle two or more squares. The features should be prominent, and possibly lie near source regions so that the additional computations required by CTSG are warranted in resolving important pollutant impact areas.

b.    **Decide on the orientation of the feature.**

The orientation of the feature is generally evident if the feature is longer in one direction than another. If there is no dominant direction to the feature, model it as a symmetric feature, and choose an orientation of north.

c.    **Obtain height-profiles along each axis of the feature.**

Choose an approximate center for the feature and draw axes through it (one axis should lie along the direction of orientation). Along each axis, measure the distance between approximate intersections of the axis with marked contours. The distances so measured should extend from the contour furthest to the south to the same contour furthest to the north (for a north-south axis). Divide each of these distances by two, and tabulate the results.

d.    **Identify the maximum elevation of the feature.**

Take the peak elevation directly from the map.

e.    **Identify the elevation at the base of the feature.**

Generally, the base of the feature will be that point at which the feature becomes indistinguishable from terrain variations around it.

f.    **Convert all elevations that were tabulated to heights above the base of the feature.**

g.    **Use optimizer program (OPTHILL) to obtain shape parameters.**

The "relief" parameter is just the peak elevation less the base elevation. The "axmax" value for each axis should be representative of the maximum extent of the feature along each axis at the elevation of the base of the feature. With these two variables fixed for each axis, the height-

profile data from step c. can be put through OPTHILL to obtain "expo" and "scale" for each axis.

Table 4-60 summarizes the OPTHILL input and output filenames. OPTHILL requires a single input file (OPTHILL.INP) which contains the user's inputs describing the terrain profile, each height, and maximum axis length. The computed values of EXPO and SCALE for one axis of the hill are listed in the output list file (OPTHILL.LST). The format and contents of the OPTHILL control file are explained in Table 4-61.

4.15.2   Example OPTHILL Application

The OPTHILL program is an optimization that takes a value of "relief" and "axmax," and a sequence of pairs of (x,ht) values along an axis, and returns a value of "expo" and "scale" that prescribes the profile function that best matches the (x,ht) pairs. Its use is illustrated by the following example.

Figure 4-2 shows the terrain surrounding the site of EPA's "Full-Scale Plume Study" (FSPS) that was performed in the Truckee River Valley near Reno, NV (Strimaitis et al., 1985), as part of the Complex Terrain Model Development Program. Nocturnal flow in this valley is frequently channeled by the high terrain to the north and south of the Tracy power plant. Elevations typical of nocturnal plume heights (4600-4800 ft. MSL) are emphasized on the figure. Given the predominant flow to the east during stable conditions, there is potential for plume impact on the feature just northeast of the plant. This feature, marked by axes in Figure 4-2, was named "Beacon Hill" during the study.

Following the procedures outlined above, axes were drawn over the feature and distances between fixed contour elevations were tabulated. After subtracting the elevation above sea level of the base of the feature (the floor of the river valley), these data were entered into two files. Table 4-62 displays the contents of both files. The files (axis1.inp and axis2.inp) contain "relief" and the value for "axmax" for each axis of the hill, followed by five pairs of (x,ht) values. The first record of each file is reserved for comments to identify the data. Values for "relief" and "axmax" are free-format, and should be entered anywhere in the open space provided on the next two lines. Pairs of (x,ht) should be entered right after the next comment record.

OPTHILL must be invoked separately for each of the two axes of the hill. This is accomplished by renaming one input file (e.g., axis1.inp) to the OPTHILL input control file name (OPTHILL.INP), executing the program, renaming the output file (OPTHILL.LST) to a new name (e.g., axis1.lst), and then repeating these steps for the second axis of the hill. The output files produced by OPTHILL for the current example are presented in Table 4-63 and 4-64. The output file lists the final values of the profile parameters, and it also lists the profile data provided by the user along with the corresponding data computed from the profile parameters.

Table 4-60

OPTHILL Input and Output Files

| Unit | File Name | Type | Format | Description |
|------|-----------|------|--------|-------------|
| 5 | OPTHILL.INP | input | formatted | Control file containing user inputs |
| 6 | OPTHILL.LST | output | formatted | List file (line printer output file) |

Table 4-61
OPTHILL Control File Inputs (OPTHILL.INP)

| Record | Variable No. | Variable Name | Columns | Type of Format | Description |
|--------|--------------|---------------|---------|----------------|-------------|
| 1 | 1 | TITLE(15) | 1-60 | 15A4 | 60 character title |
| 2 | 1 | RELIEF | * | real | Height (m) of the crest of the hill above the grid elevation |
| 3 | 1 | AXMAX | * | real | Maximum allowed axis length (m) for the axis (major or minor) being evaluated |
| 4 | 1 | - | * | - | This record is skipped by the program. May contain optional text data (see example) |
| 5 | 1 | DIST | * | real | Distance-height pairs describing the profile of the terrain.  Units: m |
| 5 | 2 | HGT | * | real | Distance-height pairs describing the profile of the terrain. Units:  m |

_____

*  Entered in FORTRAN free format.
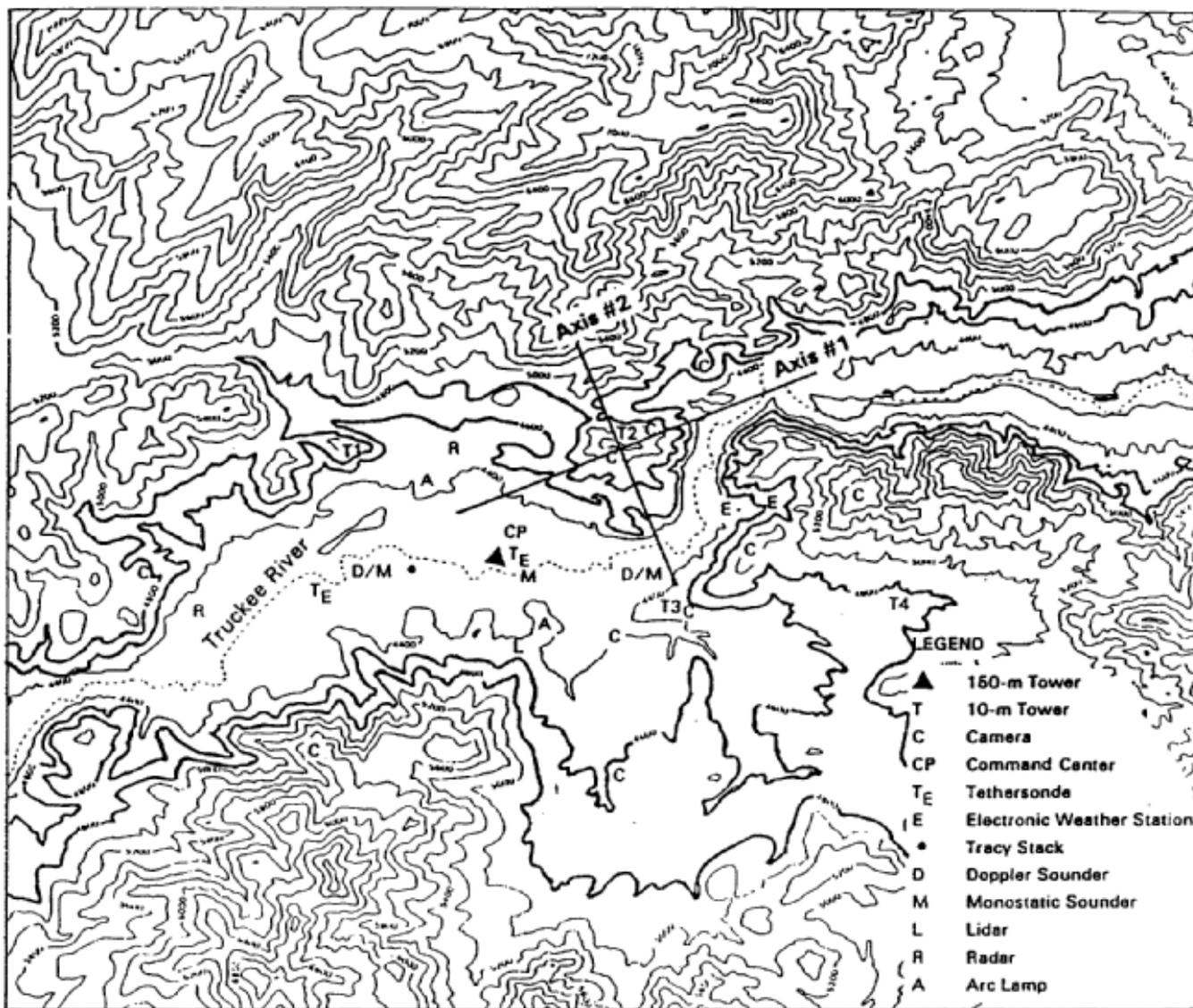
Figure 4-2.    Map of terrain surrounding the site of the FSPS, illustrating the selection and characterization of a terrain feature for CTSG modeling.

Table 4-62

Sample OPTHILL Input Files

### (a) OPTHILL.INP for Axis #1 of the hill.

```
Optimal SCALE and EXPO factors -- Axis #1 of example problem
300.      - Height (m) of hill crest above "zero-plane" elevation (RELIEF)
2000.     - Maximum allowed length (m) for this axis (AXMAX)
-------------------------------- Distance-height pairs describing hill profile -------------------------------
564.,    239.                        - Dist.(m) from crest, terrain ht (m) above "zero-plane" elev.
826.,    178.                          (Repeated for each dist.-height pair)
1062.,   150.
1193.,   117.
1508.,    56.
```

### (b) OPTHILL.INP for Axis #2 of the hill.

```
Optimal SCALE and EXPO factors -- Axis #2 of example problem
300.                     - Height (m) of hill crest above "zero-plane" elevation (RELIEF)
1500.                    - Maximum allowed length (m) for this axis (AXMAX)
-------------------------------- Distance-height pairs describing hill profile -------------------------------
302.,    239.                        - Dist.(m) from crest, terrain ht (m) above "zero-plane" elev.
551.,    178.                          (Repeated for each dist.-height pair)
708.,    150.
970.,    117.
1311.,    56.
```

Table 4-63
OPTHILL Output File for Axis #1 of Sample Hill

```
***  Optimal SCALE and EXPO factors -- Axis #1 of example problem ***

        EVOL TIME LIMIT =       60. SECONDS        SKIP = 10

NUMBER OF PARAMETERS FOR THIS STUDY :  4

PARAMETER       START VALUE     STEP CONTROL    LOWER LIMIT    UPPER LIMIT
---------       -----------     -----------     ----------     ----------


1 RELIEF        0.3000E+03      0.0000E+00      0.3000E+03     0.3000E+03
2 AXMAX         0.2000E+04      0.0000E+00      0.2000E+04     0.2000E+04
3 EXPO          0.2000E+01      0.2000E+01      0.1000E+00     0.1000E+02
4 SCALE         0.2000E+04      0.1000E+04      0.2000E+02     0.2000E+06




CALCULATIONS STARTED




RETURN VALUE:  2 NORMAL RETURN    FUNCTION VALUE: 0.50303

PARAMETER VALUES:
            RELIEF  =    300.00000
            AXMAX   =   2000.00000
            EXPO    =      1.90651
            SCALE   =   1522.94500


Distance  Height    Fitted Value

  564.0    239.0      237.4
  826.0    178.0      186.4
 1062.0    150.0      139.9
 1193.0    117.0      115.5
 1508.0     56.0       63.0
```

Table 4-64

```
.***  Optimal SCALE and EXPO factors -- Axis #2 of example problem ***

          EVOL TIME LIMIT =        60. SECONDS        SKIP = 10

NUMBER OF PARAMETERS FOR THIS STUDY :   4

PARAMETER  START VALUE   STEP CONTROL  LOWER LIMIT   UPPER LIMIT
---------- -----------   -----------   ----------    -----------


1 RELIEF   0.3000E+03    0.0000E+00    0.3000E+03    0.3000E+03
2 AXMAX    0.1500E+04    0.0000E+00    0.1500E+04    0.1500E+04
3 EXPO     0.2000E+01    0.2000E+01    0.1000E+00    0.1000E+02
4 SCALE    0.1500E+04    0.7500E+03    0.1500E+02    0.1500E+06




CALCULATIONS STARTED




RETURN VALUE:  2        NORMAL RETURN
         FUNCTION VALUE: 2.17504

PARAMETER VALUES:
          RELIEF  =    300.00000
          AXMAX   =   1500.00000
          EXPO    =      1.23912
          SCALE   =   2895.90200


Distance  Height   Fitted Value

  302.0    239.0      244.0
  551.0    178.0      189.1
  708.0    150.0      154.7
  970.0    117.0       99.5
 1311.0     56.0       33.5
```

This process is simplified somewhat if a batch file is used to manage the filenames. One such batch file for DOS (RUNOPT.BAT) is included with the testcase. It requires three filenames as arguments:

       RUNOPT   file1  file2  file3

where

| | | |
|---|---|---|
| file1 | OPTHILL.EXE | executable program file |
| file2 | user.inp | input file |
| file3 | user.out | output file |

The batch file copies file2 to OPTHILL.INP, runs OPTHILL.EXE which creates OPTHILL.LST, then renames OPTHILL.LST to the name supplied as file3. For the example above, axis #1 would be processed by typing the command:

       RUNOPT  OPTHILL.EXE   AXIS1.INP   AXIS1.LST

With these results, hill information that is independent of the choice of coordinate system and the modeling grid for the wind model can be specified:

| | |
|---|---|
| xc,yc (m) | (depends on choice of coordinates) |
| thetah (deg) | 69° |
| zgrid (m) | (depends on grid for wind model) |
| relief (m) | 300. |
| expo (1) | 1.91 |
| expo (2) | 1.24 |
| scale (1) (m) | 1523. |
| scale (2) (m) | 2896. |
| axmax (1) (m) | 2000. |
| axmax (2) (m) | 1500. |

Note that scale(2) is almost twice scale(1), even though axis 1 corresponds to the longer axis of the hill. This can occur because the "scale" parameter is a property of the entire inverse-polynomial function (Equation 4-1), rather than just the portion of the function that is fit to the profile of the terrain. In Figure 4-1, the shape of the terrain might best conform to the upper 10% of the polynomial function, in which case the "scale" parameter would exceed "axmax." In this example application of the OPTHILL program, we see that axmax(2) is substantially less than axmax(1), whereas scale(2) exceeds scale(1), indicating that a comparatively smaller portion of the polynomial function represents the terrain profile along the minor axis.

# 5. CALPOST POSTPROCESSING PROGRAM

The CALPOST program is a postprocessor designed to average and report concentration or wet/dry deposition flux results based on the hourly data contained in the CALPUFF output file. If the CALPUFF application had been configured to provide concentrations needed to assess visibility, CALPOST can also compute extinction coefficients for visibility-related impacts. A range of averaging times may be selected, and the results may be reported in a number of different formats (e.g. rank tables and plots; exceedance tables and plots). Capabilities and options include:

- User-selected processing period.
- User-selected averaging times, including option for one defined by the user.
- User-selected chemical species.
- User-selected units for reporting concentrations or deposition fluxes.
- Option to include gridded receptors, discrete receptors, and complex terrain receptors in any combination.
- Option to specify subsets of the gridded and discrete receptors.
- Option to produce tables of the "top-50" average concentration/deposition flux data (includes time and receptor information) for specified averaging times.
- Option to produce tables of up to four "top-N" (user specifies the number N) ranked average concentration/deposition flux data at the selected receptors for specified averaging times.
- Option to produce tables of the number of exceedances of user-specified threshold values at the selected receptors for specified averaging times.
- Option to produce a table of the annual (or length-of-run) average concentration/deposition flux at the selected receptors.
- Option to print concentration/deposition flux averages for selected days.
- Option to produce a file of timeseries of concentration/deposition flux averages for selected days.
- Option to produce plot-files in addition to the selected tables for the "top N" concentrations or deposition fluxes, the number of exceedances of the user-specified thresholds, and the concentration/deposition flux fields for a particular day.
- Option to scale all concentration/deposition flux data by means of a linear function of the form: $a*X + b$ (where X is concentration or deposition, and a,b are user-supplied constants).
- Option to add an hourly background concentration/deposition flux from an external file.
- Option to produce visibility parameters , signaled by setting the species name to "visib". Requires that CALPUFF is configured for visibility computations.

When CALPOST is directed to perform visibility calculations, most of the preceding options remain valid and determine how the computed extinction coefficients are averaged and reported. Additional options are provided to configure how the extinction coefficients are computed:

- Option to select which modeled species (sulfate, nitrate, fine/coarse particulate matter) are included in the extinction coefficient.
- Option to include background extinction when forming ranked tabulations, top-50 tabulations, or exceedance tabulations.
- Option to specify the extinction efficiency for each modeled species.
- User-selected method for obtaining the background extinction coefficients (non-speciated extinction coefficient, monthly speciated extinction coefficients, measured hourly extinction coefficients)

Whenever visibility processing is selected, the peak daily percent change in extinction and the corresponding change in deciview are always tabulated and reported in addition to the tables and plot-files selected to characterize the extinction coefficient results.

Table 5-1 lists the default name of each input and output file associated with CALPOST. The plot-files are named automatically, with the user able to specify a pathname and character string to make the file names unique. The name and full path of each file (except one) is assigned in the control file. The exception, the control filename itself, is assigned on the command line. For example, on a DOS system,

> CALPOST   d:\CALPUFF\CALPOST.INP

will execute the CALPOST code, and read the input and output filenames for the current run from the control file CALPOST.INP in the directory d:\CALPUFF. If the control filename is not specified on the command line, the default control filename (i.e., CALPOST.INP in the current working directory) will be used. The total number of characters in the path and filename can be up to 70 characters.

The utility routine that delivers a command line argument is system dependent. The function that provides the system clock time and system CPU time is also system or compiler-specific. All system-dependent or compiler-specific routines in CALPOST are isolated into a file called DATETM.xxx, where the file extension (.xxx) indicates the system for which the code is designed. For example, DATETM.HP contains code for Hewlett-Packard® Unix systems, DATETM.SUN is for Sun® Unix systems, DATETM.LAH is for Lahey® FORTRAN-compiled PC-applications, and DATETM.MS is for Microsoft® FORTRAN-compiled PC applications. By appending the correct system-dependent DATETM file onto the main CALPOST code, the code should run without any modifications.

CALPOST generates an output list file (default name: CALPOST.LST) and a set of optional files. The names for the optional files follow a fixed template, with one or more characters reserved for the user to specify in order to distinguish output from multiple applications. Note, however, that the "8.3"

Table 5-1

CALPOST Input and Output Files

| Unit | File Name | Type | Format | Description |
|------|-----------|------|--------|-------------|
| in2 | CALPOST.INP | input | formatted | Control file containing user inputs |
| in1 | MODEL.DAT | input | unformatted | CALPUFF output file containing modeled concentration or deposition flux data |
| in3 | VISB.DAT | input | unformatted | CALPUFF output file containing relative humidity data (required only for visibility applications) |
| in4 | BACK.DAT | input | formatted | Optional file of hourly background concentrations |
| in5 | VSRN.DAT | input | formatted | Optional file of hourly background extinction coefficients from transmissometer or nephelometer |
| io1 | CALPOST.LST | output | formatted | List file containing CALPOST tables and other generated data |
| iot1 | TS01[uuuu].DAT | ouput | formatted | Timeseries of 1-hour averages |
| iot3 | TS03[uuuu].DAT | output | formatted | Timeseries of 3-hour averages |
| iot24 | TS24[uuuu].DAT | output | formatted | Timeseries of 24-hour averages |
| iotn | TSnn[uuuu].DAT | output | formatted | Timeseries of N-hour averages |
| mapu | Rtt[uuuuu].DAT Rttii[uuu].GRD | output | formatted | Top Nth Rank Plots in DATA format Top Nth Rank Plots in GRID format |
| mapu | Xtt[uuuuu].DAT Xtt[uuuuu].GRD | output | formatted | Exceedance Plots in DATA format Exceedance Plots in GRID format |
| mapu | jjjtthh[u].DAT jjjtthh[u].GRD | output | formatted | Echo Plots in DATA format Echo Plots in GRID format |
| mapu | V24[uuuuu].DAT | output | formatted | Daily Peak Summary of Visibility |

Filenames for all plot-files are constructed using a template that includes a pathname, optional user-supplied character(s) [u], and fixed characters (R, X, V24, tt, ii, jjj, hh, DAT, and GRD), where

| | | | |
|---|---|---|---|
| tt = | averaging period (e.g. 03) | DAT = | Data format (comma-delimited ASCII file in x, y, value1, value2, ... , value4 format) |
| ii = | rank (e.g. 02) | | |
| jjj = | Julian Day | GRD = | Grid format (only for gridded receptors) compatible with Surfer® plotting software |
| hh = | ending hour (00-23) | | |

filename convention is used so the number of characters is limited.  For example, a plot-file containing the highest second-high 24-hour average concentration at each gridded receptor, in GRID format, would be called:

       R2402sen.grd

where "sen" is the user-specified run identifier.  If the user does not enter a run identifier, the file would be called R2402.grd.  A plot-file in DATA format containing the number of exceedances of a 3-hour threshold specified by the user would be called:

       X03sen.dat

where "sen" is the user-specified run identifier.  Plot-files in GRID format containing 8-hour average concentrations for Julian Day 112 would be called

       1120807s.grd
       1120815s.grd
       1120823s.grd

where "s" is the user-specified run identifier.  A visibility analysis might generate the plot-file:

       V24sen.dat

where "sen" is the user-specified run identifier.

As with CALPUFF and CALMET, CALPOST is configured by means of a parameter file, called PARAMS.PST, in which all of the array dimensions related to the number of gridded, discrete, and complex terrain receptors, the number of "top N" tables allowed, and the Fortran unit numbers associated with each input and output file are specified.  If for a particular application, the user needs to increase the number of discrete receptors, for example, beyond the current maximum, a change to the value of the discrete receptor parameter in PARAMS.PST will automatically re-size all arrays related to this parameter upon recompilation of the CALPOST code.

5.1     Input Files

5.1.1   User Control File (CALPOST.INP)

User-specified inputs to CALPOST are read from a control file whose default name is CALPOST.INP.
A description of each input variable is shown in Table 5-2, and a sample input file is presented in
Table 5-3.  This control file uses the same self-documenting control file format as CALPUFF.  See
Section 4.1 for a description of the control file input conventions.  Selections may be made by either
editing an existing control file, or by using the CALPOST GUI.  Note that you can generate a "new"
control file with all of the standard options and comments by saving the "NEW.INP" file from the GUI to
disk.

5.1.2   CALPUFF Output Files (MODEL.DAT and VISB.DAT)

The program reads the concentration/deposition flux data from an unformatted data file (default name:
MODEL.DAT) that is generated by the CALPUFF model (or CALGRID).   CALPUFF also generates a
file containing relative humidity data (default name: VISB.DAT), which is read by CALPOST if the
visibility option in CALPOST is selected.  The structure of these files is described in Section 4-13.

5.1.3   Background Concentrations/Deposition Fluxes (BACK.DAT)

As an option, a spatially uniform, hourly background concentration/deposition flux can be added to
modeled concentrations/deposition fluxes before averages are processed in CALPOST.  These values are
provided in a formatted ASCII file (default name: BACK.DAT) prepared by the user.  Table 5-4 lists the
record structure for this file, and a partial listing of a sample file is presented in Table 5-5.

Units for the background values may be different from those requested from CALPOST.  Therefore, the
scaling factor placed in the header record is an important feature.  It converts the native units for the
background concentrations to $g/m^3$ , or it converts the native units for background deposition fluxes to
$g/m^2$ /s.  These are the internal units used in the CALPUFF output file.  Any units conversion specified in
the control file (parameter IPRTU) can then be applied uniformly to both the CALPUFF and background
values.  Note that the multiplicative and additive scaling factors (A, B) are not applied to the background
values.

5.1.4   Visibility Measurements (VSRN.DAT)

CALPOST allows the use of visibility measurements to establish hourly background extinction for use in
assessing the change in visibility resulting from modeled emissions.  Two formats are supported for these

data, and both are taken from the data files available on CD-ROM from the Interagency Monitoring of Protected Visual Environments (IMPROVE) program.  When background extinction method number 4 is selected in the control file (MVISBK = 4), transmissometer measurements must be provided in the IMPROVE format.  Example records for this file are listed in Table 5-6.  When background extinction method number 5 is selected in the control file (MVISBK = 5), nephelometer measurements must be provided in the IMPROVE format.  Example records for this file are listed in Table 5-7.

CALPOST uses the content of one field in the file header record to identify which type of file is provided (it must be consistent with the MVISBK selection).  The first 26 characters are read, and the characters in position 24-26 must be 'INS' for the nephelometer data file.  Subsequent data records are read using the following statements, where the variable "meas" is the extinction coefficient ($Mm^{-1}$):

Transmissometer Data —
```
    read(in5,102) iyr,ijday,ihr,meas,ivflag,irh
102   format(7x,i2,5x,i3,1x,i2,2x,i5,22x,i2,17x,i2)
```

Nephelometer Data —
```
    read(in5,101) iyr,ijday,ihr,meas,ivflag,rh
101   format(7x,i2,5x,i3,1x,i2,8x,i6,8x,i2,40x,40x,40x,11x,f7.2)
```

If similar measurements are available from other sources, they may be used in CALPOST by adhering to this file structure.  Note that the transmissometer measurements are assumed to provide the total extinction coefficient, whereas the nephelometer measurements provide just the extinction coefficient due to particle scattering.

Table 5-2
CALPOST Control File Inputs - Input group 0
Input and Output File Names

| Variable | Type | Description | Default |
|----------|------|-------------|---------|
| MODDAT | character*70 | File name of modeled concentration/deposition data file, including full path if desired | MODEL.DAT |
| VISDAT | character*70 | File name of input relative humidity data file, including full path if desired (for visibility) | VISB.DAT |
| BACKDAT | character*70 | File name of input hourly background concentration or deposition flux data file, including full path if desired | BACK.DAT |
| VSRDAT | character*70 | File name of input hourly background light extinction data, including full path if desired | VSRN.DAT |
| PSTLST | character*70 | File name of list file of output from CALPOST, including full path if desired | CALPOST.LST |
| PLPATH | character*70 | Pathname for plot-files (optional: must not be blank if supplied) | (blank) |
| TUNAM | character*8 | User-supplied characters for Top-N plot-file names (optional: must not be blank if supplied) | (blank) |
| XUNAM | character*8 | User-supplied characters for Exceedance plot-file names (optional: must not be blank if supplied) | (blank) |
| EUNAM | character*8 | User-supplied characters for Echo plot-file names (optional: must not be blank if supplied) | (blank) |
| VUNAM | character*8 | User-supplied characters for Visibility plot-file names (optional: must not be blank if supplied) | (blank) |
| TSUNAM | character*8 | User-supplied characters for Timeseries file names (optional: must not be blank if supplied) | (blank) |
| LCFILES | logical | Control flag for converting file names to lower case if T, or to upper case if F | T |

Table 5-2 (Continued)
CALPOST Control File Inputs - Input Group 1
General Run Control Parameters

| Variable | Type | Description | Default |
|---|---|---|---|
| METRUN | integer | Option to run all periods in CALPUFF file (0,1)<br>0 = no, run the period defined by ISYR, ISMO, ISDY, ISHR, and NHRS<br>1 = yes, run all periods found in the file instead of any period defined by ISYR, ISMO, ISDY, ISHR, and NHRS | 0 |
| ISYR | integer | Starting year of data to process (four digits) | - |
| ISMO | integer | Starting month [a] | - |
| ISDY | integer | Starting day [a] | - |
| ISHR | integer | Starting hour [a] (0-23). Uses ending hour convention (e.g., Hour 1 refers to the period from 0:00 - 1:00). | - |
| NHRS | integer | Number of hours to process [a] | - |
| NREP | integer | Process every "NREP[th] "hour of data<br>1 = process every hour<br>2 = process every 2nd hour<br>5 = process every 5th hour | 1 |
| ASPEC | character*12 | Name of "species" to process [b] | - |
| ILAYER | integer | Code indicating layer of concentrations (always "1" when processing concentrations from CALPUFF, "-1" for dry deposition fluxes, "-2" for wet deposition fluxes, and "-3" for total deposition fluxes) | 1 |
| A | real | Multiplicative scaling factor applied to modeled concentrations or deposition fluxes (not applied if A = B = 0.0) | 0.0 |
| B | real | Additive factor applied to modeled concentrations or deposition fluxes (not applied if A = B = 0.0) | 0.0 |
| LBACK | logical | Add background concentrations/deposition fluxes from external file? | F |

[a] Used only if METRUN = 0.

[b] Sample values of ASPEC: SO2, SO4, NOX, HNO3, NO3. For visibility calculations, the species name must be entered as VISIB, which is not a species name actually used in the CALPUFF run: the species included in the visibility calculations are selected by the LVSO4, LVNO3, etc. parameters.

| Variable | Type | Description | Default |
|---|---|---|---|
| LG | logical | Process Gridded receptors? | F |
| LD | logical | Process Discrete receptors? | F |
| LCT | logical | Process CTSG complex terrain receptors? | F |
| NDRECP | integer aray | Select specific discrete receptors (used only if LD=T)<br>-1 = process ALL discrete receptors[c]<br>0 = discrete receptor not processed<br>1 = discrete receptor processed<br>(Enter NREC values using repeated-value notation)[d] | -1 |
| IBGRID | integer | X grid index of lower left corner of subset of gridded receptors to process if LG = T (-1[e] or 1 to NX) | -1[c] |
| JBGRID | integer | Y grid index of lower left corner of subset of gridded receptors to process if LG = T (-1[e] or 1 to NY) | -1[c] |
| IEGRID | integer | X grid index of upper right corner of subset of gridded receptors to process if LG = T (-1[e] or IBGRID to NX) | -1[c] |
| JEGRID | integer | Y grid index of upper right corner of subset of gridded receptors to process if LG = T (-1[e] or JBGRID to NY) | -1[c] |
| NGONOFF | integer | Number of gridded receptor rows provided in Subgroup 1a to identify specific gridded receptors to process | 0 |
| (Optional Input Group 1a - Specific Gridded Receptors) | | | |
| NGXRECP | integer array | Sequence of 0,1 values (one for each gridded receptor in a row of the sampling grid) used to select individual gridded receptors<br>0 = gridded receptor not processed<br>1 = gridded receptor processed<br>(Repeated value notation may be used)[f] | 1 |

[c] Use -1 for the first discrete receptor to signal the use of all discrete receptors in the CALPUFF file.

[d] Explicitly turn each discrete receptor on/off (1/0). NREC receptors were used in the CALPUFF run, so NREC entries are needed in this array. These may be entered in groups: 3*1,2*0 is equivalent to 1,1,1,0,0.

[e] Use -1 for all 4 grid cell indices to signal the use of all gridded receptors.

[f] Enter NGONOFF lines which represent rows of the sampling grid, starting with the northernmost row that contains receptors to be excluded and ending with row 1 to the south (none may be skipped).

| Variable | Type | Description | Default |
|----------|------|-------------|---------|
| RHMAX | real | Maximum relative humidity (%) used in the particle growth equation for visibility processing | 98 |
| LVSO4 | logical | Include modeled sulfate in extinction (T/F) | T |
| LVNO3 | logical | Include modeled nitrate in extinction (T/F) | T |
| LVOC | logical | Include modeled organic carbon in extinction (T/F) | T |
| LVPMC | logical | Include modeled coarse particulates in extinction (T/F) | T |
| LVPMF | logical | Include modeled fine particulates in extinction (T/F) | T |
| LVBK | logical | Include background in extinction when ranking for top-n, top-50, or exceedance tables (T/F) | T |
| SPECPMC | character*12 | Species name for coarse particulates in MODEL. DAT | PMC |
| SPECPMF | character*12 | Species name for coarse particulates in MODEL. DAT | PMF |

----- Extinction Efficiencies ($m^2/g$) -----

| Variable | Type | Description | Default |
|----------|------|-------------|---------|
| EEPMC | real | Modeled coarse particulates | 0.6 |
| EEPMF | real | Modeled fine particulates | 1.0 |
| EEPMCBK | real | Background coarse particulates | 0.6 |
| EESO4 | real | Ammonium Sulfate | 3.0 |
| EENO3 | real | Ammonium Nitrate | 3.0 |
| EEOC | real | Organic Carbon | 4.0 |
| EESOIL | real | Soil Dust | 1.0 |
| EEEC | real | Elemental Carbon (soot) | 10.0 |

| Variable | Type | Description | Default |
|----------|------|-------------|---------|
| MVISBK | integer | Method used to obtain background extinction:<br>1 = Supply single light extinction and hygroscopic fraction<br>  - IWAQM (1993) RH adjustment applied to hygroscopic background and modeled sulfate and nitrate<br>2 = Compute extinction from speciated PM measurements (A)<br>  - Hourly RH adjustment applied to observed and modeled sulfate and nitrate<br>  - RH factor is capped at RHMAX<br>3 = Compute extinction from speciated PM measurements (B)<br>  - Hourly RH adjustment applied to observed and modeled sulfate and nitrate<br>  - Receptor-hour excluded if RH>RHMAX<br>  - Receptor-day excluded if fewer than 6 valid receptor-hours<br>4 = Read hourly transmissometer background extinction data<br>  - Hourly RH adjustment applied to modeled sulfate and nitrate<br>  - Hour excluded if measurement invalid (missing, interference, or large RH)<br>  - Receptor-hour excluded if RH>RHMAX<br>  - Receptor-day excluded if fewer than 6 valid receptor-hours<br>5 = Read hourly nephelometer background extinction measurements<br>  - Rayleigh extinction value (BEXTRAY) added to measurement<br>  - Hourly RH adjustment applied to modeled sulfate and nitrate<br>  - Hour excluded if measurement invalid (missing, interference, or large RH)<br>  - Receptor-hour excluded if RH>RHMAX<br>6 = Compute extinction from speciated PM measurements<br>  - FLAG RH adjustment factor applied to observed and modeled sulfate and nitrate.<br><br>----- Additional MVISBK = 1 Inputs ----- | 6 |
| BEXTBK | real | Background light extinction coefficient ($Mm^{-1}$) | - |
| RHFRAC | real | Percentage of particles affected by relative humidity | - |
| | | ----- Additional MVISBK = 6 Inputs ----- | |
| RHFAC | integer array | Monthly relative humidity factors for adjusting extinction coefficients for hygroscopic species | - |

| Variable | Type | Description | Default |
|----------|------|-------------|---------|
| ----- Additional MVISBK = 2,3,6 Inputs ----- | | | |
| BKSO4 | real | Background Ammonium Sulfate Concentration ($\mu g/m^3$) | - |
| BKNO3 | real | Background Ammonium Nitrate Concentration ($\mu g/m^3$) | - |
| BKPMC | real | Background Coarse Particulate Concentration ($\mu g/m^3$) | - |
| BKOC | real | Background Organic Carbon Concentration ($\mu g/m^3$) | - |
| BKSOIL | real | Background Soil Dust Concentration ($\mu g/m^3$) | - |
| BKEC | real | Background Elemental Carbon Concentration ($\mu g/m^3$) | - |
| ----- Additional MVISBK = 2,3,5,6 Inputs ----- | | | |
| BEXTRAY | real | Extinction due to Rayleigh Scattering ($Mm^{-1}$) | 10. |

| Variable | Type | Description | Default |
|----------|------|-------------|---------|
| IPRTU | integer | Output units flag: (always Mm$^{-1}$ for extinction) | 1 |
| | | For concentrations     For deposition fluxes | |
| | | 1 = g/m$^3$     g/m$^2$/s | |
| | | 2 = mg/m$^3$     mg/m$^2$/s | |
| | | 3 = ug/m$^3$     ug/m$^2$/s | |
| | | 4 = ng/m$^3$     ng/m$^2$/s | |
| | | 5 = odour units     - | |
| NAVG | integer | User-specified averaging time (hours) | 0 |
| L1HR | logical | Report 1-hr averages? | T |
| L3HR | logical | Report 3-hr averages? | T |
| L24HR | logical | Report 24-hr averages? | T |
| LRUNL | logical | Report length-of-run averages? | T |
| LT50 | logical | Produce top 50 tables? | T |
| LTOPN | logical | Produce "top N" tables? | F |
| NTOP | integer | Number of "top" values at each receptor (must be $\leq$ 4) | 4 |
| ITOP(4) | integer array | Specific ranks of "top" values reported (e.g., values of 1, 2, 5 and 48 would produce the highest, 2nd highest, 5th highest, and 48th highest concentrations at each receptor) | 1,2,3,4 |
| LEXCD | logical | Produce exceedance tables? | F |
| THRESH1 | real | Exceedance threshold (output units) for 1-hr averages | -1[g] |
| THRESH3 | real | Exceedance threshold (output units) for 3-hr averages | -1[g] |
| THRESH24 | real | Exceedance threshold (output units) for 24-hr averages | -1[g] |
| THRESHN | real | Exceedance threshold (output units) for NAVG-hr averages | -1[g] |

[g] Exceedance processing is only performed for selected averaging times with thresholds greater than or equal to zero.

Table 5-2 (Concluded)

CALPOST Control File Inputs - Input Group 3

Output Options

| Variable | Type | Description | Default |
|----------|------|-------------|---------|
| ----- Multiple Exceedance Processing ----- | | | |
| NDAY | integer | Number of days to accumulate exceedance counts when reporting violations (NDAY > 0 activates this processing option) | 0 |
| NCOUNT | integer | Number of exceedances allowed in a single NDAY period | 1 |
| LECHO | logical | Output selected averages on selected days? | F |
| IECHO(366) | integer array | Array of days selected to print data for all selected averaging times (0 = do not print, 1 = print) | 366*0 |
| LTIME | logical | Output timeseries for all selected receptors for all selected days for all selected averaging times? | F |
| LPLT | logical | Generate plot-file output? | F |
| LGRD | logical | Write plot-files in GRID[h] format when available? | F |
| LDEBUG | logical | Activate special debug output statements? | F |

[h] GRID format is compatible with the Surfer® plotting software. Only processed values obtained at gridded receptors are written in this format. If the GRID option is not selected, processed values obtained at all receptors are written in the comma-delimited DATA format (x, y, value1, value2, ... , value4).

Table 5-3

Sample CALPOST Control File (CALPOST.INP)

```
CALPUFF Application with met data from CALMET
Visibility Processing Example
Produce tables of peak 3-hour average extinction
---------------- Run title (3 lines) -------------------------------------------
                     CALPOST MODEL CONTROL FILE
                     --------------------------
--------------------------------------------------------------------------------
INPUT GROUP: 0 -- Input and Output File Names
--------------
Input Files
-----------
File                    Default File Name
----                    -----------------
Conc/Dep Flux File      MODEL.DAT         ! MODDAT =PUFFVIS.CON   !
Relative Humidity File  VISB.DAT          ! VISDAT =VISB.DAT    !
Background Data File     BACK.DAT          *BACKDAT =     *
Transmissometer/        VSRN.DAT          *VSRDAT =    *
Nephelometer Data File

Output Files
------------
File                    Default File Name
----                    -----------------
List File               CALPOST.LST       ! PSTLST =SAMPVIS.LST   !

Pathname for Timeseries Files   (blank)    * TSPATH =    *
(activate with exclamation points only if
providing NON-BLANK character string)

Pathname for Plot Files   (blank)          * PLPATH =    *
(activate with exclamation points only if
 providing NON-BLANK character string)

User Character String (U) to augment default filenames
(activate with exclamation points only if
 providing NON-BLANK character string)

Timeseries              TSttUUUU.DAT      * TSUNAM =    *

Top Nth Rank Plot        RttUUUU.DAT
                    or  RttiiUUU.GRD       * TUNAM =    *

Exceedance Plot          XttUUUUU.DAT
                    or  XttUUUUU.GRD       * XUNAM =    *

Echo Plot                jjjtthhU.DAT
(Specific Days)     or  jjjtthhU.GRD       * EUNAM =    *

Visibility Plot          V24UUUUU.DAT      * VUNAM =    *
(Daily Peak Summary)
--------------------------------------------------------------------------------
All file names will be converted to lower case if LCFILES = T
Otherwise, if LCFILES = F, file names will be converted to UPPER CASE
        T = lower case       ! LCFILES = T !
        F = UPPER CASE
NOTE: (1) file/path names can be up to 70 characters in length
NOTE: (2) Filenames for ALL PLOT and TIMESERIES FILES are constructed
        using a template that includes a pathname, user-supplied
        character(s), and fixed strings (tt,ii,jjj, and hh), where
            tt = Averaging Period (e.g. 03)
            ii = Rank (e.g. 02)
            jjj= Julian Day
            hh = Hour(ending)
        are determined internally based on selections made below.
        If a path or user-supplied character(s) are supplied, each
        must contain at least 1 non-blank character.
!END!
--------------------------------------------------------------------------------
```

Table 5-3 (Continued)

Sample CALPOST Control File (CALPOST.INP)

```
INPUT GROUP: 1 -- General run control parameters
--------------

     Option to run all periods found
     in the met. file(s) (METRUN)         Default: 0   ! METRUN =   0  !

         METRUN = 0 - Run period explicitly defined below
         METRUN = 1 - Run all periods in CALPUFF data file(s)

     Starting date:    Year  (ISYR) --   No default   ! ISYR  = 1988   !
     (used only if     Month (ISMO) --   No default   ! ISMO  = 7  !
      METRUN = 0)      Day   (ISDY) --   No default   ! ISDY  = 7  !
                       Hour  (ISHR) --   No default   ! ISHR  = 1   !

     Number of hours to process (NHRS) -- No default   ! NHRS  = 24  !

     Process every hour of data?(NREP) -- Default: 1  ! NREP  = 1  !
       (1 = every hour processed,
        2 = every 2nd hour processed,
        5 = every 5th hour processed, etc.)

Species & Concentration/Deposition Information
----------------------------------------------

        Species to process (ASPEC)       -- No default   ! ASPEC = VISIB  !
        (ASPEC = VISIB for visibility processing)

        Layer/deposition code (ILAYER)  -- Default: 1   ! ILAYER =  1  !
          '1'  for CALPUFF concentrations,
          '-1' for dry deposition fluxes,
          '-2' for wet deposition fluxes,
          '-3' for wet+dry deposition fluxes.

        Scaling factors of the form:    -- Defaults:   ! A =  0.0    !
            X(new) = X(old) * A + B        A = 0.0    ! B =  0.0    !
          (NOT applied if A = B = 0.0)     B = 0.0

        Add Hourly Background Concentrations/Fluxes?
                            (LBACK) -- Default: F   ! LBACK =  F !

Receptor information
--------------------

  Gridded receptors processed?    (LG) -- Default: F   ! LG  = T  !
  Discrete receptors processed?   (LD) -- Default: F   ! LD  = F  !
  CTSG Complex terrain receptors processed?
                              (LCT) -- Default: F   ! LCT = F  !

--Select range of DISCRETE receptors (only used when LD = T):

  Select ALL DISCRETE receptors by setting NDRECP flag to -1;
                          OR
  Select SPECIFIC DISCRETE receptors by entering a flag (0,1) for each
     0 = discrete receptor not processed
     1 = discrete receptor processed
  using repeated value notation to select blocks of receptors:
     23*1, 15*0, 12*1
  Flag for all receptors after the last one assigned is set to 0
  (NDRECP) -- Default: -1
                                       ! NDRECP =  -1  !


--Select range of GRIDDED receptors (only used when LG = T):

        X index of LL corner (IBGRID) -- Default: -1     ! IBGRID = 10 !
            (-1 OR 1 <= IBGRID <= NX)

        Y index of LL corner (JBGRID) -- Default: -1     ! JBGRID = 10 !
            (-1 OR 1 <= JBGRID <= NY)
```

Table 5-3 (Continued)

Sample CALPOST Control File (CALPOST.INP)

```
      X index of UR corner (IEGRID) -- Default: -1     ! IEGRID =  15  !
          (-1 OR 1 <= IEGRID <= NX)

      Y index of UR corner (JEGRID) -- Default: -1     ! JEGRID =  15  !
          (-1 OR 1 <= JEGRID <= NY)

 Note: Entire grid is processed if IBGRID=JBGRID=IEGRID=JEGRID=-1


--Specific gridded receptors can also be excluded from CALPOST
  processing by filling a processing grid array with 0s and 1s.  If the
  processing flag for receptor index (i,j) is 1 (ON), that receptor
  will be processed if it lies within the range delineated by IBGRID,
  JBGRID,IEGRID,JEGRID and if LG=T. If it is 0 (OFF), it will not be
  processed in the run.  By default, all array values are set to 1 (ON).

  Number of gridded receptor rows provided in Subgroup (1a) to
  identify specific gridded receptors to process
                           (NGONOFF) -- Default: 0       ! NGONOFF =  0  !

!END!



--------------
Subgroup (1a) -- Specific gridded receptors included/excluded
--------------

    Specific gridded receptors are excluded from CALPOST processing
    by filling a processing grid array with 0s and 1s.  A total of
    NGONOFF lines are read here.  Each line corresponds to one 'row'
    in the sampling grid, starting with the NORTHERNMOST row that
    contains receptors that you wish to exclude, and finishing with
    row 1 to the SOUTH (no intervening rows may be skipped).  Within
    a row, each receptor position is assigned either a 0 or 1,
    starting with the westernmost receptor.
       0 = gridded receptor not processed
       1 = gridded receptor processed

    Repeated value notation may be used to select blocks of receptors:
       23*1, 15*0, 12*1

    Because all values are initially set to 1, any receptors north of
    the first row entered, or east of the last value provided in a row,
    remain ON.

    (NGXRECP) -- Default: 1
```

Table 5-3 (Continued)

Sample CALPOST Control File (CALPOST.INP)

```
--------------------------------------------------------------------------------
INPUT GROUP: 2 -- Visibility Parameters (ASPEC = VISIB)
--------------

    Maximum relative humidity (%) used in particle growth curve
                              (RHMAX) -- Default: 98   ! RHMAX  = 98.0 !

    Modeled species to be included in computing the light extinction
     Include SULFATE?          (LVSO4) -- Default: T   ! LVSO4  = T   !
     Include NITRATE?          (LVNO3) -- Default: T   ! LVNO3  = T   !
     Include ORGANIC CARBON?   (LVOC)  -- Default: T   ! LVOC   = F   !
     Include COARSE PARTICLES? (LVPMC) -- Default: T   ! LVPMC  = F   !
     Include FINE PARTICLES?   (LVPMF) -- Default: T   ! LVPMF  = F   !

    And, when ranking for TOP-N, TOP-50, and Exceedance tables,
     Include BACKGROUND?        (LVBK) -- Default: T   ! LVBK   = T   !

    Species name used for particulates in MODEL.DAT file
                  COARSE    (SPECPMC) -- Default: PMC ! SPECPMC = PMC !
                  FINE      (SPECPMF) -- Default: PMF ! SPECPMF = PMF !

Extinction Efficiency (1/Mm per ug/m**3)
----------------------------------------
    MODELED particulate species:
            PM  COARSE     (EEPMC) -- Default: 0.6 ! EEPMC  = 0.6 !
            PM  FINE       (EEPMF) -- Default: 1.0 ! EEPMF  = 1.0 !
    BACKGROUND particulate species:
            PM  COARSE     (EEPMCBK) -- Default: 0.6 ! EEPMCBK = 0.6 !
    Other species:
            AMMONIUM SULFATE (EESO4) -- Default: 3.0 ! EESO4  = 3.0 !
            AMMONIUM NITRATE (EENO3) -- Default: 3.0 ! EENO3  = 3.0 !
            ORGANIC CARBON  (EEOC)  -- Default: 4.0 ! EEOC   = 4.0 !
            SOIL            (EESOIL)-- Default: 1.0 ! EESOIL = 1.0 !
            ELEMENTAL CARBON (EEEC) -- Default: 10. ! EEEC   = 10.0 !

Background Extinction Computation
---------------------------------
    Method used for background light extinction
                              (MVISBK) -- Default: 6   ! MVISBK = 2  !

        1 = Supply single light extinction and hygroscopic fraction
              - IWAQM (1993) RH adjustment applied to hygroscopic background
                and modeled sulfate and nitrate
        2 = Compute extinction from speciated PM measurements (A)
              - Hourly RH adjustment applied to observed and modeled sulfate
                and nitrate
              - RH factor is capped at RHMAX
        3 = Compute extinction from speciated PM measurements (B)
              - Hourly RH adjustment applied to observed and modeled sulfate
                and nitrate
              - Receptor-hour excluded if RH>RHMAX
              - Receptor-day excluded if fewer than 6 valid receptor-hours
        4 = Read hourly transmissometer background extinction measurements
              - Hourly RH adjustment applied to modeled sulfate and nitrate
              - Hour excluded if measurement invalid (missing, interference,
                or large RH)
              - Receptor-hour excluded if RH>RHMAX
              - Receptor-day excluded if fewer than 6 valid receptor-hours
        5 = Read hourly nephelometer background extinction measurements
              - Rayleigh extinction value (BEXTRAY) added to measurement
              - Hourly RH adjustment applied to modeled sulfate and nitrate
              - Hour excluded if measurement invalid (missing, interference,
                or large RH)
              - Receptor-hour excluded if RH>RHMAX
              - Receptor-day excluded if fewer than 6 valid receptor-hours
        6 = Compute extinction from speciated PM measurements
              - FLAG RH adjustment factor applied to observed and
                modeled sulfate and nitrate
```

Table 5-3 (Continued)

Sample CALPOST Control File (CALPOST.INP)

```
    Additional inputs used for MVISBK = 1:
    -------------------------------------
     Background light extinction (1/Mm)
                             (BEXTBK) -- No default    ! BEXTBK = 21.0 !
      Percentage of particles affected by relative humidity
                             (RHFRAC) -- No default    ! RHFRAC = 7.0 !

    Additional inputs used for MVISBK = 6:
    -------------------------------------
     Extinction coefficients for hygroscopic species (modeled and
     background) are computed using a monthly RH adjustment factor
     in place of an hourly RH factor (VISB.DAT file is NOT needed).
     Enter the 12 monthly factors here (RHFAC).  Month 1 is January.

     (RHFAC)  -- No default     ! RHFAC = 0.0, 0.0, 0.0, 0.0,
                                            0.0, 0.0, 0.0, 0.0,
                                            0.0, 0.0, 0.0, 0.0 !

    Additional inputs used for MVISBK = 2,3,6:
    -----------------------------------------
     Background extinction coefficients are computed from monthly
     CONCENTRATIONS of ammonium sulfate (BKSO4), ammonium nitrate (BKNO3),
     coarse particulates (BKPMC), organic carbon (BKOC), soil (BKSOIL), and
     elemental carbon (BKEC).  Month 1 is January.
     (ug/m**3)

     (BKSO4)  -- No default     ! BKSO4 = 0.2, 0.3, 0.3, 0.4,
                                           0.4, 0.4, 0.3, 0.3,
                                           0.3, 0.2, 0.2, 0.2 !
     (BKNO3)  -- No default     ! BKNO3 = 0.1, 0.2, 0.2, 0.2,
                                           0.3, 0.3, 0.2, 0.2,
                                           0.2, 0.1, 0.1, 0.1 !
     (BKPMC)  -- No default     ! BKPMC = 1.0, 1.0, 2.0, 2.0,
                                           2.0, 1.0, 2.0, 3.2,
                                           4.0, 3.33, 2.0, 1.0 !
     (BKOC)   -- No default     ! BKOC  = 0.0, 0.0, 0.0, 0.0,
                                           0.0, 0.0, 0.0, 0.0,
                                           0.0, 0.0, 0.0, 0.0 !
     (BKSOIL) -- No default     ! BKSOIL= 2.0, 3.0, 3.0, 3.0,
                                           4.0, 4.0, 3.0, 3.0,
                                           4.0, 3.0, 2.0, 2.0 !
     (BKEC)   -- No default     ! BKEC  = 0.0, 0.0, 0.0, 0.0,
                                           0.0, 0.0, 0.0, 0.0,
                                           0.0, 0.0, 0.0, 0.0 !

    Additional inputs used for MVISBK = 2,3,5,6:
    -------------------------------------------
     Extinction due to Rayleigh scattering is added (1/Mm)
                             (BEXTRAY) -- Default: 10.0 ! BEXTRAY = 10.0 !
!END!
--------------------------------------------------------------------------------
INPUT GROUP: 3 -- Output options
-------------

Output Units
------------
    Units for All Output      (IPRTU) -- Default: 1   ! IPRTU =  1   !
                    for            for
                Concentration   Deposition
        1 =        g/m**3         g/m**2/s
        2 =        mg/m**3        mg/m**2/s
        3 =        ug/m**3        ug/m**2/s
        4 =        ng/m**3        ng/m**2/s
        5 =       Odour Units

    Visibility: extinction expressed in 1/Mega-meters (IPRTU is ignored)
```

Table 5-3 (Continued)

Sample CALPOST Control File (CALPOST.INP)

```
Averaging time(s) reported
--------------------------

     1-hr averages          (L1HR) -- Default: T   !   L1HR = F   !

     3-hr averages          (L3HR) -- Default: T   !   L3HR = T   !

     24-hr averages         (L24HR) -- Default: T  !   L24HR = F  !

     Run-length averages    (LRUNL) -- Default: T  !   LRUNL = F  !

     User-specified averaging time in hours - results for
     an averaging time of NAVG hours are reported for
     NAVG greater than 0:
                            (NAVG) -- Default: 0   !   NAVG =  0  !


Types of tabulations reported
-----------------------------

  1) Visibility: daily visibility tabulations are always reported
                 for the selected receptors when ASPEC = VISIB.
                 In addition, any of the other tabulations listed
                 below may be chosen to characterize the light
                 extinction coefficients.
                 [List file or Plot/Analysis File]

  2) Top 50 table for each averaging time selected
     [List file only]
                            (LT50) -- Default: T   !   LT50 = F   !

  3) Top 'N' table for each averaging time selected
     [List file or Plot file]
                            (LTOPN) -- Default: F  !   LTOPN = T  !

       -- Number of 'Top-N' values at each receptor
          selected (NTOP must be <= 4)
                            (NTOP) -- Default: 4   ! NTOP = 1   !

       -- Specific ranks of 'Top-N' values reported
          (NTOP values must be entered)
                  (ITOP(4) array) -- Default:      ! ITOP = 1   !
                                       1,2,3,4

  4) Threshold exceedance counts for each receptor and each averaging
     time selected
     [List file or Plot file]
                            (LEXCD) -- Default: F  !   LEXCD = F  !

       -- Identify the threshold for each averaging time by assigning a
          non-negative value (output units).

                                    -- Default: -1.0
          Threshold for  1-hr averages  (THRESH1) !  THRESH1 = -1.0  !
          Threshold for  3-hr averages  (THRESH3) !  THRESH3 = -1.0  !
          Threshold for 24-hr averages  (THRESH24) ! THRESH24 = -1.0  !
          Threshold for NAVG-hr averages (THRESHN) !  THRESHN = -1.0  !


       -- Counts for the shortest averaging period selected can be
          tallied daily, and receptors that experience more than NCOUNT
          counts over any NDAY period will be reported.  This type of
          exceedance violation output is triggered only if NDAY > 0.

          Accumulation period(Days)
                            (NDAY) -- Default: 0   !   NDAY =  0  !
          Number of exceedances allowed
                            (NCOUNT) -- Default: 1  !   NCOUNT =  1  !
```

Table 5-3 (Concluded)
## Sample CALPOST Control File (CALPOST.INP)

```
   5) Selected day table(s)

      Echo Option -- Many records are written each averaging period
      selected and output is grouped by day
      [List file or Plot file]
                              (LECHO) -- Default: F   !  LECHO = F  !

      Timeseries Option -- Averages at all selected receptors for
      each selected averaging period are written to timeseries files.
      Each file contains one averaging period, and all receptors are
      written to a single record each averaging time.
      [TSttUUUU.DAT files]
                              (LTIME) -- Default: F   !  LTIME = F  !

        -- Days selected for output
                    (IECHO(366)) -- Default: 366*0
           ! IECHO  = 366*0  !
           (366 values must be entered)

Plot output options
-------------------

      Plot files can be created for the Top-N, Exceedance, and Echo
      tables selected above.  Two formats for these files are available,
      DATA and GRID.  In the DATA format, results at all receptors are
      listed along with the receptor location [x,y,val1,val2,...].
      In the GRID format, results at only gridded receptors are written,
      using a compact representation.  The gridded values are written in
      rows (x varies), starting with the most southern row of the grid.
      The GRID format is given the .GRD extension, and includes headers
      compatible with the SURFER(R) plotting software.

      A plotting and analysis file can also be created for the daily
      peak visibility summary output, in DATA format only.

      Generate Plot file output in addition to writing tables
      to List file?
                              (LPLT) -- Default: F   ! LPLT  = F !

      Use GRID format rather than DATA format,
      when available?
                              (LGRD) -- Default: F   ! LGRD  = F !

Additional Debug Output
-----------------------

   Output selected information to List file
    for debugging?
                              (LDEBUG) -- Default: F  ! LDEBUG  = F !

 !END!
```

Table 5-4

BACK.DAT Record Structure

Header Record

| Record No. | Variable | Type | Description | Sample Values |
|---|---|---|---|---|
| 1 | CONFACT | real | Multiplicative factor to convert background concentrations to $g/m^3$, or to convert background deposition fluxes to $g/m^2/s$. For example, CONFACT = .000001 indicates that the background values are in either $\mu g/m^3$ or $\mu g/m^2/s$. | .000001 |

Data Records (free format)

| Variable No. | Variable | Type | Description | Sample Values |
|---|---|---|---|---|
| 1 | NYR | integer | Year for record (YYYY) | 1994 |
| 2 | NJDAY | integer | Julian Day for record (JJJ) | 210 |
| 3 | NHR | integer | Hour for record (00-23, time ending) | 13 |
| 4 | XMHBU | real | Background Concentration/Deposition Flux | 32.8 |

Table 5-5

Sample Background Concentration File (BACK.DAT)

```
0.000001
1994   2    1    23.57
1994   2    2    20.95
1994   2    3    20.95
1994   2    4    15.71
1994   2    5    23.57
1994   2    6    28.81
1994   2    7    28.81
1994   2    8    26.19
1994   2    9    31.43
1994   2   10    23.57
1994   2   11    20.95
1994   2   12    18.33
1994   2   13    15.71
1994   2   14    15.71
1994   2   15    13.09
1994   2   16    13.09
1994   2   17    13.09
1994   2   18    10.48
1994   2   19    13.09
1994   2   20    15.71
1994   2   21    13.09
1994   2   22    10.48
1994   2   23    10.48
1994   3    0    13.09
```

Table 5-6

Sample Transmissometer File (VSRN.DAT)

(Partial Listing)

```
SITE YYYYMMDD  JD HHMM BEXT  UC  #  #  UT   DT MAX V A    AT  U  C   RH   U  C  DV
YOSE 19890317  76    0   19   2  1  0 -99 -991105 0      0  1  0   78   5  0  64
YOSE 19890317  76  100   17   2  1  0 -99 -991105 0     -1  1  0   84   5  0  53
YOSE 19890317  76  200   16   2  1  0 -99 -991105 0      0  1  0   80   5  0  47
YOSE 19890317  76  300   14   2  1  0 -99 -991105 0      1  1  0   65   5  0  34
YOSE 19890317  76  400   18   2  1  0 -99 -991105 0     -1  1  0   76   5  0  59
YOSE 19890317  76  500   16   2  1  0 -99 -991105 0     -1  1  0   79   5  0  47
YOSE 19890317  76  600   12   2  1  0 -99 -991105 0     -1  1  0   71   5  0  18
YOSE 19890317  76  700   16   2  1  0 -99 -991105 0      1  1  0   67   5  0  47
YOSE 19890317  76  800   16   2  1  0 -99 -991105 0      4  1  0   48   5  0  47
YOSE 19890317  76  900   20   2  1  0 -99 -991105 0     11  1  0   34   5  0  69
YOSE 19890317  76 1000   21   2  1  0 -99 -991105 0      9  1  0   32   5  0  74
YOSE 19890317  76 1100   25   2  1  0 -99 -991105 0     10  1  0   30   5  0  92
YOSE 19890317  76 1200   33   2  1  0 -99 -991105 0      9  1  0   45   5  0 119
YOSE 19890317  76 1300   45   2  1  0 -99 -991105 0      9  1  0   51   5  0 150
YOSE 19890317  76 1400   55   2  1  0 -99 -991105 0     10  1  0   58   5  0 170
YOSE 19890317  76 1500   67   2  1  0 -99 -991105 0     10  1  0   62   5  0 190
YOSE 19890317  76 1600   99   2  1  0 -99 -991105 0      8  1  0   70   5  0 229
YOSE 19890317  76 1700   60   2  1  0 -99 -991105 0      9  1  0   74   5  0 179
YOSE 19890317  76 1800   42   2  1  0 -99 -991105 0      6  1  0   84   5  0 144
YOSE 19890317  76 1900   37   2  0  1 -99 -991105 1 A    5  1  0   92   5  0 131
YOSE 19890317  76 2000   33   2  1  0 -99 -991105 0      6  1  0   82   5  0 119
YOSE 19890317  76 2100   29   2  1  0 -99 -991105 0      6  1  0   82   5  0 106
YOSE 19890317  76 2200   32   2  1  0 -99 -991105 0      6  1  0   83   5  0 116
YOSE 19890317  76 2300   30   2  1  0 -99 -991105 0      6  1  0   83   5  0 110
YOSE 19890318  77    0   35   2  1  0 -99 -991105 0      7  1  0   80   5  0 125
```

| Field | Description |
|---|---|
| SITE | Site abbreviation |
| YYYYMMDD | Date (4-digit year/month/day) |
| JD | Julian Date |
| HHMM | Time using a 24-hour clock in hour/minute format |
| BEXT | bext ($Mm^{-1}$) |
| UC | bext uncertainty ($Mm^{-1}$) |
| # | Number of readings in average |
| # | Number of readings not in average due to weather |
| UT | Uncertainty threshold ($Mm^{-1}$) |
| DT | threshold ($Mm^{-1}$) |
| MAX | Maximum threshold ($Mm^{-1}$) |
| V | bext validity code (0=valid, 1=interference, 2=invalid, 9=suspect) |
| A | bext validity interference subcode |
| AT | Temperature ($^{\circ}C$) |
| U | Temperature uncertainty ($^{\circ}C$) |
| C | Temperature validity code |
| RH | Relative humidity (%) |
| U | Relative humidity uncertainty (%) |
| C | Relative humidity validity code (0=valid, 2=invalid, 9=suspect) |
| DV | Haziness (deciview x 10) |

Table 5-7
## Sample Nephelometer File (VSRN.DAT)
### (Partial Listing)

| SITE | YYYYMMDD | JD | HHMM | INS | BSP | PREC | V | A | RAW-M | RAW-SD | # | N/A | SD/M | DEL | MAX | RH | 0123456789mPM0T | YINTER | SLOPE | AT | AT-SD | # | AT-PR | CT | CT-SD | # | CT-PR | RH | RH-SD | # | RH-PR N/A |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| MOZ2 | 19941009 | 282 | 0000 | 048 | 22 | 0.140 | 0 | | 43.33 | 1.60 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -18.9 | 1.12 | -3.58 | 0.19 | 12 | 1.00 | -3.01 | 0.14 | 12 | 1.00 | 85.17 | 1.06 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 0100 | 048 | 17 | 0.140 | 0 | | 38.87 | 1.36 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -18.9 | 1.12 | -3.67 | 0.23 | 12 | 1.00 | -2.79 | 0.10 | 12 | 1.00 | 82.03 | 0.93 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 0200 | 048 | 18 | 0.140 | 0 | | 40.24 | 0.71 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -18.8 | 1.12 | -3.94 | 0.10 | 12 | 1.00 | -2.94 | 0.05 | 12 | 1.00 | 84.49 | 0.72 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 0300 | 048 | 19 | 0.140 | 0 | | 40.54 | 1.47 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -18.7 | 1.12 | -4.07 | 0.07 | 12 | 1.00 | -3.06 | 0.04 | 12 | 1.00 | 84.49 | 1.40 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 0400 | 048 | 16 | 0.140 | 0 | | 38.57 | 1.72 | 10 | -99.0 | 10.0 | 50 | 5000 | 90 | 0A2000000000003 | -18.7 | 1.12 | -4.30 | 0.11 | 12 | 1.00 | -3.19 | 0.09 | 9 | 1.00 | 82.56 | 0.84 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 0500 | 048 | 18 | 0.140 | 0 | | 39.50 | 1.40 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -18.7 | 1.12 | -4.40 | 0.21 | 12 | 1.00 | -3.33 | 0.13 | 12 | 1.00 | 82.87 | 1.13 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 0600 | 048 | 15 | 0.140 | 0 | | 37.24 | 1.04 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -18.7 | 1.12 | -4.16 | 0.16 | 12 | 1.00 | -3.05 | 0.20 | 12 | 1.00 | 79.12 | 1.44 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 0700 | 048 | 13 | 0.140 | 0 | | 35.60 | 1.34 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -18.7 | 1.12 | -3.62 | 0.43 | 12 | 1.00 | -2.23 | 0.41 | 12 | 1.00 | 76.14 | 2.20 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 0800 | 048 | 10 | 0.140 | 0 | | 32.62 | 1.26 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -18.7 | 1.12 | -2.02 | 0.48 | 12 | 1.00 | -0.29 | 0.63 | 11 | 1.00 | 69.82 | 1.82 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 0900 | 048 | 10 | 0.140 | 0 | | 32.75 | 1.42 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -18.7 | 1.12 | -0.69 | 0.31 | 12 | 1.00 | 1.32 | 0.33 | 12 | 1.00 | 65.75 | 1.18 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 1000 | 048 | 10 | 0.140 | 0 | | 32.94 | 1.73 | 10 | -99.0 | 10.0 | 50 | 5000 | 90 | 0A2000000000003 | -18.7 | 1.12 | 0.24 | 0.30 | 12 | 1.00 | 2.03 | 0.40 | 9 | 1.00 | 63.34 | 1.71 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 1100 | 048 | 15 | 0.140 | 0 | | 37.18 | 1.47 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -18.8 | 1.12 | 1.23 | 0.29 | 12 | 1.00 | 3.13 | 0.28 | 12 | 1.00 | 66.90 | 1.48 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 1200 | 048 | 15 | 0.140 | 0 | | 37.44 | 1.76 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -19.1 | 1.12 | 2.13 | 0.23 | 12 | 1.00 | 4.27 | 0.27 | 12 | 1.00 | 64.31 | 1.93 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 1300 | 048 | 12 | 0.140 | 0 | | 35.03 | 1.17 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -19.3 | 1.12 | 2.74 | 0.32 | 12 | 1.00 | 4.74 | 0.35 | 12 | 1.00 | 57.82 | 4.01 | 10 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 1400 | 048 | 9 | 0.140 | 0 | | 32.69 | 0.83 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -19.6 | 1.12 | 3.86 | 0.34 | 12 | 1.00 | 5.73 | 0.34 | 12 | 1.00 | 51.25 | 2.95 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 1500 | 048 | 10 | 0.140 | 0 | | 33.59 | 0.98 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -19.8 | 1.12 | 4.35 | 0.17 | 12 | 1.00 | 5.94 | 0.20 | 12 | 1.00 | 50.14 | 1.11 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 1600 | 048 | 10 | 0.140 | 0 | | 34.10 | 1.64 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000001 | -20.1 | 1.12 | 3.82 | 0.22 | 12 | 1.00 | 5.25 | 0.23 | 11 | 1.00 | 51.88 | 1.66 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 1700 | 048 | 11 | 0.140 | 0 | | 34.78 | 1.66 | 10 | -99.0 | 10.0 | 50 | 5000 | 90 | 0A2000000000002 | -20.3 | 1.12 | 2.18 | 0.75 | 12 | 1.00 | 3.46 | 0.93 | 10 | 1.00 | 57.44 | 2.77 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 1800 | 048 | 11 | 0.140 | 0 | | 35.13 | 0.73 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -20.4 | 1.12 | 1.12 | 0.22 | 12 | 1.00 | 2.01 | 0.23 | 12 | 1.00 | 58.90 | 1.04 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 1900 | 048 | 10 | 0.140 | 0 | | 34.22 | 0.96 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -20.4 | 1.12 | 0.71 | 0.13 | 12 | 1.00 | 1.56 | 0.11 | 12 | 1.00 | 56.36 | 1.23 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 2000 | 048 | 10 | 0.140 | 0 | | 34.27 | 1.51 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -20.4 | 1.12 | 0.02 | 0.13 | 12 | 1.00 | 0.89 | 0.16 | 12 | 1.00 | 56.45 | 0.99 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 2100 | 048 | 9 | 0.140 | 0 | | 33.52 | 0.64 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -20.4 | 1.12 | -0.17 | 0.06 | 12 | 1.00 | 0.61 | 0.06 | 12 | 1.00 | 55.21 | 0.41 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 2200 | 048 | 9 | 0.140 | 0 | | 33.48 | 0.89 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -20.5 | 1.12 | -0.33 | 0.04 | 12 | 1.00 | 0.43 | 0.03 | 12 | 1.00 | 54.33 | 1.55 | 12 | 2.00XXXX |
| MOZ2 | 19941009 | 282 | 2300 | 048 | 8 | 0.140 | 0 | | 32.90 | 0.77 | 10 | -99.0 | 10.0 | 50 | 5000 | 90 | 0A2000000000003 | -20.5 | 1.12 | -0.26 | 0.08 | 12 | 1.00 | 0.50 | 0.07 | 9 | 1.00 | 47.41 | 0.78 | 12 | 2.00XXXX |
| MOZ2 | 19941010 | 283 | 0000 | 048 | 8 | 0.140 | 0 | | 32.44 | 0.63 | 12 | -99.0 | 10.0 | 50 | 5000 | 90 | 0C0000000000000 | -20.4 | 1.12 | -0.42 | 0.16 | 12 | 1.00 | 0.41 | 0.11 | 12 | 1.00 | 48.51 | 1.46 | 12 | 2.00XXXX |

| Field | Description |
|---|---|
| SITE | Site Abbreviation |
| YYYYMMDD | Date (4-digit year/month/day) |
| JD | Julian Date |
| HHMM | Time using a 24-hour clock in hour/minute format |
| INS | Nephelometer Serial Number |
| BSP | bsp (Mm$^{-1}$) — Particle scattering coefficient = Total - Rayleigh |
| PREC | bsp Estimated Precision (%/100) |
| V | bsp Validity Code(0=valid, 1=interference, 2=invalid, 9=suspect) |
| A | bsp Interference Code |
| RAW-M | Raw Nephelometer Hourly Average (Counts) |
| RAW-SD | Standard Deviation of Raw Nephelometer Average (Counts) |
| # | Number of Data Points in Hourly Nephelometer Average |
| N/A | (Not Used) |
| SD/M | Standard Deviation/Mean Interference Threshold |
| DEL | bsp Rate of Change Interference Threshold |
| MAX | Maximum bsp Interference Threshold |
| RH | Relative Humidity Interference Threshold |
| 0123456789mPMOT | Composite Nephelometer Code Summary |
| YINTER | Y-intercept of Calibration Line Used to Calculate bsp |
| SLOPE | Slope of Calibration Line Used to Calculate bsp |
| AT | Average Ambient Temperature (ºC) |
| AT-SD | Standard Deviation of Hourly AT Average |
| # | Number of Data Points in Hourly AT Average |
| AT-PR | Estimated Precision of Ambient Temperature |
| CT | Average Nephelometer Chamber Temperature (ºC) |
| CD-SD | Standard Deviation of Hourly CT Average |
| # | Number of Data Points in Hourly CT Average |
| CT-PR | Estimated Precision of Chamber Temperature |
| RH | Average Relative Humidity (%) |
| RH-SD | Standard Deviation of Hourly RH Average |
| # | Number of Data Points in Hourly RH Average |
| RH-PR | Estimated Precision of Relative Humidity |

5.2        Output Files

5.2.1        List File (CALPOST.LST)

The list file has four logical sections.  The first section contains an image of the control file inputs; the second section contains a summary of these inputs and it documents the content of the CALPUFF output file that is processed; the third section contains the tabulations of CALPOST results requested by the user;  and the fourth section reports the peak value(s) obtained for each averaging time processed.  An example list file is shown in Table 5-8, with the first logical section removed (the input file for this example was shown in Table 5-3).

Each table contains specific reference to the averaging time, the pollutant species (CALPOST processes a single species at a time), concentration/deposition units, receptor locations, and the date and time (marked at the end of the averaging period).  When visibility is assessed, the modeled extinction in inverse megameters (1/Mm) is processed and reported just like concentration or deposition.  In addition, the peak daily average visibility reduction is reported for each day processed, characterized as either a percent change in extinction (from background), or as a change in deciview, as defined in Section 2.13.

5.2.2        Visibility File (V24uuuuu.DAT)

When visibility processing is selected and plot-files are requested, the peak daily average visibility reduction tabulations written to the list file are written to disk as a visibility file as well.  This facilitates the use of subsequent analysis tools, such as spreadsheets.  The record format is the same as that used in the list file.  The user may accept the default filname (V24.DAT), or augment the default name with up to five additional characters.

5.2.3        Plot-file(s)

CALPOST can generate a set of optional plot-files containing the "top N" highest concentrations/deposition fluxes at each receptor, the number of exceedances of user-specified threshold values at each receptor and averaging time, or the values of concentration/deposition flux for user-specified time periods.  Two formats are available for these plot-files.  The first, called DATA format, is of the form: receptor (X, Y), value1, ... , value4 as described in Table 5-9.  This comma-delimited format is suitable for both gridded and discrete receptor data.  It is compatible with many of the popular PC-based graphics and analysis packages.  An example of this format is shown in Table 5-10.  The second format, called the GRID format is appropriate for gridded receptor fields only.  It is directly compatible with the contouring option of the Surfer® plotting package (i.e., it bypasses the need to first interpolate the data to a regular rectangular grid by the plotting package).  Its record structure is described in Table 5-11, and an example is shown in Table 5-12.

5.2.4        Timeseries File(s)

CALPOST can generate a set of optional timeseries files for the concentration, deposition flux, or extinction coefficient identified in the CALPOST control file, at each receptor selected, for each averaging time selected.  Each averaging time is placed in a separate file, so there may be as many as four timeseries files generated (1-hour, 3-hour, 24-hour and N-hour averages).  The period covered by the timeseries is controlled by the selected day option as well as the period processed.  No timeseries output is generated if no days are selected.  All averages in the period processed are written to the timeseries file(s) if all days are selected.

For a given time (e.g, the 3-hour period ending at 0900 on Julian day 310), the current averages for all selected receptors are written as a single "record".  The length of the record grows as the number of receptors increases.  Therefore, the timeseries option should be used with a manageable subset of the receptors contained in the CALPUFF simulation.

The format of the timeseries file is described in Table 5-13.  The file contains a number of header records that identify the parameter that is reported, its units and averaging time, and the number of receptors included.  The location of each receptor is provided.  Data records follow, with a single record for each time period.  An example timeseries file for 1-hour averages of $SO_2$ at two gridded receptors for a single 24-hour period is shown in Table 5-14.

## Table 5-8

## Sample CALPOST Output File (CALPOST.LST)

## (Partial Listing)

```
*************************************************************************************************************************
                                    CALPOST   Version 5.2          Level 991104
*************************************************************************************************************************

  CALPOST Control File Input Summary ------------------------

    Replace run data with data in Puff file 1=Y:    0
                      Run starting date -- year: 1988
                                          month:    7
                                            day:    7
                                     Julian day:  189
         Time at beginning of run  -  hour(0-23):    0
                                -      second:    0
                          Run length (hours):   24


 Every hour of data processed -- NREP = 1


  Species & Concentration/Deposition Information
                                        Species: VISIB
                      Layer of processed data:    1
     (>0=conc, -1=dry flux, -2=wet flux, -3=wet & dry flux)
                  Multiplicative scaling factor: 0.0000E+00
                        Additive scaling factor: 0.0000E+00
               Hourly background values used?: F


  Receptor information
                    Gridded receptors processed?: T
                   Discrete receptors processed?: F
     CTSG Complex terrain receptors processed?: F

  Gridded Receptors Processed


                                    Begin at ix:   10.00
                                      End at ix:   15.00
                                    Begin at iy:   10.00
                                      End at iy:   15.00



  Visibility Processing Selected

  Extinction Computation includes:
                              SULFATES
                              NITRATES
                              BACKGROUND
            Max. RH % for particle growth (%):  98.000

  Extinction Efficiency (1/Mm per ug/m**3)
                              ammonium sulfate:    3.00
                              ammonium nitrate:    3.00
                                organic carbon:    4.00
                                          soil:    1.00
                              elemental carbon:   10.00
                              MODELED coarse PM:    0.60
                              MODELED   fine PM:    1.00
                              BACKGRND coarse PM:    0.60

  Background Extinction Calculation Method 2
          Rayleigh scattering extinction (1/Mm):   10.00
             Monthly background conc. (ug/m**3):

       (NH4)2SO4    (NH4)NO3      PM-C         OC        SOIL        EC
    1  .2000E+00   .1000E+00   .1000E+01   .0000E+00   .2000E+01   .0000E+00
    2  .3000E+00   .2000E+00   .1000E+01   .0000E+00   .3000E+01   .0000E+00
    3  .3000E+00   .2000E+00   .2000E+01   .0000E+00   .3000E+01   .0000E+00
    4  .4000E+00   .2000E+00   .2000E+01   .0000E+00   .3000E+01   .0000E+00
    5  .4000E+00   .3000E+00   .2000E+01   .0000E+00   .4000E+01   .0000E+00
    6  .4000E+00   .3000E+00   .1000E+01   .0000E+00   .4000E+01   .0000E+00
    7  .3000E+00   .2000E+00   .2000E+01   .0000E+00   .3000E+01   .0000E+00
    8  .3000E+00   .2000E+00   .3200E+01   .0000E+00   .3000E+01   .0000E+00
    9  .3000E+00   .2000E+00   .4000E+01   .0000E+00   .4000E+01   .0000E+00
   10  .2000E+00   .1000E+00   .3330E+01   .0000E+00   .3000E+01   .0000E+00
   11  .2000E+00   .1000E+00   .2000E+01   .0000E+00   .2000E+01   .0000E+00
   12  .2000E+00   .1000E+00   .1000E+01   .0000E+00   .2000E+01   .0000E+00



  Output options
               Units requested for output:   (1/Mega-m)

  Averaging time(s) selected
      User-specified averaging time (NAVG hours):     0
                               1-hr averages:     F
                               3-hr averages:     T
                              24-hr averages:     F
                            NAVG-hr averages:     F
                       Length of run averages:     F

  Output components selected
                                      Top-50:     F
```

```
                 Top-N values at each receptor:      T
           Exceedance counts at each receptor:       F
     Output selected information for debugging:      F
                 Echo tables for selected days:      F
                 Time-series for selected days:      F

  Top "n" table control
         Number of "top" values at each receptor:    1
         Specific ranks of "top" values reported:    1


  Plot file option
                            Plot files created:      F

IDENTIFICATION OF PROCESSED MODEL FILE ----------

CALPUFF     5.2         991104

CALPUFF test case run - 3 point sources : Visibility Test Case
24-Hour Simulation using CALMET met. data
Gridded receptors on 17x17 20-km met grid

Averaging time for values reported from model:
          1   HOUR

Number of averaging periods in file from model:
           24

Chemical species names for each layer in model:
SO2          1
SO4          1
NOX          1
HNO3         1
NO3          1

--------------------------------------------------------------------------------------------------------------------------
          INPUT FILES

 Default Name      Unit No.     File Name and Path
 ------------      --------     ------------------
  CALPOST.INP         5         SAMPVIS.INP
    MODEL.DAT         4         puffvis.con
    VISB.DAT          9         visb.dat


--------------------------------------------------------------------------------------------------------------------------
          OUTPUT FILES

 Default Name      Unit No.     File Name and Path
 ------------      --------     ------------------
  CALPOST.LST         8         sampvis.lst

*****************************************************************************************************************************
                              CALPOST  Version 5.2        Level 991104
*****************************************************************************************************************************

                                           VISIB    B_SN___

 1 RANKED    3   HOUR AVERAGE   EXTINCTION   VALUES AT EACH GRIDDED RECEPTOR  (YEAR,DAY,ENDING TIME)  (1/Mega-m)

RECEPTOR      COORDINATES (km)            1 RANK
 10, 10     310.000  4760.000    2.3055E+01 (1988,189,0600)
 10, 11     310.000  4780.000    2.3055E+01 (1988,189,0600)
 10, 12     310.000  4800.000    2.3055E+01 (1988,189,0600)
 10, 13     310.000  4820.000    2.3055E+01 (1988,189,0600)
 10, 14     310.000  4840.000    2.3055E+01 (1988,189,0600)
 10, 15     310.000  4860.000    2.3055E+01 (1988,189,0600)
 11, 10     330.000  4760.000    2.3055E+01 (1988,189,0600)
 11, 11     330.000  4780.000    2.3055E+01 (1988,189,0600)
 11, 12     330.000  4800.000    2.3055E+01 (1988,189,0600)
 11, 13     330.000  4820.000    2.3055E+01 (1988,189,0600)
 11, 14     330.000  4840.000    2.3055E+01 (1988,189,0600)
 11, 15     330.000  4860.000    2.2586E+01 (1988,189,0600)
 12, 10     350.000  4760.000    2.3055E+01 (1988,189,0600)
 12, 11     350.000  4780.000    2.3055E+01 (1988,189,0600)
 12, 12     350.000  4800.000    2.3055E+01 (1988,189,0600)
 12, 13     350.000  4820.000    2.2586E+01 (1988,189,0600)
 12, 14     350.000  4840.000    2.2586E+01 (1988,189,0600)
 12, 15     350.000  4860.000    2.2586E+01 (1988,189,0600)
 13, 10     370.000  4760.000    2.2586E+01 (1988,189,0600)
 13, 11     370.000  4780.000    2.2887E+01 (1988,189,0600)
 13, 12     370.000  4800.000    2.2586E+01 (1988,189,0600)
 13, 13     370.000  4820.000    2.2586E+01 (1988,189,0600)
 13, 14     370.000  4840.000    2.2586E+01 (1988,189,0600)
 13, 15     370.000  4860.000    2.2586E+01 (1988,189,0600)
 14, 10     390.000  4760.000    2.2586E+01 (1988,189,0600)
 14, 11     390.000  4780.000    2.4164E+01 (1988,189,0600)
 14, 12     390.000  4800.000    2.2668E+01 (1988,189,0600)
```

```
 14, 13    390.000  4820.000   2.2586E+01 (1988,189,0600)
 14, 14    390.000  4840.000   2.2586E+01 (1988,189,0600)
 14, 15    390.000  4860.000   2.2586E+01 (1988,189,0600)
 15, 10    410.000  4760.000   2.2603E+01 (1988,189,0600)
 15, 11    410.000  4780.000   2.4171E+01 (1988,189,0600)
 15, 12    410.000  4800.000   2.2881E+01 (1988,189,0600)
 15, 13    410.000  4820.000   2.2586E+01 (1988,189,0600)
 15, 14    410.000  4840.000   2.2586E+01 (1988,189,0600)
 15, 15    410.000  4860.000   2.2586E+01 (1988,189,0600)

  1 - RANK HIGHEST VALUES FOR PERIOD

Multiply all values by 10 ** -2

 15 I 2306  2259  2259  2259  2259  2259
    I   +     +     +     +     +     +
 14 I 2306  2306  2259  2259  2259  2259
    I   +     +     +     +     +     +
 13 I 2306  2306  2259  2259  2259  2259
    I   +     +     +     +     +     +
 12 I 2306  2306  2306  2259  2267  2288
    I   +     +     +     +     +     +
 11 I 2306  2306  2306  2289  2416  2417
    I   +     +     +     +     +     +
 10 I 2306  2306  2306  2259  2259  2260
    I   +     +     +     +     +     +
    ---------------------------------
       10    11    12    13    14    15
```

```
*******************************************************************************************************************************
                                     CALPOST  Version 5.2        Level 991104
*******************************************************************************************************************************

                                         24HR VISIBILITY
                                       VISIB    B_SN__
                                         (1/Mega-m)

                                                               Modeled Extinction by Species
YEAR DAY HR  RECEPTOR      COORDINATES (km)  TYPE BEXT(Model) BEXT(BKG) BEXT(Total) %CHANGE  F(RH) bxSO4  bxNO3   bxOC  bxPMC  bxPMF
1988 190  0    15, 11    410.000  4780.000  G      0.370      18.023     18.392     2.05    2.548  0.210  0.159  0.000  0.000  0.000

 --- Number of days with Extinction Change  =>   5.0 % :        0
 --- Number of days with Extinction Change  =>  10.0 % :        0
 ---           Largest Extinction Change  =                  2.05 %

*******************************************************************************************************************************
                                     CALPOST  Version 5.2        Level 991104
*******************************************************************************************************************************


                                     Run-Length VISIBILITY


                                       VISIB    B_SN__


                                         (1/Mega-m)


            RECEPTOR      COORDINATES (km)  TYPE BEXT(Model) BEXT(BKG) BEXT(Total) %CHANGE  F(RH)

              15, 11    410.000  4780.000  G      0.370      18.023     18.392     2.05    2.548

 --- Number of recs with Extinction Change  >    1.0 % :        5
 ---           Largest Extinction Change  =                  2.05 %

*******************************************************************************************************************************
                                     CALPOST  Version 5.2        Level 991104
*******************************************************************************************************************************


                                         24HR VISIBILITY


                                       VISIB    B_SN__


                                         (deciview)

                                                               % of Modeled Extinction by Species
YEAR DAY HR  RECEPTOR      COORDINATES (km)  TYPE  DV(Total)   DV(BKG)  DELTA DV  F(RH)  %_SO4  %_NO3   %_OC  %_PMC  %_PMF
1988 190  0    15, 11    410.000  4780.000  G      6.093       5.890     0.203   2.548  56.92  43.08   0.00   0.00   0.00

 --- Number of days with Delta-Deciview  =>   0.50:        0
 --- Number of days with Delta-Deciview  =>   1.00:        0
 ---           Largest Delta-Deciview  =              0.203
```

```
********************************************************************************************************************************
                                      CALPOST  Version 5.2         Level 991104
********************************************************************************************************************************

                                          Run-Length VISIBILITY

                                           VISIB    B_SN__

                                             (deciview)

                 RECEPTOR     COORDINATES (km)  TYPE  DV(Total)    DV(BKG)   DELTA DV  F(RH)

                  15, 11    410.000  4780.000   G       6.093      5.890      0.203   2.548

 --- Number of recs with Delta-Deciview  >    0.10:        5
 ---             Largest Delta-Deciview  =          0.203

********************************************************************************************************************************
                                      CALPOST  Version 5.2         Level 991104
********************************************************************************************************************************


                                             SUMMARY SECTION

                                           VISIB    B_SN__

                                             (1/Mega-m)

 RECEPTOR      COORDINATES (km)    TYPE     PEAK (YEAR,DAY,ENDING TIME)     FOR RANK    FOR AVERAGE PERIOD

  15, 11    410.000  4780.000   GRIDDED   2.4171E+01 (1988,189,0600)      RANK  1        3   HOUR
```

Table 5-9

Plot-File "DATA" Record Structure

Header Records

| Record No. | Variable | Type | Description |
|---|---|---|---|
| 1 | Line 1 | character | Title line identifying averaging time, type of output, and units |
| 2 | (blank) | | |
| 3 | Line 2 | character | Species Processed |
| 4 | (blank) | | |
| 5 | Line 3 | character | Column Headings |
| 6 | (blank) | | |

Data Records (free format)

| Variable No. | Variable | Type | Description | Sample Values |
|---|---|---|---|---|
| 1 | X | real | X-coordinate of receptor (km) | 94.02 |
| 2 | Y | real | Y-coordinate of receptor (km) | 210.89 |
| 3 | V1 | real | Value 1 | 213.8 |
| 4 | V2 | real | Value 2 (optional) | 132.6 |
| 5 | V3 | real | Value 3 (optional) | 16.88 |
| 6 | V4 | real | Value 4 (optional) | .009 |

## Table 5-10
## Sample "DATA" Plot-File
## (Partial Listing)

```
 2 RANKED        1-HOUR AVERAGE  CONCENTRATION VALUES AT EACH RECEPTOR  ( g/m**3)

        SO2            1

   RECEPTOR (x,y) km       1 RANK        2 RANK

   270.000   4720.000     7.8952E-09    1.9814E-09
   290.000   4720.000     5.9128E-08    1.5432E-08
   310.000   4720.000     8.2049E-08    3.7027E-08
   330.000   4720.000     7.2441E-08    5.9440E-08
   350.000   4720.000     7.9033E-08    5.8254E-08
   370.000   4720.000     7.0579E-08    4.8233E-08
   390.000   4720.000     1.3587E-07    9.4182E-08
   410.000   4720.000     4.7199E-08    4.6522E-08
   270.000   4740.000     4.6755E-12    1.6541E-12
   290.000   4740.000     9.4266E-10    6.2788E-10
   310.000   4740.000     7.0272E-09    3.6496E-09
   330.000   4740.000     1.8139E-08    1.2038E-08
   350.000   4740.000     3.8828E-08    1.9662E-08
   370.000   4740.000     5.8562E-08    4.9597E-08
   390.000   4740.000     5.3909E-08    5.2398E-08
   410.000   4740.000     4.5306E-07    2.8328E-07
   270.000   4760.000     0.0000E+00    0.0000E+00
   290.000   4760.000     1.7201E-10    1.2712E-10
   310.000   4760.000     1.3340E-09    1.1862E-09
   330.000   4760.000     4.5722E-09    4.4274E-09
   350.000   4760.000     1.0541E-08    1.0369E-08
   370.000   4760.000     3.2621E-07    6.5301E-08
   390.000   4760.000     8.6671E-07    4.7615E-07
   410.000   4760.000     5.4748E-07    4.4530E-07
   270.000   4780.000     0.0000E+00    0.0000E+00
   290.000   4780.000     1.8996E-11    1.7348E-11
   310.000   4780.000     5.3253E-10    5.0730E-10
   330.000   4780.000     2.2485E-09    2.2173E-09
   350.000   4780.000     6.2623E-09    6.2032E-09
   370.000   4780.000     1.0701E-06    1.6573E-07
   390.000   4780.000     6.4020E-07    6.0337E-07
   410.000   4780.000     6.3429E-07    4.6677E-07
   270.000   4800.000     0.0000E+00    0.0000E+00
   290.000   4800.000     0.0000E+00    0.0000E+00
   310.000   4800.000     1.9163E-10    1.6276E-10
   330.000   4800.000     1.1810E-09    9.1738E-10
   350.000   4800.000     2.6353E-08    4.7434E-09
   370.000   4800.000     1.2015E-06    1.0502E-06
   390.000   4800.000     2.4910E-07    1.9500E-07
   410.000   4800.000     2.9590E-07    2.0784E-07
   270.000   4820.000     0.0000E+00    0.0000E+00
   290.000   4820.000     0.0000E+00    0.0000E+00
   310.000   4820.000     5.6655E-11    5.0932E-11
   330.000   4820.000     5.0676E-10    4.5829E-10
   350.000   4820.000     5.7000E-09    3.2322E-09
   370.000   4820.000     8.0446E-07    4.9414E-07
   390.000   4820.000     6.8545E-07    5.6447E-07
   410.000   4820.000     2.5748E-07    2.0238E-07
```

# Table 5-11
## Plot-File "GRID" Record Structure

### Header Records (free format)

| Record No. | Variable No. | Variable | Type | Description | Sample Values |
|---|---|---|---|---|---|
| 1 | 1 | ID | character | File type code (must be 'DSAA' for ASCII file) | DSAA |
| 2 | 1 | NX | integer | Number of receptors in easting direction | 34 |
| 2 | 2 | NY | integer | Number of receptors in northing direction | 51 |
| 3 | 1 | XBEG | real | X-coordinate (km) of first gridded receptor (southwest) | 213.75 |
| 3 | 2 | YBEG | real | Y-coordinate (km) of first gridded receptor (southwest) | 439.00 |
| 4 | 1 | XEND | real | X-coordinate (km) of last gridded receptor (northeast) | 222.00 |
| 4 | 2 | YEND | real | Y-coordinate (km) of last gridded receptor (northeast) | 451.50 |
| 5 | 1 | VMIN | real | Minimum value in grid | 0.001 |
| 5 | 2 | VMAX | real | Maximum value in grid | 159.0 |

### Data Records (free format)

| Record No. | Variable | Type | Description |
|---|---|---|---|
| 1 | V1 | real array | NX values in first row of grid (southernmost row) |
| 2 | V2 | real array | NX values in second row of grid |
| ... | ... | ... | |
| NY | VNY | real array | NX values in last row of grid (northernmost row) |

Table 5-11 (Concluded)

Plot-File "GRID" Record Structure

Footer Records

| Record No. | Variable | Type | Description |
|---|---|---|---|
| 1-5 | (blank) | | |
| 6 | Line 1 | character | Title line identifying averaging time, type of output, and units |
| 7 | (blank) | | |
| 8 | Line 2 | character | Species Processed or other information (varies with type of data) |
| 9 | (blank) | | |
| 10 | Line 3 | character | Species Processed or other information (varies with type of data) |

Table 5-12
Sample "GRID" Plot-File

```
DSAA
          8            8
    270.000     410.000
   4720.000    4860.000
  0.0000E+00  0.1202E-05
7.8952E-09  5.9128E-08  8.2049E-08  7.2441E-08  7.9033E-08  7.0579E-08  1.3587E-07  4.7199E-08
4.6755E-12  9.4266E-10  7.0272E-09  1.8139E-08  3.8828E-08  5.8562E-08  5.3909E-08  4.5306E-07
0.0000E+00  1.7201E-10  1.3340E-09  4.5722E-09  1.0541E-08  3.2621E-07  8.6671E-07  5.4748E-07
0.0000E+00  1.8996E-11  5.3253E-10  2.2485E-09  6.2623E-09  1.0701E-06  6.4020E-07  6.3429E-07
0.0000E+00  0.0000E+00  1.9163E-10  1.1810E-09  2.6353E-08  1.2015E-06  2.4910E-07  2.9590E-07
0.0000E+00  0.0000E+00  5.6655E-11  5.0676E-10  5.7000E-09  8.0446E-07  6.8545E-07  2.5748E-07
0.0000E+00  0.0000E+00  0.0000E+00  2.0870E-10  2.1584E-09  3.1430E-08  5.1841E-07  2.4384E-07
0.0000E+00  0.0000E+00  0.0000E+00  6.9000E-11  4.3005E-10  1.0159E-08  1.3561E-07  3.3995E-07



     1-HOUR AVERAGE  CONCENTRATION VALUES AT EACH RECEPTOR  ( g/m**3)

  SO2           1

  RANK          1
```

## Table 5-13
## Timeseries File Record Structure

### Header Records

| Record No. | Variable | Type | Description |
|---|---|---|---|
| 1 | Line 1 | character | Title line identifying file type and species processed |
| 2 | (blank) | | |
| 3 | Line 2 | character | Averaging time, type of output, and units |
| 4 | Line 3 | character | Number of receptors processed |
| 5 | (blank) | | |
| 6 | Line 4 | character | Receptor type for each receptor processed |
| 7 | Line 5 | character | Receptor ID or Easting cell index for each receptor processed |
| 8 | Line 6 | character | Northing cell index for each receptor processed |
| 9 | Line 7 | character | Easting coordinate (km) for each receptor processed |
| 10 | Line 8 | character | Northing coordinate (km) for each receptor processed |
| 11 | (blank) | | |
| 12 | Line 9 | character | Heading for year, day, time columns |
| 13 | (blank) | | |

### Data Records (free format)

| Variable No. | Variable | Type | Description | Sample Values |
|---|---|---|---|---|
| 1 | IYR | integer | Year (YYYY format) | 1996 |
| 2 | JDAY | integer | Julian Day (JJJ format) | 216 |
| 3 | ITIME | integer | Time at end of averaging period (HHMM format) | 0800 |
| 4 to NREC+3 | V | real array | Value for each of the NREC receptors processed | 5.473498E-07 |

Table 5-14

Sample Timeseries File

```
TIMESERIES Output  --------  SO2           1

        1    HOUR Average   CONCENTRATION Values at Selected Receptors  ( g/m**3)
        2    Receptors are Included

           Type:            GRID          GRID
            ix:                6             8
            iy:                4             5
          x(km):  2.300000E+02  2.700000E+02
          y(km):  4.640000E+03  4.660000E+03

 YYYY JDY HHMM

 1988 189 0100    0.000000E+00  0.000000E+00
 1988 189 0200    1.916138E-08  0.000000E+00
 1988 189 0300    3.400294E-07  0.000000E+00
 1988 189 0400    3.968533E-07  0.000000E+00
 1988 189 0500    1.251997E-07  0.000000E+00
 1988 189 0600    5.473498E-07  0.000000E+00
 1988 189 0700    4.170044E-08  1.020110E-09
 1988 189 0800    0.000000E+00  8.213156E-10
 1988 189 0900    0.000000E+00  0.000000E+00
 1988 189 1000    0.000000E+00  0.000000E+00
 1988 189 1100    3.724512E-08  0.000000E+00
 1988 189 1200    9.805949E-08  6.046957E-09
 1988 189 1300    9.109576E-08  2.053027E-08
 1988 189 1400    8.968187E-08  3.515141E-08
 1988 189 1500    1.855247E-07  4.744752E-08
 1988 189 1600    2.432677E-07  6.169984E-08
 1988 189 1700    1.831459E-07  9.404808E-08
 1988 189 1800    9.832471E-08  1.438350E-07
 1988 189 1900    3.688035E-08  1.607274E-07
 1988 189 2000    4.669193E-09  1.218663E-07
 1988 189 2100    1.730192E-10  5.904977E-08
 1988 189 2200    3.505524E-11  2.744583E-08
 1988 189 2300    0.000000E+00  4.535747E-09
 1988 190 0000    0.000000E+00  3.198288E-10
```

# 6. REFERENCES

Anthes, R.A., E.Y. Hsie, and Y.H. Kuo, 1987: Description of the Penn State/NCAR mesoscale model version 4 (MM4). NCAR Tech Note, NCAR/TN-282+STR, Available from the National Center for Atmospheric Research, PO Box 3000, Boulder, CO 80307, 66 pp.

Arya, S.P.S., 1984: Parametric relations for the atmospheric boundary layer. *Bound. Layer Meteor.*, **30**, 57-73.

Atkinson, R., A.C. Lloyd and L. Winges, 1982: An updated chemical mechanism for hydrocarbon/$NO_x$/$SO_x$ photo oxidation suitable for inclusion in atmospheric simulation models. *Atmospheric Environ.*, **16**, 1341.

Barrie, L.A., 1981: The prediction of rain acidity and $SO_2$ scavenging in eastern North America. *Atmospheric Environ.*, **15**, 31-41.

Benkley, C.W. and A. Bass, 1979: Development of Mesoscale Air Quality Simulation Models. Volume 3. User's Guide to MESOPUFF (Mesoscale Puff) Model. EPA 600/7-79-XXX, Environmental Protection Agency, Research Triangle Park, NC, 124 pp.

Blackadar, A.K. and H. Tennekes, 1968: Asymptotic similarity in neutral barotropic planetary boundary layers. *J. Atmos. Sci.*, **25**, 1025-1020.

Bowers, J.F. and A.J. Anderson, 1981: An evaluation study for the Industrial Source Complex (ISC) dispersion model. EPA 450/4-81-002, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Briggs, G.A., 1969: Plume Rise. U.S. Atomic Energy Commission. TID-25075. Oak Ridge, TN.

Briggs, G.A., 1973: Diffusion estimates for small emissions (Draft). Air Resources Atmospheric Turbulence and Diffusion Laboratory. ATOL No. 79.

Briggs, G.A., 1975: Plume rise predictions. In: *Lectures on Air Pollution and Environmental Impact Analyses*. American Meteorological Society, Boston, MA, pp. 59-111.

Briggs, G.A., 1985: Analytical parameterizations of diffusion: The convective boundary layer. *J. Clim. and Appl. Meteor.*, **24**, 1167-1186.

Brighton, P.W.M., 1978:  Strongly stratified flow past three-dimensional obstacles.  *Quart. J.R. Met. Soc.*, **104**, 289-307.

Britter, R.E., J.C.R. Hunt and K.J. Richards, 1981:  Airflow over a two-dimensional hill:  Studies of velocity speed-up, roughness effects and turbulence.  *Quart. J.R. Met. Soc.*, **107**, 92-110.

Brost, R.A. and J.C. Wyngaard, 1978:  A model study of the stably stratified planetary boundary layer.  *J. Atmos. Sci.*, **35**, 1427-1400.

Calvert, J.G., F. Su, J.W. Bottenheim and O.P. Strausz, 1978:  Mechanism of the homogeneous oxidation of sulfur dioxide in the troposphere.  *Atmospheric Environ.*, **12**, 1978.

Caughey, S.J., 1981:  Observed characteristics of the atmospheric boundary layer.  In:  *Atmospheric Turbulence and Air Pollution Modeling*.  F.T.M. Nieuwstadt and H. Van Dop, Eds.,  D. Reidel Publishing Company, Boston, MA.

Ching, J.K.S., J.M. Godowitch, J.F. Clarke and A.H. Auer, 1983:  Urban scale variations of turbulence parameters and fluxes.  AMS Specialty Conference on Air Quality Modeling of the Urban Boundary Layer, Baltimore, MD.

Deardorff, J.W. and G.E. Willis, 1975:  A parameterization of diffusion into the mixed layer.  *J. Appl. Meteor.*, **14**, 1451-1458.

Deardorff, J.W. and G.E. Willis, 1982:  Ground-level concentrations due to fumigation into an entraining mixed-layer.  *Atmospheric Environ.*, **16**, 1159-1170.

Douglas, S. and R. Kessler, 1988:  User's guide to the diagnostic wind model.  California Air Resources Board, Sacramento, CA.

Draxler, R.R., 1976:  Determination of atmospheric diffusion parameters.  *Atmospheric Environ.*, **10**, 99-105.

Drazin, P.G., 1961:  On the steady flow of a fluid of variable density past an obstacle.  *Tellus*, **13**, 239-251.

EPA, 1988:  User's guide to SDM -- A Shoreline Dispersion Model (EPA-450/4-88-017).  U.S. Environmental Protection Agency, Research Triangle Park, NC.

EPA, 1993a:  Interagency Workgroup on Air Quality Modeling (IWAQM) Phase I report: Interim recommendations for modeling long range transport and impacts on regional visibility.  U.S. EPA,  Research Triangle Park, NC.

EPA, 1993b:  User's guide to the Building Profile Input Program (BPIP).  U.S. Environmental Protection Agency, Research Triangle Park, NC.

EPA, 1995:  User's guide for the Industrial Source Complex (ISC3) dispersion models. Vol. I - User instructions (EPA-454/B-95-003a). Vol. II - Description of model algorithms (EPA - 454/B-95-003b). Vol III - Guide to programmers (EPA - 454/B-95-003c).  U.S. Environmental Protection Agency, Research Triangle Park, NC.

EPA, 1995:  Testing of meteorological and dispersion models for use in regional air quality modeling.  Report prepared for U.S. EPA by Sigma Research/EARTH TECH, Concord, MA.

Forrest, J., R.W. Garber and L. Newman, 1981:  Conversion rates in power plant plumes based on filter pack data:  The coal-fired cumberland plume.  *Atmospheric Environ.*, **15**, 2273.

Fowler, D. and M.H. Unsworth, 1979:  Turbulent transfer of sulphur dioxide to a wheat crop.  *Quart. J.R. Meteor. Soc.*, **105**, 767-784.

Garratt, J.R., 1992:  *The Atmospheric Boundary Layer*.  Cambridge University Press, Great Britain.

Geller, M. and E. Ng, 1971:  Tables of Integrals of the Error Functions — II:  Additions and Corrections.  *J. Research of the National Bureau of Standards, Part B, Mathematical Sciences,* **75B**, 149-163.

Gifford, F.A., Jr., 1976:  Turbulent Diffusion--Typing schemes: A Review.  *Nucl. Saf.*, **17**, 68-86.

Grell, G., J. Dudhia, and D. Stauffer, 1996: A description of the fifth generation Penn State/NCAR Mesoscale Model (MM5), NCAR/TN-398+STR

Hales, J.M., D.C. Powell and T.D. Fox, 1977:  STRAM--An Air Pollution Model Incorporating Non-linear Chemistry, Variable Trajectories, and Plume Segment Diffusion.  EPA 450/3-77-012. Environmental Protection Agency, Research Triangle Park, NC, 147 pp.

Hanna, S.R., G.A. Briggs, J. Deardorff, B.A. Egan, F.A. Gifford and F. Pasquill, 1977:  AMS workshop on stability classification schemes and sigma curves - summary of recommendations.  *Bull. Am. Meteor. Soc.*, **58**, 1305-1309.

Hanna, S.R. and J.C. Chang, 1991: Modifications of the Hybrid Plume Dispersion Model (HPDM) for urban conditions and its evaluation using the Indianapolis data set, Volume I: User's Guide for HPDM-URBAN. EPRI Project No. RFP-02736-1, Palo Alto, CA 94303.

Hanna, S.R., L.L. Schulman, R.J. Paine, J.E. Pleim and M. Baer, 1985: Development and evaluation of the offshore and coastal dispersion model. *JAPCA*, **35**, 1039-1047.

Hanna, S.R., J.C. Weil and R.J. Paine, 1986: Plume model development and evaluation. Report Number D034-500. Electric Power Research Institute, Palo Alto, CA.

Heffter, J.L., 1965: The variations of horizontal diffusion parameters with time for travel periods of one hour or longer. *J. Appl. Meteor.*, **4**, 153-156.

Hicks, B.B., 1982: In: *Critical Assessment Document on Acid Deposition (Chapter VII-Dry Deposition)*. ATDL Contribution File No. 81/24. Atmospheric Turbulence and Diffusion Laboratory, NOAA, Oak Ridge, TN.

Hicks, B.B., 1985: Behavior of turbulence statistics in the convective boundary layer. *J. Clim. and Appl. Meteor.*, **24**, 607-614.

Hosker, R.P., 1974: A comparison of estimation procedures for overwater plume dispersion. Proceedings of the Symposium on Atmospheric Diffusion and Air Pollution. American Meteorological Society, Boston, MA.

Hosker, R.P., 1984: Flow and diffusion near obstacles. In: *Atmospheric Science and Power Production*. R. Randerson, Ed., DOE/TIC-27601, National Technical Information Service, Springfield, VA.

Hosker, R.P., Jr. and S.E. Lindberg, 1982: Review: Atmospheric deposition and plant assimilation of gases and particles. *Atmospheric Environ.*, **16**, 889-910.

Hoult, D.P. and J.C. Weil, 1972: A turbulent plume in a laminar crossflow. *Atmos. Environ.,* **6**, 513-531.

Huber, A.H. 1977: Incorporating building/terrain wake effects on stack effluents. Preprint volume for the Joint Conference on Applications of Air Pollution Meteorology, American Meteorological Society, Boston, MA.

Huber, A.H. and W.H. Snyder, 1976:  Building wake effects on short stack effluents.  Preprint volume for the Third Symposium on Atmospheric Diffusion and Air Quality, American Meteorological Society, Boston, MA.

Huber, A.H. and W.H. Snyder, 1982:  Wind tunnel investigation of the effects of a rectangular-shaped building on dispersion of effluents from short adjacent stacks.  *Atmospheric Environ.*, **17**, 2837-2848.

Hunt, J.C.R., 1982:  Diffusion in the stable boundary layer.  In:  *Atmospheric Turbulence and Air Pollution Modeling*.  F.T.M. Nieuwstadt and H. van Dop, Eds., D. Reidel Publishing Co., Boston, MA.

Hunt, J.C.R. and R.J. Mulhearn, 1973:  Turbulent dispersion from sources near two-dimensional obstacles.  *J. Fluid Mech.*, **61**, 245-274.

Hunt, J.C.R., J.S. Puttock and W.H. Snyder, 1979:  Turbulent diffusion from a point source in stratified and neutral flows around a three-dimensional hill (Part I - Diffusion equation analysis).  *Atmospheric Environ.*, **13**, 1227-1239.

Hunt, J.C.R. and W.H. Snyder, 1980:  Experiments on stably and neutrally stratified flow over a model three-dimensional hill.  *J. Fluid Mech.*, **96**, 671-704.

Irwin, J.S., 1979:  Scheme for estimating dispersion parameters as a function of release height.  EPA-600/4-79-062, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Irwin, J.S., 1983:  Estimating plume dispersion - a comparison of several sigma schemes.  *J. Clim. and Appl. Meteor.*, **22**, 92-114.

Kessler, R.C., 1989:  User's Guide.  Systems Applications, Inc. Version of the Colorado State University Mesoscale Model.  California Air Resources Board, Sacramento, CA.

Lamb, R.G., 1981:  Diffusion in the convective boundary layer.  In:  *Atmospheric Turbulence and Air Pollution Modeling*.  T.F.M. Nieuwstadt and K. van Dop, Eds., D. Reidel Publishing Company, Boston, MA.

LeMone, M., 1978:  The marine boundary layer.  In:  *Proceedings of Workshop on the Planetary Boundary Layer*.  American Meteorological Society, Boston, MA, pp 182-234.

Levine, S.Z. and S.E. Schwartz, 1982:  In-cloud and below-cloud of scavenging of nitric acid vapor. *Atmospheric Environ.*, **16**, 1725-1734.

Lorimer, G., 1986:  The AUSPLUME Gaussian plume dispersion model. Environmental Protection Authority of Victoria, Melbourne, Victoria, Australia.

Ludwig, F.L., L.S. Gasiorek and R.E. Ruff, 1977:  Simplification of a Gaussian puff model for real-time minicomputer use.  *Atmospheric Environ.*, **11**, 431-436.

Lyons, W. and H. Cole, 1973:  Fumigation and plume trapping on the shores of Lake Michigan during stable onshore flow.  *J. Appl. Meteor.*, **12**, 494-510.

Maul, P.R., 1980:  Atmospheric transport of sulfur compound pollutants.  Central Electricity Generating Bureau MID/SSD/80/0026/R, Nottingham, England.

Manins, P.C., 1979:  Partial penetration of an elevated inversion layer by chimney plumes.  *Atmospheric Environ.*, **13**, 733-741.

Manins, P.C., 1984:  Chimney plume penetration of the sea-breeze inversion.  *Atmospheric Environ.*, **18**, 2339-2344.

McElroy, J.L. and F. Pooler, 1968:  The St. Louis dispersion study.  U.S. Public Health Service, National Air Pollution Control Administration, Report AP-53.

Mills, M.T., R.J. Paine, E.M. Insley and B.A. Egan, 1987:  The complex terrain dispersion model (CTDM) terrain preprocessor system--user guide and program descriptions.  U.S. Environmental Protection Agency, Atmospheric Sciences Research Laboratory, Research Triangle Park, NC.

Misra, P.K., 1980:  Dispersion from tall stacks into a shoreline environment.  *Atmospheric Environ.*, **14**, 397-400.

Moller U. and G. Shumann, 1970:  Mechanisms of transport from the atmosphere to the earth's surface.  *J. Geophy. Res.*, **75**, 3013-3019.

Morris, R.E., R.C. Kessler, S.G. Douglas, K.R. Styles, and G.E. Moore, 1988:  Rocky Mountain Acid Deposition Model Assessment: Acid Rain Mountain Mesoscale Model (ARM3).   U.S. Environmental Protection Agency, Atmospheric Sciences Research Laboratory, Research Triangle Park, NC.

Nieuwstadt, F.T.M., 1977:  The dispersion of pollutants over a water surface.  Eighth International Technical Meeting on Air Pollution, Modeling, and It's Application, NATO/CCMS Doc. No. 80, pp. 337-359.

Nieuwstadt, F.T.M., 1984:  Some aspects of the turbulent stable boundary layer.  *Bound. Layer Meteor.*, **30**, 31-55.

O'Dell, R.A., M. Taheri and R.L. Kabel, 1977:  A model for uptake of pollutants by vegetation. *JAPCA*, **27**, 1104-1109.

Padro J., G.D. Hartog, and H.H. Neumann, 1991: An investigation of the ADOM dry deposition module using summertime $O_3$ measurements above a deciduous forest.  *Atmospheric Environ.*, **25A**, 1689-1704.

Paine, R.J., D.G. Strimaitis, M.G. Dennis, R.J. Yamartino, M.T. Mills and E.M. Insley, 1987:  User's guide to the complex terrain dispersion model.  Vol. 1., EPA-600/8-87-058a, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Panofsky, H.A., H. Tennekes, D.H. Lenschow and J.C. Wyngaard, 1977:  The characteristics of turbulent velocity components in the surface layer under convective conditions. *Bound. Layer Meteor.*, **11**, 355-361.

Pasquill, F., 1976:  Atmospheric dispersion parameters in Gaussian plume modeling: Part II.  Possible requirements for change in the Turner workbook values.  EPA-600/4-76-030b, U.S. Environmental Protection Agency, Research Triangle Park, NC, 53 pp.

Perry, S.G., D.J. Burns, L.H. Adams, R.J. Paine, M.G. Dennis, M.T. Mills, D.G. Strimaitis, R.J. Yamartino, E.M. Insley, 1989:  User's Guide to the Complex Terrain Dispersion Model Plus Algorithms for Unstable Situations (CTDMPLUS) Volume 1: Model Description and User Instructions.  EPA/600/8-89/041, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Petersen, W.B., 1986:  A demonstration of INPUFF with the MATS data base. *Atmospheric Environ.*, **20**, 1341-1346.

Pleim, J., A. Venkatram and R.J. Yamartino, 1984: ADOM/TADAP model development program. Volume 4. The dry deposition model. Ontario Ministry of the Environment, Rexdale, Ontario, Canada.

Riley, J.J., H.T. Liu and E.W. Geller, 1976: A numerical and experimental study of stably stratified flow around complex terrain. EPA Report No. EPA-600/4-76-021, Research Triangle Park, NC, 41 p.

Rittmann, B.E., 1982: Application of the two-thirds law to plume rise from industrial-sized sources. *Atmospheric Environ.*, **16**, 2575-2579.

Schulman, L.L. and S.R. Hanna, 1986: Evaluation of downwash modifications to the Industrial Source Complex Model. *JAPCA*, **36**, 258-264.

Schulman, L.L. and J.S. Scire, 1980: Buoyant Line and Point Source (BLP) dispersion model user's guide. Document P-7304-B, Environmental Research & Technology, Inc., Concord, MA.

Schulman, L.L. and J.S. Scire, 1981: The development and capabilities of the BLP Model. In: *Proceedings APCA Specialty Conference on Dispersion Modeling from Complex Sources*. St. Louis, MO.

Scire, J.S., E.M. Insley and R.J. Yamartino, 1990a: Model formulation and user's guide for the CALMET meteorological model. Prepared for the California Air Resources Board by Sigma Research Corporation, Concord, MA.

Scire, J.S., D.G. Strimaitis and R.J. Yamartino, 1990b: Model formulation and user's guide for the CALPUFF dispersion model. Prepared for the California Air Resources Board by Sigma Research Corporation, Concord, MA.

Scire J.S., F.R. Robe, M.E. Fernau, and R.J. Yamartino, 1998: A User's Guide for the CALMET Meteorological Model (Version 5.0). Earth Tech, Inc., Concord, MA.

Scire, J.S., F.W. Lurmann, A. Bass and S.R. Hanna, 1984a: Development of the MESOPUFF II dispersion model. EPA-600/3-84-057, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Scire, J.S., F.W. Lurmann, A. Bass and S.R. Hanna, 1984b: User's guide to the MESOPUFF II model and related processor programs. EPA-600/8-84-013, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Scire, J.S. and L.L. Schulman, 1980: Modeling plume rise from low-level buoyant line and point sources. *Proceedings Second Point Conference on Applications of Air Pollution Meteorology*, 24-28 March, New Orleans, LA, 133-139.

Scire, J.S. and L.L. Schulman, 1981: Evaluation of the BLP and ISC models with $SF_6$ tracer data and $SO_2$ measurements at aluminum reduction plants. In: *Proceedings APCA Specialty Conference on Dispersion Modeling from Complex Sources*, St. Louis, MO.

Scire, J.S. and A. Venkatram, 1985: The contribution of in-cloud oxidation of $SO_2$ to wet scavenging of sulfur in convective clouds. *Atmospheric Environ.*, **19**, 637-650.

Scire, J.S., R.J. Yamartino, G.R. Carmichael and Y.S. Chang, 1989: CALGRID: A Mesoscale Photochemical/Grid Model. Volume II: User's Guide. California Air Resources Board, Sacramento, CA.

Sehmel, G.A., 1980: Particle and gas dry deposition - a review. *Atmospheric Environ.*, **14**, 983-1011.

Sehmel, G.A. and S.L. Sutter, 1974: Particle deposition rates on a water surface as a function of particle diameter and air velocity. *J. Rechs Atmos.*, **III**, 911-918.

Shepherd, J.G., 1974: Measurements of the direct deposition of sulphur dioxide onto grass and water by the profile method. *Atmospheric Environ.*, **8**, 69-74.

Sheppard, P.A., 1956: Airflow over mountains. *Quart. J.R. Meteor. Soc.*, **82**, 528-529.

Slinn, S.A. and W.G.N. Slinn, 1980: Predictions for particle deposition on natural waters. *Atmospheric Environ.*, **14**, 1013-1016.

Slinn, W.G.N., L. Hasse, B.B. Hicks, A.W. Hogan, D. Lal, P.S. Liss, K.O. Munnich, G.A. Sehmel and O. Vittori, 1978: Some aspects of the transfer of atmospheric trace constituents past the air-sea interface. *Atmospheric Environ.*, **12**, 2055-2087.

Smith F.B., 1972: A scheme for estimating the vertical dispersion of a plume from a source near ground level. Proceedings of the NATO Expert Panel on Air Pollution Modelling, Oct. 1972. Report NATO-CCMS-14. North Atlantic Treaty Organization: Brussels.

Snyder, W.H., 1980: Towing tank studies in support of field experiments at Cinder Cone Butte, Idaho, Phase III: Verification of formula for prediction of dividing streamline height. Fluid Modeling Facility Internal Rpt., Aug. 29, Environmental Protection Agency, Research Triangle Park, NC, 12 p.

Snyder, W.H. and J.C.R. Hunt, 1984: Turbulent diffusion from a point source in stratified and neutral flow around a three-dimensional hill (Part II - Laboratory measurement of surface concentrations). *Atmospheric Environ.*, **18**, 1969-2002.

Stelson, A.W., M.E. Bassett and J.H. Seinfeld, 1983: *Thermodynamic Equilibrium Properties of Aqueous Solutions of Nitrate, Sulfate and Ammonium. Acid Precipitation, Chemistry of Particles, Fog and Rain.* J. Teasley, ed. Ann Arbor Science, Woburn, MA.

Stelson, A.W. and J.H. Seinfeld, 1982: Relative humidity and temperature dependence of the ammonium nitrate dissociation constant. *Atmospheric Environ.*, **16**, 983-992.

Strimaitis D.G., T.F. Lavery, A. Venkatram, D.C. DiCristofaro, B.R. Greene, and B.A. Egan, 1985: EPA complex terrain model development Fourth Milestone Report. EPA/600/3-84/110, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Strimaitis, D.G., R.J. Paine, B.A. Egan and R.J. Yamartino, 1988: EPA complex terrain model development final report. EPA-600/53-88-006, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Strimaitis, D.G., R.J. Yamartino, E.M. Insley, J.S. Scire, 1995: A User's Guide for the Kinematic Simulation Particle (KSP) Model. Prepared for Institut fuer Meteorologie, Freie Universitaet Berlin, Germany, and Umwelbundesamt, Berlin, Germany, Document No. 1274-2, by Earth Tech, Inc, Concord, MA

Thuillier, R.H., 1982: Dispersion characteristics in the lee of complex structures. *JAPCA*, **32**, 526-532.

Turner, D.B., 1970: Workbook of Atmospheric Dispersion Estimates. U.S. EPA Office of Air Programs Publication No. AP-26. Research Triangle Park, NC.

van Egmond, N.D. and H. Kesseboom, 1983: Mesoscale air pollution dispersion models - II. Lagrangian Puff model and comparison with Eulerian grid model. *Atmospheric Environ.*, **17**, 267-274.

Voldner, E.C., L.A. Barrie and A. Sirois, 1986:  A literature review of dry deposition of oxides of sulphur and nitrogen with emphasis on long-range transport modeling in North America. *Atmospheric Environ.*, **20**, 2101-2123.

Weil, J.C., 1985:  Updating applied diffusion models.  *J. Clim. Appl. Meteor.*, **24**, 1111-1130.

Weil, J.C., 1988:  Dispersion in the convective boundary layer. *Lectures on Air Pollution Modeling*. Editors, Venkatram A. and Wyngaard, J.C., 167-227.

Weil, J.C., 1988:  Plume rise. *Lectures on Air Pollution Modeling*.  Editors, Venkatram A. and Wyngaard, J.C., 119-166.

Weil, J.C., 1990: A diagnosis of the asymmetry in top-down and bottom-up diffusion using a Lagrangian stochastic model.  *J. Atmos. Sci.*, **47**, 501-515.

Weil, J.C., and R.P. Brower, 1984:  An updated Gaussian plume model for tall stacks.  *J. Air Pollut. Control Assoc.*, **34**, 818-827.

Weil, J.C., L.A.Corio, and R.P. Brower, 1997:  A PDF Model for Buoyant Plumes in the Convective Boundary Layer.  *J. Appl. Meteor.*, **36**, 982-1003.

Wesely, M.L. and B.B. Hicks, 1977:  Some factors that affect the deposition rates of sulfur dioxide and similar gases on vegetation.  *J. Air Poll. Control Assoc.*, **27**, 1110-1116.

Wilson, W.E., 1981:  Sulfate formation in point source plumes:  A review of recent field studies. *Atmospheric Environ.*, **15**, 2573.

Wyngaard, J.C., 1988: Structure of the PBL.  *Lectures on Air Pollution Modeling*.  Editors, Venkatram A. and Wyngaard, J.C., 9-61.

Yamartino, R.J., J.S. Scire, S.R. Hanna, G.R. Carmichael and Y.S. Chang, 1989:  CALGRID: A Mesoscale Photochemical Grid Model.  Volume I:  Model Formulation Document.  California Air Resources Board, Sacramento, CA.

Yamartino, R.J., J.S. Scire, S.R. Hanna, G.R. Carmichael and Y.S. Chang, 1992:  The CALGRID mesoscale photochemical grid model - I. Model formulation. *Atmospheric Environ.*, **26A**, 1493-1512.

Yamartino, R.J., D.G. Strimaitis, J.S. Scire, E.M. Insley, and M.J. Spitzak, 1996: Final Report on the Phase I Development of the Kinematic Simulation Particle (KSP) Atmospheric Dispersion Model, prepared for Institut fuer Meteorologie, Freie Universitaet Berlin, Germany, and Umwelbundesamt, Berlin, Germany, Document No. 1274-3m, by Earth Tech, Inc, Concord, MA

Zannetti, P., 1981:  An improved puff algorithm for plume dispersion simulation.  *J. Appl. Meteor.*, **20**, 1203-1211.

Zhang, X., 1993:  A computational analysis for the rise, dispersion, and deposition of buoyant plumes. Ph.D. Thesis, Massachusetts Institute of Technology, Cambridge.

# APPENDIX A

## Tree Diagram of the CALPUFF Model
## and Subroutine/Function Calling Structure

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|

```
PROGRAM CALPUFF
.       UNDER0
.       SETUP
.       .       DATETM
.       .       .       DATE
.       .       .       TIME
.       .       .       ETIME
.       .       COMLINE
.       .       .       GETCL
.       .       READCF
.       .       .       READFN
.       .       .       .       READIN
.       .       .       .       .       DEBLNK
.       .       .       .       .       ALLCAP
.       .       .       .       .       ALTONU
.       .       .       .       .       SETVAR
.       .       .       .       FILCASE
.       .       .       WRIVL
.       .       .       YR4C
.       .       .       READIN
.       .       .       .       DEBLNK
.       .       .       .       ALLCAP
.       .       .       .       ALTONU
.       .       .       .       SETVAR
.       .       .       QAYR4
.       .       .       QUADAREA
.       .       .       .       TRIAREA
.       .       .       QAINP
.       .       WRFILES
.       .       SETCOM
.       .       OPENOT
.       .       .       OPENAB
.       .       MET1
.       .       .       YR4
.       .       .       RDR1D
.       .       .       METQA
.       .       .       RDR2D
.       .       .       RDI2D
.       .       .       OUT
.       .       .       .       WRT
.       .       .       .       WRT2
.       .       MET2
.       .       .       YR4
.       .       .       JULDAY
```

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | INCR | | | | | | | |
| . | . | . | GRDAY | | | | | | | |
| . | . | . | INITR2D | | | | | | | |
| . | . | . | INITI2D | | | | | | | |
| . | . | . | OUT | | | | | | | |
| . | . | . | . | WRT | | | | | | |
| . | . | . | . | WRT2 | | | | | | |
| . | . | MET3 | | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | . | JULDAY | | | | | | | |
| . | . | . | INCR | | | | | | | |
| . | . | . | GRDAY | | | | | | | |
| . | . | . | INITR2D | | | | | | | |
| . | . | . | INITI2D | | | | | | | |
| . | . | . | OUT | | | | | | | |
| . | . | . | . | WRT | | | | | | |
| . | . | . | . | WRT2 | | | | | | |
| . | . | MET4 | | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | . | JULDAY | | | | | | | |
| . | . | . | INCR | | | | | | | |
| . | . | . | GRDAY | | | | | | | |
| . | . | . | INITR2D | | | | | | | |
| . | . | . | INITI2D | | | | | | | |
| . | . | . | OUT | | | | | | | |
| . | . | . | . | WRT | | | | | | |
| . | . | . | . | WRT2 | | | | | | |
| . | . | RDHDEM2 | | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | RDHDEM3 | | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | RDHDEM4 | | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | RDHDEM5 | | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | CHEMI | | | | | | | | |
| . | . | . | RDCHEM | | | | | | | |
| . | . | . | . | READIN | | | | | | |
| . | . | . | . | . | DEBLNK | | | | | |
| . | . | . | . | . | ALLCAP | | | | | |
| . | . | . | . | . | ALTONU | | | | | |
| . | . | . | . | . | SETVAR | | | | | |
| . | . | . | RDHDOZ | | | | | | | |
| . | . | . | . | YR4 | | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | RDTIOZ | | | | | | | |
| . | . | . | OUT | | | | | | | |
| . | . | . | . | WRT | | | | | | |
| . | . | . | . | WRT2 | | | | | | |
| . | . | . | SSLATLON | | | | | | | |
| . | . | EMQA | | | | | | | | |
| . | . | . | QCHECK | | | | | | | |
| . | . | RDTIEM2 | | | | | | | | |
| . | . | RDTIEM3 | | | | | | | | |
| . | . | RDTIEM5 | | | | | | | | |
| . | . | ELEVI | | | | | | | | |
| . | . | . | GETELEV | | | | | | | |
| . | . | SIGSET | | | | | | | | |
| . | . | SLUGI | | | | | | | | |
| . | . | DRYI | | | | | | | | |
| . | . | . | RDVD | | | | | | | |
| . | . | . | . | READIN | | | | | | |
| . | . | . | . | . | DEBLNK | | | | | |
| . | . | . | . | . | ALLCAP | | | | | |
| . | . | . | . | . | ALTONU | | | | | |
| . | . | . | . | . | SETVAR | | | | | |
| . | . | . | VDP1 | | | | | | | |
| . | . | TRELIEF | | | | | | | | |
| . | . | . | TERAVG | | | | | | | |
| . | . | VWIDTH | | | | | | | | |
| . | . | CTINIT | | | | | | | | |
| . | . | . | INPTER | | | | | | | |
| . | . | . | . | KLOSE | | | | | | |
| . | . | . | INPREC | | | | | | | |
| . | . | NUMPR1 | | | | | | | | |
| . | . | RESTARTQ | | | | | | | | |
| . | . | . | INCR | | | | | | | |
| . | . | . | JULDAY | | | | | | | |
| . | . | TIBLSET | | | | | | | | |
| . | . | WRIVL | | | | | | | | |
| . | . | MFLXSET | | | | | | | | |
| . | . | MFLXHDR | | | | | | | | |
| . | . | MBALHDR | | | | | | | | |
| . | . | WROUT1 | | | | | | | | |
| . | . | . | JULDAY | | | | | | | |
| . | . | . | WRINT | | | | | | | |
| . | . | . | XTRACTI | | | | | | | |
| . | . | . | WRDAT | | | | | | | |
| . | COMP | | | | | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|---|---|---|---|---|---|---|---|---|---|---|
| . | . | JULDAY | | | | | | | | |
| . | . | RESTARTI | | | | | | | | |
| . | . | . | INCR | | | | | | | |
| . | . | . | RDI1D | | | | | | | |
| . | . | . | RDR1D | | | | | | | |
| . | . | . | RDR2D | | | | | | | |
| . | . | . | RDR3D | | | | | | | |
| . | . | . | RDQA | | | | | | | |
| . | . | RDMET | | | | | | | | |
| . | . | . | RDR2D | | | | | | | |
| . | . | . | NEXTFIL | | | | | | | |
| . | . | . | . | MET1 | | | | | | |
| . | . | . | . | . | YR4 | | | | | |
| . | . | . | . | . | RDR1D | | | | | |
| . | . | . | . | . | METQA | | | | | |
| . | . | . | . | . | RDR2D | | | | | |
| . | . | . | . | . | RDI2D | | | | | |
| . | . | . | . | . | OUT | | | | | |
| . | . | . | . | . | . | WRT | | | | |
| . | . | . | . | . | . | WRT2 | | | | |
| . | . | . | RDI2D | | | | | | | |
| . | . | . | RDR1D | | | | | | | |
| . | . | . | RDI1D | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | . | OUT | | | | | | | |
| . | . | . | . | WRT | | | | | | |
| . | . | . | . | WRT2 | | | | | | |
| . | . | RDISC | | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | . | JULDAY | | | | | | | |
| . | . | . | INCR | | | | | | | |
| . | . | . | GRDAY | | | | | | | |
| . | . | . | INITR2D | | | | | | | |
| . | . | . | POWLAW | | | | | | | |
| . | . | . | INITR2D | | | | | | | |
| . | . | . | INITI2D | | | | | | | |
| . | . | . | INITAR | | | | | | | |
| . | . | . | INITAI | | | | | | | |
| . | . | . | OUT | | | | | | | |
| . | . | . | . | WRT | | | | | | |
| . | . | . | . | WRT2 | | | | | | |
| . | . | RDPLM | | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | . | JULDAY | | | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | INCR | | | | | | | |
| . | . | . | GRDAY | | | | | | | |
| . | . | . | STAB2L | | | | | | | |
| . | . | . | POWLAW | | | | | | | |
| . | . | . | INITR2D | | | | | | | |
| . | . | . | INITI2D | | | | | | | |
| . | . | . | INITAR | | | | | | | |
| . | . | . | INITAI | | | | | | | |
| . | . | . | OUT | | | | | | | |
| . | . | . | . | WRT | | | | | | |
| . | . | . | . | WRT2 | | | | | | |
| . | . | RDMET4 | | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | . | JULDAY | | | | | | | |
| . | . | . | INCR | | | | | | | |
| . | . | . | GRDAY | | | | | | | |
| . | . | . | INITR2D | | | | | | | |
| . | . | . | LSTAB | | | | | | | |
| . | . | . | RDPROF | | | | | | | |
| . | . | . | . | YR4 | | | | | | |
| . | . | . | . | JULDAY | | | | | | |
| . | . | . | . | INCR | | | | | | |
| . | . | . | . | GRDAY | | | | | | |
| . | . | . | XTPRF | | | | | | | |
| . | . | . | . | PSIM | | | | | | |
| . | . | . | STPRF | | | | | | | |
| . | . | . | INITI2D | | | | | | | |
| . | . | . | INITAR | | | | | | | |
| . | . | . | INITAI | | | | | | | |
| . | . | . | OUT | | | | | | | |
| . | . | . | . | WRT | | | | | | |
| . | . | . | . | WRT2 | | | | | | |
| . | . | RDPROF | | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | . | JULDAY | | | | | | | |
| . | . | . | INCR | | | | | | | |
| . | . | . | GRDAY | | | | | | | |
| . | . | SUNDATA | | | | | | | | |
| . | . | RDOZ | | | | | | | | |
| . | . | . | YR4 | | | | | | | |
| . | . | INCR | | | | | | | | |
| . | . | GRDAY | | | | | | | | |
| . | . | INITR2D | | | | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|---|---|---|---|---|---|---|---|---|---|---|
| . | . | MFLXINI | | | | | | | | |
| . | . | . | INITR2D | | | | | | | |
| . | . | MBALINI | | | | | | | | |
| . | . | GETPRFP | | | | | | | | |
| . | . | . | XTPRF | | | | | | | |
| . | . | . | . | PSIM | | | | | | |
| . | . | HDUN | | | | | | | | |
| . | . | GETPRFM | | | | | | | | |
| . | . | SPLIT | | | | | | | | |
| . | . | . | ROLLDN | | | | | | | |
| . | . | . | . | SWAP | | | | | | |
| . | . | . | SWAP | | | | | | | |
| . | . | INITPUF | | | | | | | | |
| . | . | . | POINTS1 | | | | | | | |
| . | . | . | . | RLSMET | | | | | | |
| . | . | . | . | . | ZFIND | | | | | |
| . | . | . | . | . | WINDSET | | | | | |
| . | . | . | . | . | . | POWLAW | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | TURBSET | | | | | |
| . | . | . | . | . | . | SIGWV | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | PTLAPS | | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | VEMFAC | | | | | | |
| . | . | . | . | SETCSIG | | | | | | |
| . | . | . | . | STKTIP | | | | | | |
| . | . | . | . | PRFIN | | | | | | |
| . | . | . | . | PRFINSH | | | | | | |
| . | . | . | . | PTLAPS | | | | | | |
| . | . | . | . | . | XTPRF | | | | | |
| . | . | . | . | . | . | PSIM | | | | |
| . | . | . | . | PRFPP | | | | | | |
| . | . | . | . | PRM | | | | | | |
| . | . | . | . | DWSIGS | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |
| . | . | . | . | . | HEFTRAN | | | | | |
| . | . | . | . | . | . | SIGTY | | | | |
| . | . | . | . | . | . | . | XVY | | | |
| . | . | . | . | . | . | SIGTZ | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | . | . | . | . | XVZ | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | . | . | SIGTY | | | | | | |
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | . | PRSS | | | | | | |
| . | . | . | . | . | SSCM | | | | | |
| . | . | . | . | . | SSCB | | | | | |
| . | . | . | . | . | ROOT3 | | | | | |
| . | . | . | . | . | . | ROOT2 | | | | |
| . | . | . | . | ROLLDN | | | | | | |
| . | . | . | . | . | SWAP | | | | | |
| . | . | . | . | SWAP | | | | | | |
| . | . | . | . | INJECT | | | | | | |
| . | . | . | RDEM2 | | | | | | | |
| . | . | . | . | YR4 | | | | | | |
| . | . | . | POINTS2 | | | | | | | |
| . | . | . | . | RLSMET | | | | | | |
| . | . | . | . | . | ZFIND | | | | | |
| . | . | . | . | . | WINDSET | | | | | |
| . | . | . | . | . | . | POWLAW | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | TURBSET | | | | | |
| . | . | . | . | . | . | SIGWV | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | PTLAPS | | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | SETCSIG | | | | | | |
| . | . | . | . | STKTIP | | | | | | |
| . | . | . | . | PRFIN | | | | | | |
| . | . | . | . | PRFINSH | | | | | | |
| . | . | . | . | PTLAPS | | | | | | |
| . | . | . | . | . | XTPRF | | | | | |
| . | . | . | . | . | . | PSIM | | | | |
| . | . | . | . | PRFPP | | | | | | |
| . | . | . | . | PRM | | | | | | |
| . | . | . | . | DWSIGS | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | . | . | HEFTRAN | | | | | |
| . | . | . | . | . | . | SIGTY | | | | |
| . | . | . | . | . | . | . | XVY | | | |
| . | . | . | . | . | . | SIGTZ | | | | |
| . | . | . | . | . | . | . | XVZ | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | . | . | SIGTY | | | | | | |
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | . | PRSS | | | | | | |
| . | . | . | . | . | SSCM | | | | | |
| . | . | . | . | . | SSCB | | | | | |
| . | . | . | . | . | ROOT3 | | | | | |
| . | . | . | . | . | . | ROOT2 | | | | |
| . | . | . | . | ROLLDN | | | | | | |
| . | . | . | . | . | SWAP | | | | | |
| . | . | . | . | SWAP | | | | | | |
| . | . | . | . | INJECT | | | | | | |
| . | . | . | LINES1 | | | | | | | |
| . | . | . | . | RLSMET | | | | | | |
| . | . | . | . | . | ZFIND | | | | | |
| . | . | . | . | . | WINDSET | | | | | |
| . | . | . | . | . | . | POWLAW | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | TURBSET | | | | | |
| . | . | . | . | . | . | SIGWV | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | PTLAPS | | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | VEMFAC | | | | | | |
| . | . | . | . | SETCSIG | | | | | | |
| . | . | . | . | SIGTY | | | | | | |
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | HEFTRAN | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | . | . | SETLINE | | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | . | . | ROOT3 | | | | | |
| . | . | . | . | . | . | ROOT2 | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | . | ROLLDN | | | | | | |
| . | . | . | . | . | SWAP | | | | | |
| . | . | . | . | SWAP | | | | | | |
| . | . | . | . | INJECT | | | | | | |
| . | . | . | RDEM5 | | | | | | | |
| . | . | . | . | YR4 | | | | | | |
| . | . | . | LN2FILL | | | | | | | |
| . | . | . | LINES2 | | | | | | | |
| . | . | . | . | RLSMET | | | | | | |
| . | . | . | . | . | ZFIND | | | | | |
| . | . | . | . | . | WINDSET | | | | | |
| . | . | . | . | . | . | POWLAW | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | TURBSET | | | | | |
| . | . | . | . | . | . | SIGWV | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | PTLAPS | | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | SETCSIG | | | | | | |
| . | . | . | . | SIGTY | | | | | | |
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | HEFTRAN | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | . | . | SETLINE | | | | | | |
| . | . | . | . | . | ROOT3 | | | | | |
| . | . | . | . | . | . | ROOT2 | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | . | ROLLDN | | | | | | |
| . | . | . | . | . | SWAP | | | | | |
| . | . | . | . | SWAP | | | | | | |
| . | . | . | . | INJECT | | | | | | |
| . | . | . | AREAS1 | | | | | | | |
| . | . | . | . | RLSMET | | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | . | . | ZFIND | | | | | |
| . | . | . | . | . | WINDSET | | | | | |
| . | . | . | . | . | . | POWLAW | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | TURBSET | | | | | |
| . | . | . | . | . | . | SIGWV | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | PTLAPS | | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | VEMFAC | | | | | | |
| . | . | . | . | ROLLDN | | | | | | |
| . | . | . | . | . | SWAP | | | | | |
| . | . | . | . | SYAREA | | | | | | |
| . | . | . | . | SWAP | | | | | | |
| . | . | . | . | INJECT | | | | | | |
| . | . | . | RDEM3 | | | | | | | |
| . | . | . | . | YR4 | | | | | | |
| . | . | . | QUADAREA | | | | | | | |
| . | . | . | AREAS2 | | | | | | | |
| . | . | . | . | RLSMET | | | | | | |
| . | . | . | . | . | ZFIND | | | | | |
| . | . | . | . | . | WINDSET | | | | | |
| . | . | . | . | . | . | POWLAW | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | TURBSET | | | | | |
| . | . | . | . | . | . | SIGWV | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | PTLAPS | | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | NUMMET | | | | | | |
| . | . | . | . | . | POWLAW | | | | | |
| . | . | . | . | NUMRISE | | | | | | |
| . | . | . | . | . | ZMET | | | | | |
| . | . | . | . | . | LUMP | | | | | |
| . | . | . | . | . | RATE | | | | | |
| . | . | . | . | . | MARCHING | | | | | |
| . | . | . | . | . | UNLUMP | | | | | |
| . | . | . | . | SYAREA | | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | . | ROLLDN | | | | | | |
| . | . | . | . | . | SWAP | | | | | |
| . | . | . | . | SWAP | | | | | | |
| . | . | . | . | INJECT | | | | | | |
| . | . | . | VOLS1 | | | | | | | |
| . | . | . | . | RLSMET | | | | | | |
| . | . | . | . | . | ZFIND | | | | | |
| . | . | . | . | . | WINDSET | | | | | |
| . | . | . | . | . | . | POWLAW | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | TURBSET | | | | | |
| . | . | . | . | . | . | SIGWV | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | PTLAPS | | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | VEMFAC | | | | | | |
| . | . | . | . | ROLLDN | | | | | | |
| . | . | . | . | . | SWAP | | | | | |
| . | . | . | . | SWAP | | | | | | |
| . | . | . | . | INJECT | | | | | | |
| . | . | . | RDEM4 | | | | | | | |
| . | . | . | . | YR4 | | | | | | |
| . | . | . | . | RDEMREC | | | | | | |
| . | . | . | VOLS2 | | | | | | | |
| . | . | . | . | RLSMET | | | | | | |
| . | . | . | . | . | ZFIND | | | | | |
| . | . | . | . | . | WINDSET | | | | | |
| . | . | . | . | . | . | POWLAW | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | TURBSET | | | | | |
| . | . | . | . | . | . | SIGWV | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | . | PTLAPS | | | | | |
| . | . | . | . | . | . | XTPRF | | | | |
| . | . | . | . | . | . | . | PSIM | | | |
| . | . | . | . | ROLLDN | | | | | | |
| . | . | . | . | . | SWAP | | | | | |
| . | . | . | . | SWAP | | | | | | |
| . | . | . | . | INJECT | | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | ZFIND | | | | | | | | |
| . | . | PUFFDZ | | | | | | | | |
| . | . | ADVECT | | | | | | | | |
| . | . | . | POWLAW | | | | | | | |
| . | . | . | ADVWND | | | | | | | |
| . | . | . | . | ZFIND | | | | | | |
| . | . | . | XTPRF | | | | | | | |
| . | . | . | . | PSIM | | | | | | |
| . | . | MBALSUM | | | | | | | | |
| . | . | RISEWIND | | | | | | | | |
| . | . | ADVWND | | | | | | | | |
| . | . | . | ZFIND | | | | | | | |
| . | . | GETOZ | | | | | | | | |
| . | . | . | FINDR | | | | | | | |
| . | . | TIBLON | | | | | | | | |
| . | . | TIBLGRO | | | | | | | | |
| . | . | EXMET | | | | | | | | |
| . | . | . | FINDR | | | | | | | |
| . | . | . | FINDI | | | | | | | |
| . | . | VMASS | | | | | | | | |
| . | . | TURBSET | | | | | | | | |
| . | . | . | SIGWV | | | | | | | |
| . | . | . | XTPRF | | | | | | | |
| . | . | . | . | PSIM | | | | | | |
| . | . | PDFVARS | | | | | | | | |
| . | . | PTLAPS | | | | | | | | |
| . | . | . | XTPRF | | | | | | | |
| . | . | . | . | PSIM | | | | | | |
| . | . | SETPUF | | | | | | | | |
| . | . | . | SETCSIG | | | | | | | |
| . | . | . | SIGTY | | | | | | | |
| . | . | . | . | XVY | | | | | | |
| . | . | . | HEFTRAN | | | | | | | |
| . | . | . | . | SIGTY | | | | | | |
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | WALLTRAP | | | | | | | |
| . | . | . | SIGTZ | | | | | | | |
| . | . | . | . | XVZ | | | | | | |
| . | . | . | CTADJ2 | | | | | | | |
| . | . | . | . | GETELEV | | | | | | |
| . | . | SETSLG | | | | | | | | |
| . | . | . | SETCSIG | | | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|---|---|---|---|---|---|---|---|---|---|---|
| . | . | . | SIGTY | | | | | | | |
| . | . | . | . | XVY | | | | | | |
| . | . | . | HEFTRAN | | | | | | | |
| . | . | . | . | SIGTY | | | | | | |
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | SIGTZ | | | | | | | |
| . | . | . | . | XVZ | | | | | | |
| . | . | . | CTADJ2 | | | | | | | |
| . | . | . | . | GETELEV | | | | | | |
| . | . | . | WALLTRAP | | | | | | | |
| . | . | CHEM | | | | | | | | |
| . | . | . | CHEMTF | | | | | | | |
| . | . | . | . | CHEMII | | | | | | |
| . | . | . | . | CHEMEQ | | | | | | |
| . | . | . | . | . | TRPF | | | | | |
| . | . | . | CHEMRIV | | | | | | | |
| . | . | WET | | | | | | | | |
| . | . | DRY | | | | | | | | |
| . | . | . | VDCOMP | | | | | | | |
| . | . | . | . | VDP | | | | | | |
| . | . | . | VCBAR | | | | | | | |
| . | . | . | . | GETELEV | | | | | | |
| . | . | . | . | CTADJ | | | | | | |
| . | . | . | . | VCOUP | | | | | | |
| . | . | TRACK | | | | | | | | |
| . | . | MFLXCMP | | | | | | | | |
| . | . | CALCPF | | | | | | | | |
| . | . | . | PFSCRN | | | | | | | |
| . | . | . | PUFRECS | | | | | | | |
| . | . | . | . | SLGFRAC | | | | | | |
| . | . | . | . | SETCSIG | | | | | | |
| . | . | . | . | DWSIGS | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |
| . | . | . | . | . | HEFTRAN | | | | | |
| . | . | . | . | . | . | SIGTY | | | | |
| . | . | . | . | . | . | . | XVY | | | |
| . | . | . | . | . | . | SIGTZ | | | | |
| . | . | . | . | . | . | . | XVZ | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | . | . | PRSS | | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | . | . | SSCM | | | | | |
| . | . | . | . | . | SSCB | | | | | |
| . | . | . | . | . | ROOT3 | | | | | |
| . | . | . | . | . | . | ROOT2 | | | | |
| . | . | . | . | GRISE | | | | | | |
| . | . | . | . | . | PRM | | | | | |
| . | . | . | . | . | PRB | | | | | |
| . | . | . | . | . | PRSHEAR | | | | | |
| . | . | . | . | . | PRTAB | | | | | |
| . | . | . | . | . | PRBL | | | | | |
| . | . | . | . | . | . | PRTAB | | | | |
| . | . | . | . | STKTIP | | | | | | |
| . | . | . | . | SIGTY | | | | | | |
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | HEFTRAN | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | . | CTADJ | | | | | | |
| . | . | . | . | PUFFCT2 | | | | | | |
| . | . | . | . | GETELEV | | | | | | |
| . | . | . | PDFPATH | | | | | | | |
| . | . | . | PFSAMP | | | | | | | |
| . | . | . | ASDF | | | | | | | |
| . | . | | | .ERFDIF | | | | | | |
| . | . | . | . | . | ERF | | | | | |
| . | . | . | . | . | ERFC | | | | | |
| . | . | CALCSL | | | | | | | | |
| . | . | . | SLGXLIM | | | | | | | |
| . | . | . | . | VECMAX | | | | | | |
| . | . | . | . | VECMIN | | | | | | |
| . | . | . | SETCSIG | | | | | | | |
| . | . | . | AREAINT | | | | | | | |
| . | . | . | . | XY2UWCW | | | | | | |
| . | . | . | . | EXTREME | | | | | | |
| . | . | . | . | VECMAX | | | | | | |
| . | . | . | . | VECMIN | | | | | | |
| . | . | . | . | CWYVALS | | | | | | |
| . | . | . | . | CPQROMB | | | | | | |
| . | . | . | . | . | CPTRAP | | | | | |
| . | . | . | . | . | . | RECSPEC0 | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|---|---|---|---|---|---|---|---|---|---|---|
| . | . | . | . | . | . | . | HEFTRAN | | | |
| . | . | . | . | . | . | . | . | SIGTY | | |
| . | . | . | . | . | . | . | . | . | XVY | |
| . | . | . | . | . | . | . | . | SIGTZ | | |
| . | . | . | . | . | . | . | . | . | XVZ | |
| . | . | . | . | . | . | . | SIGTY | | | |
| . | . | . | . | . | . | . | . | XVY | | |
| . | . | . | . | . | . | . | SIGTZ | | | |
| . | . | . | . | . | . | . | . | XVZ | | |
| . | . | . | . | . | . | . | GRISE | | | |
| . | . | . | . | . | . | . | . | PRM | | |
| . | . | . | . | . | . | . | . | PRB | | |
| . | . | . | . | . | . | . | . | PRSHEAR | | |
| . | . | . | . | . | . | . | . | PRTAB | | |
| . | . | . | . | . | . | . | . | PRBL | | |
| . | . | . | . | . | . | . | . | . | PRTAB | |
| . | . | . | . | . | . | . | CTADJ | | | |
| . | . | . | . | . | . | LSSLINT | | | | |
| . | . | . | . | . | . | . | CWYVALS | | | |
| . | . | . | . | . | . | . | PDFPATH | | | |
| . | . | . | . | . | . | . | XERFDIF | | | |
| . | . | . | . | . | . | . | . | ERF | | |
| . | . | . | . | . | . | . | ERF | | | |
| . | . | . | . | . | . | . | ERFDIF | | | |
| . | . | . | . | . | . | . | . | ERF | | |
| . | . | . | . | . | . | . | . | ERFC | | |
| . | . | . | . | . | . | . | VCOUP | | | |
| . | . | . | . | . | . | POLINT | | | | |
| . | . | . | SLGRECS | | | | | | | |
| . | . | . | . | SLGFRAC | | | | | | |
| . | . | . | . | SETCSIG | | | | | | |
| . | . | . | . | DWSIGS | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |
| . | . | . | . | . | HEFTRAN | | | | | |
| . | . | . | . | . | . | SIGTY | | | | |
| . | . | . | . | . | . | . | XVY | | | |
| . | . | . | . | . | . | SIGTZ | | | | |
| . | . | . | . | . | . | . | XVZ | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | . | . | PRSS | | | | | | |
| . | . | . | . | . | SSCM | | | | | |
| . | . | . | . | . | SSCB | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | . | . | ROOT3 | | | | | |
| . | . | . | . | . | . | ROOT2 | | | | |
| . | . | . | . | GRISE | | | | | | |
| . | . | . | . | . | PRM | | | | | |
| . | . | . | . | . | PRB | | | | | |
| . | . | . | . | . | PRSHEAR | | | | | |
| . | . | . | . | . | PRTAB | | | | | |
| . | . | . | . | . | PRBL | | | | | |
| . | . | . | . | . | . | PRTAB | | | | |
| . | . | . | . | SIGTY | | | | | | |
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | HEFTRAN | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | . | STKTIP | | | | | | |
| . | . | . | . | CTADJ | | | | | | |
| . | . | . | . | SLUGCT2 | | | | | | |
| . | . | . | . | . | SLGFRAC | | | | | |
| . | . | . | . | GETELEV | | | | | | |
| . | . | . | PDFPATH | | | | | | | |
| . | . | . | SLUGAVE | | | | | | | |
| . | . | . | . | SLGFRAC | | | | | | |
| . | . | . | . | VCOUP | | | | | | |
| . | . | . | . | ERF | | | | | | |
| . | . | . | . | XERFDIF | | | | | | |
| . | . | . | . | . | ERF | | | | | |
| . | . | . | . | SLUGINT | | | | | | |
| . | . | . | . | . | SLGFRAC | | | | | |
| . | . | . | . | . | VCOUP | | | | | |
| . | . | . | . | . | ERF | | | | | |
| . | . | . | . | . | ERFDIF | | | | | |
| . | . | . | . | . | . | ERF | | | | |
| . | . | . | . | . | . | ERFC | | | | |
| . | . | . | . | . | ASDF | | | | | |
| . | . | . | . | . | . | ERFDIF | | | | |
| . | . | . | . | . | . | . | ERF | | | |
| . | . | . | . | . | . | . | ERFC | | | |
| . | . | . | . | SLGTLIM | | | | | | |
| . | . | . | . | . | ROOT2 | | | | | |
| . | . | . | . | . | ROOT3 | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | . | . | . | ROOT2 | | | | |
| . | . | . | . | . | FINLINI | | | | | |
| . | . | . | . | ROMBTIN | | | | | | |
| . | . | . | . | . | TRAPSL | | | | | |
| . | . | . | . | . | . | SLUGSNP | | | | |
| . | . | . | . | . | . | . | SLGFRAC | | | |
| . | . | . | . | . | . | . | VCOUP | | | |
| . | . | . | . | . | . | . | ERF | | | |
| . | . | . | . | . | . | . | ASDF | | | |
| . | . | . | . | . | . | . | . | ERFDIF | | |
| . | . | . | . | . | . | . | . | . | ERF | |
| . | . | . | . | . | . | . | . | . | ERFC | |
| . | . | . | . | . | POLINT | | | | | |
| . | . | PFSCRN | | | | | | | | |
| . | . | PUFRECS | | | | | | | | |
| . | . | . | SLGFRAC | | | | | | | |
| . | . | . | SETCSIG | | | | | | | |
| . | . | . | DWSIGS | | | | | | | |
| . | . | . | . | SIGTY | | | | | | |
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | HEFTRAN | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | PRSS | | | | | | | |
| . | . | . | . | SSCM | | | | | | |
| . | . | . | . | SSCB | | | | | | |
| . | . | . | . | ROOT3 | | | | | | |
| . | . | . | . | . | ROOT2 | | | | | |
| . | . | . | GRISE | | | | | | | |
| . | . | . | . | PRM | | | | | | |
| . | . | . | . | PRB | | | | | | |
| . | . | . | . | PRSHEAR | | | | | | |
| . | . | . | . | PRTAB | | | | | | |
| . | . | . | . | PRBL | | | | | | |
| . | . | . | . | . | PRTAB | | | | | |
| . | . | . | STKTIP | | | | | | | |
| . | . | . | SIGTY | | | | | | | |
| . | . | . | . | XVY | | | | | | |
| . | . | . | HEFTRAN | | | | | | | |
| . | . | . | . | SIGTY | | | | | | |

# APPENDIX A
## Subroutine/Function Calling Structure - Tree Diagram

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | SIGTZ | | | | | | | |
| . | . | . | . | XVZ | | | | | | |
| . | . | . | CTADJ | | | | | | | |
| . | . | . | PUFFCT2 | | | | | | | |
| . | . | . | GETELEV | | | | | | | |
| . | . | CTSG | | | | | | | | |
| . | . | . | CTPAR | | | | | | | |
| . | . | . | . | ROTATE | | | | | | |
| . | . | . | . | KLOSE | | | | | | |
| . | . | . | . | XINTRP | | | | | | |
| . | . | . | . | SIGMA | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | . | . | AXIS | | | | | | |
| . | . | . | . | MUNU | | | | | | |
| . | . | . | . | HILROT | | | | | | |
| . | . | . | . | SPEED | | | | | | |
| . | . | . | . | PATH | | | | | | |
| . | . | . | . | . | R1MACH | | | | | |
| . | . | . | . | . | . | XERMSG | | | | |
| . | . | . | . | . | . | . | J4SAVE | | | |
| . | . | . | . | . | . | . | XERPRN | | | |
| . | . | . | . | . | . | . | . | XGETUA | | |
| . | . | . | . | . | . | . | . | . | J4SAVE | |
| . | . | . | . | . | . | . | XERHLT | | | |
| . | . | . | . | . | . | . | XERSVE | | | |
| . | . | . | . | . | . | . | . | XGETUA | | |
| . | . | . | . | . | . | . | . | . | J4SAVE | |
| . | . | . | . | . | . | . | XERCNT | | | |
| . | . | . | . | . | . | . | FDUMP | | | |
| . | . | . | . | . | HILHGT | | | | | |
| . | . | . | . | . | FLOPUFF | | | | | |
| . | . | . | . | . | . | ERF | | | | |
| . | . | . | . | . | . | SPEED | | | | |
| . | . | . | . | . | XSETF | | | | | |
| . | . | . | . | . | . | J4SAVE | | | | |
| . | . | . | . | . | . | XERMSG (+) | | | | |
| . | . | . | . | . | SNSQE | | | | | |
| . | . | . | . | . | . | SNSQ | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | . | . | . | . | R1MACH | | | |
| . | . | . | . | . | . | . | . | XERMSG (+) | | |
| . | . | . | . | . | . | . | PATH0 | | | |
| . | . | . | . | . | . | . | . | HILHGT | | |
| . | . | . | . | . | . | . | . | FLOPUFF | | |
| . | . | . | . | . | . | . | . | . | ERF | |
| . | . | . | . | . | . | . | . | . | SPEED | |
| . | . | . | . | . | . | . | ENORM | | | |
| . | . | . | . | . | . | . | FDJAC1 | | | |
| . | . | . | . | . | . | . | . | R1MACH | | |
| . | . | . | . | . | . | . | . | . | XERMSG (+) | |
| . | . | . | . | . | . | . | . | PATH0 | | |
| . | . | . | . | . | . | . | . | . | HILHGT | |
| . | . | . | . | . | . | . | . | . | FLOPUFF | |
| . | . | . | . | . | . | . | . | . | . | ERF |
| . | . | . | . | . | . | . | . | . | . | SPEED |
| . | . | . | . | . | . | . | QRFAC | | | |
| . | . | . | . | . | . | . | . | R1MACH | | |
| . | . | . | . | . | . | . | . | . | XERMSG (+) | |
| . | . | . | . | . | . | . | . | ENORM | | |
| . | . | . | . | . | . | . | QFORM | | | |
| . | . | . | . | . | . | . | DOGLEG | | | |
| . | . | . | . | . | . | . | R1UPDT | | | |
| . | . | . | . | . | . | . | . | R1MACH | | |
| . | . | . | . | . | . | . | . | . | XERMSG (+) | |
| . | . | . | . | . | . | . | R1MPYQ | | | |
| . | . | . | . | . | . | XERMSG (+) | | | | |
| . | . | . | CTREC | | | | | | | |
| . | . | . | . | ROTATE | | | | | | |
| . | . | . | . | MUNU | | | | | | |
| . | . | . | . | IREG | | | | | | |
| . | . | . | PUFFC | | | | | | | |
| . | . | . | . | ERF | | | | | | |
| . | . | . | . | ERFDIF | | | | | | |
| . | . | . | . | . | ERF | | | | | |
| . | . | . | . | . | ERFC | | | | | |
| . | . | . | UPPER | | | | | | | |
| . | . | . | . | FCTY | | | | | | |
| . | . | . | . | . | TFAC | | | | | |
| . | . | . | . | FCTZ | | | | | | |
| . | . | . | . | . | TFAC | | | | | |
| . | . | . | . | QATR | | | | | | |
| . | . | . | . | FLOPUFF | | | | | | |
| . | . | . | . | . | ERF | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | . | . | SPEED | | | | | |
| . | . | . | . | BI | | | | | | |
| . | . | . | . | BJI | | | | | | |
| . | . | . | . | ERF | | | | | | |
| . | . | . | . | ERFDIF | | | | | | |
| . | . | . | . | . | ERF | | | | | |
| . | . | . | . | . | ERFC | | | | | |
| . | . | . | LOWER | | | | | | | |
| . | . | . | . | MUNU | | | | | | |
| . | . | . | . | BJIL | | | | | | |
| . | . | . | . | . | ERF | | | | | |
| . | . | . | . | BI | | | | | | |
| . | . | . | . | ERF | | | | | | |
| . | . | . | . | SIGMA | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | SLG2PUF | | | | | | | | |
| . | . | PLGRECS | | | | | | | | |
| . | . | . | SLGFRAC | | | | | | | |
| . | . | . | SETCSIG | | | | | | | |
| . | . | . | DWSIGS | | | | | | | |
| . | . | . | . | SIGTY | | | | | | |
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | HEFTRAN | | | | | | |
| . | . | . | . | . | SIGTY | | | | | |
| . | . | . | . | . | . | XVY | | | | |
| . | . | . | . | . | SIGTZ | | | | | |
| . | . | . | . | . | . | XVZ | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | PRSS | | | | | | | |
| . | . | . | . | SSCM | | | | | | |
| . | . | . | . | SSCB | | | | | | |
| . | . | . | . | ROOT3 | | | | | | |
| . | . | . | . | . | ROOT2 | | | | | |
| . | . | . | GRISE | | | | | | | |
| . | . | . | . | PRM | | | | | | |
| . | . | . | . | PRB | | | | | | |
| . | . | . | . | PRSHEAR | | | | | | |
| . | . | . | . | PRTAB | | | | | | |
| . | . | . | . | PRBL | | | | | | |
| . | . | . | . | . | PRTAB | | | | | |

| Lev0 | Lev1 | Lev2 | Lev3 | Lev4 | Lev5 | Lev6 | Lev7 | Lev8 | Lev9 | Lev10 |
|------|------|------|------|------|------|------|------|------|------|-------|
| . | . | . | STKTIP | | | | | | | |
| . | . | . | SIGTY | | | | | | | |
| . | . | . | . | XVY | | | | | | |
| . | . | . | HEFTRAN | | | | | | | |
| . | . | . | . | SIGTY | | | | | | |
| . | . | . | . | . | XVY | | | | | |
| . | . | . | . | SIGTZ | | | | | | |
| . | . | . | . | . | XVZ | | | | | |
| . | . | . | SIGTZ | | | | | | | |
| . | . | . | . | XVZ | | | | | | |
| . | . | OUTPUT | | | | | | | | |
| . | . | . | MFLXGRP | | | | | | | |
| . | . | . | COMPRS | | | | | | | |
| . | . | . | . | WRDAT | | | | | | |
| . | . | . | WRDAT | | | | | | | |
| . | . | . | XTRACT | | | | | | | |
| . | . | . | WRINT | | | | | | | |
| . | . | . | OUTSAM | | | | | | | |
| . | . | . | . | WRT | | | | | | |
| . | . | . | . | WRT2 | | | | | | |
| . | . | . | MFLXOUT | | | | | | | |
| . | . | . | MBALOUT | | | | | | | |
| . | . | RESTARTO | | | | | | | | |
| . | . | . | ROLLDN | | | | | | | |
| . | . | . | WRTI1D | | | | | | | |
| . | . | . | WRTR1D | | | | | | | |
| . | . | . | WRTR2D | | | | | | | |
| . | . | . | WRTR3D | | | | | | | |
| . | FIN | | | | | | | | | |
| . | . | DATETM | | | | | | | | |
| . | . | YR4C | | | | | | | | |
| . | . | JULDAY | | | | | | | | |
| . | . | DELTT | | | | | | | | |

APPENDIX A
Subroutine/Function Calling Table
(* indicates no routines called)

| SUBROUTINE | CALLED BY | CALLS |
|---|---|---|
| advect | comp | powlaw, advwnd, xtprf |
| advwnd | advect, comp | zfind |
| allcap | readin | * |
| altonu | readin | * |
| areaint | calcsl | xy2uwcw, extreme, cwyvals, cpqromb, vecmax, vecmin |
| areas1 | initpuf | r1smet, rolldn, syarea, swap, inject, vemfac |
| areas2 | initpuf | r1smet, rolldn, nummet, numrise, syarea, swap, inject |
| asdf | calcpf, slugint, slugsnp | erfdif |
| axis | ctpar | * |
| bi | lower, upper | * |
| bji | upper | * |
| bjil | lower | erf |
| calcpf | comp | asdf, pdfpath, pfscrn, pufrecs, pfsamp, vcoup |
| calcsl | comp | pdfpath, slgxlim, setcsig, areaint, slgrecs, slugave |
| chem | comp | chemtf, chemriv |
| chemeq | chemtf | trpf |
| chemi | setup | rdchem, rdhdoz, rdtioz, out, sslatlon |
| chemii | chemtf | * |
| chemriv | chem | * |
| chemtf | chem | chemii, chemeq |
| comline | setup | getcl |
| comp | main | restarti, initr2d, getprfp, hdun, getprfm, split, initpuf, julday, rdmet, rdisc, rdplm, rdmet4, rdsig, rdoz, rdprof, sundata, puffdz, zfind, advect, advwnd, risewind, turbset, exmet, ptlaps, getoz, tiblon, tiblgro, pdfvars vmass, setpuf, setslg, chem, wet, dry, calcpf, calcsl, pfscrn, pufrecs, ctsg, slg2puf, plgrecs, track, output, incr, grday, mbalini, mbalsum, mflxcmp, mflxini |
| comprs | output | wrdat |
| cpqromb | areaint | cptrap, polint |
| cptrap | cpqromb | recspec0, lsslint |
| ctadj | pufrecs, slgrecs, vcbar, rescpec0, calcpf | * |
| ctadj2 | setpuf, setslg | getelev |
| ctinit | setup | inpter, inprec |
| ctpar | ctsg | rotate, axis, munu, hilrot, path, klose, sigma, speed, xintrp |
| ctrec | ctsg | rotate, munu, ireg |
| ctsg | comp | ctpar, ctrec, puffc, upper, lower |
| cwyvals | areaint, lsslint | * |

| SUBROUTINE | CALLED BY | CALLS |
|---|---|---|
| date | datetm | * |
| datetm | fin, setup | date, time, etime |
| deblnk | readin | * |
| deltt | fin | * |
| dogleg | snsq | * |
| dry | comp | vdcomp, vcbar |
| dryi | setup | rdvd, vdp1 |
| dwsigs | pufrecs, slgrecs, plgrecs, points1, points2 | sigty, sigtz, heftran |
| elevi | setup | getelev |
| emqa | setup | qcheck |
| enorm | snsq, qrfac | * |
| erf | lsslint, pfsamp, bji, bjil, puffc, vdp1, flopuff, lower, upper, slugave, slugsnp, slugint, xerfdif, erfdif | * |
| erfc | erfdif | * |
| erfdif | lsslint, pfsamp, puffc, upper, slugint, slugsnp, asdf | erf, erfc |
| etime | datetm | * |
| exmet | comp | findr, findi |
| extreme | areaint | * |
| fcty | upper | tfac |
| fctz | upper | tfac |
| fdjac1 | snsq | r1mach |
| fdump | r1mach | * |
| filcase | readfn | * |
| fin | main | datetm, julday, deltt, yr4c |
| findi | exmet | * |
| findr | getoz, exmet | * |
| finlini | slgtlim | * |
| flopuff | path, path0, upper | erf, speed |
| getelev | ctadj2, elevi, vcbar, slgrecs, pufrecs | * |
| getcl | comline | * |
| getoz | comp | findr |
| getprfm | comp | * |
| getprfp | comp | xtprf |
| grday | met3, met4, rdplm, rdmet4, comp, rdprof, met2, rdisc | * |

| SUBROUTINE | CALLED BY | CALLS |
|---|---|---|
| grise | pufrecs, slgrecs, plgrecs, recspec0 | prm, prb, prshear, prtab, prbl |
| hdun | comp | * |
| heftran | pufrecs, slgrecs, plgrecs, recspec0, lines1, lines2, dwsigs, setpuf, setslg | sigty, sigtz |
| hilhgt | path, path0 | * |
| hilrot | ctpar | * |
| incr | rdmet4, met3, met4, rdplm, comp, rdprof, met2, rdisc, restarti, restartq | * |
| initai | rdisc, rdplm, rdmet4 | * |
| initar | rdisc, rdplm, rdmet4 | * |
| initi2d | met2, rdisc, met3, rdplm, met4, rdmet4 | * |
| initpuf | comp | points1, points2, rdem2, lines1, areas1, rdem3, quadarea, areas2, vols1, rdem4, vols2, rden5, ln2fill, lines2 |
| initr2d | comp, met2, rdisc, met3, met4, rdplm, rdmet4, mflxini | * |
| inject | areas1, areas2, vols1, vols2, points1, points2, lines1, lines2 | * |
| inprec | ctinit | * |
| inpter | ctinit | klose |
| ireg | ctrec | * |
| j4save | xermsg, xgetua, xsetf | * |
| julday | comp, fin, rdprof, met2, rdisc, rdplm, rdmet4, met3, met4, wrout1, restartq | * |
| klose | ctpar, inpter | * |
| lines1 | initpuf | rlsmet, setcsig, sigty, sigtz, heftran, setline, rolldn, swap, inject, vemfac |
| lines2 | initpuf | rlsmet, setcsig, sigty, sigtz, heftran, setline, rolldn, swap, inject |
| ln2fill | initpuf | * |
| lower | ctsg | munu, bjil, bi, erf, sigma |
| lsslint | cptrap | cwyvals, xerfdif, erf, erfdif, vcoup, pdfpath |
| lstab | rdmet4 | * |
| lump | numrise | * |
| marching | numrise | * |

| SUBROUTINE | CALLED BY | CALLS |
|---|---|---|
| mbalhdr | setup | * |
| mbalini | comp | * |
| mbalout | output | * |
| mbalsum | comp | * |
| met1 | setup, nextfil | rdr1d, rdr2d, metqa, out, rdi2d, yr4 |
| met2 | setup | julday, incr, grday, initr2d, out, initi2d, yr4 |
| met3 | setup | julday, incr, grday, initr2d, out, initi2d, yr4 |
| met4 | setup | julday, incr, grday, initr2d, out, initi2d, yr4 |
| metqa | met1 | * |
| mflxcmp | comp | * |
| mflxgrp | output | * |
| mflxhdr | setup | * |
| mflxini | comp | initr2d |
| mflxout | output | * |
| mflxset | setup | * |
| munu | ctpar, ctrec, lower | * |
| nextfil | rdmet | met1 |
| nummet | areas2 | powlaw |
| numpr1 | setup | * |
| numrise | areas2 | zmet, lump, rate, marching, unlump |
| openot | setup | openab |
| openab | openot | * |
| out | chem, met1, rdmet, met2, met3, met4, rdplm, rdisc, rdmet4, chemi | wrt, wrt2 |
| output | comp | comprs, wrdat, xtract, wrint, outsam, mbalout, mflxgrp, mflxout |
| outsam | output | wrt, wrt2 |
| path | ctpar | flopuff, xsetf, snsqe, hilhgt, r1mach |
| path0 | snsq, fdjac1 | flopuff, hilhgt |
| pdfpath | calcpf, lsslint, slgrecs | * |
| pdfvars | comp | * |
| pfsamp | calcpf | * |
| pfscrn | calcpf, comp | * |
| plgrecs | comp | setcsig, dwsigs, prss, grise, stktip, heftran, sigty, sigtz, slgfrac |
| points1 | initpuf | rlsmet, rolldn, setcsig, stktip, prfin, prfinish, ptlaps, prfpp, prm, dwsigs, sigtz, sigty, prss, swap, inject, vemfac |

| SUBROUTINE | CALLED BY | CALLS |
|---|---|---|
| points2 | initpuf | rlsmet, rolldn, setcsig, stktip, prfin, prfinish, ptlaps, prfpp, prm, dwsigs, sigtz, sigty, prss, swap, inject |
| polint | cpqromb, rombtin | * |
| powlaw | advect, rdisc, rdplm, windset, nummet | * |
| prb | grise | * |
| prbl | grise | prtab |
| prfin | points1, points2 | * |
| prfinsh | points1, points2 | * |
| prfpp | points1, points2 | * |
| prm | points1, points2, grise | * |
| prshear | grise | * |
| prss | pufrecs, slgrecs, plgrecs, points1, points2 | sscm, sscb, root3 |
| prtab | grise, prbl | * |
| psim | rdplm, xtprf | * |
| ptlaps | comp, points1, points2, rlsmet | xtprf |
| puffc | ctsg | erf, erfdif |
| puffct2 | pufrecs | * |
| puffdz | comp | * |
| pufrecs | calcpf, comp | setcsig, dwsigs, prss, grise, stktip, heftran, sigty, sigtz, ctadj, slgfrac, puffct2 |
| qainp | readcf | * |
| qatr | upper | * |
| qayr4 | readcf | * |
| qcheck | emqa | * |
| qform | snsq | * |
| qrfac | snsq | enorm, r1macha |
| quadarea | initpuf, readcf | triarea |
| r1mach | path, snsq, fdjac1, qrfac, r1updt | xermsg |
| r1mpyq | snsq | * |
| r1updt | snsq | r1mach |
| rate | numrise | * |
| rdchem | chemi | readin |
| rdem2 | initpuf | yr4 |
| rdem3 | initpuf | yr4 |
| rdem4 | initpuf | rdemrec, yr4 |

Subroutine/Function Calling Table
(* indicates no routines called)

| SUBROUTINE | CALLED BY | CALLS |
|---|---|---|
| rdem5 | initpuf | yr4 |
| rdemrec | rdem4 | * |
| rdhdem2 | setup | yr4 |
| rdhdem3 | setup | yr4 |
| rdhdem4 | setup | yr4 |
| rdhdem5 | setup, initpuf | yr4 |
| rdhdoz | chemi | yr4 |
| rdi1d | rdmet, restarti | * |
| rdi2d | met1, rdmet | * |
| rdisc | comp | julday, incr, grday, init2d, powlaw, initar, initai, out, initi2d, initr2d, yr4 |
| rdmet | comp | rdr1d, rdr2d, out, rdi1d, rdi2d, yr4 |
| rdmet4 | comp | julday, incr, grday, initr2d, xtprf, stprf, initar, initai, out, initi2d, lstab, rdprof, yr4, nextfil |
| rdoz | comp | yr4 |
| rdplm | comp | julday, incr, grday, stab21, powlaw, initr2d, initar, initai, out, initi2d, yr4 |
| rdprof | comp, rdmet4 | julday, incr, grday, yr4 |
| rdqa | restarti | * |
| rdr1d | met1, rdmet, restarti | * |
| rdr2d | met1, rdmet, restarti | * |
| rdr3d | restarti | * |
| rdtiem2 | setup | * |
| rdtiem3 | setup | * |
| rdtiem5 | setup | * |
| rdtioz | chem | * |
| rdvd | dryi | readin |
| readcf | setup | readfn, readin, quadarea, qainp, qayr4, yr4c, wrivl |
| readfn | readcf | readin, filcase |
| readin | rdchem, rdvd, readcf, readfn | deblnk, allcap, altonu, setvar |
| recspec0 | cptrap | heftran, sigty, sigtz, grise, ctadj |
| restarti | comp | incr, rdi1d, rdr1d, rdr2d, rdr3d, rdqa |
| restarto | comp | rolldn, wrti1d, wrtr1d, wrtr2d, wrtr3d |
| restartq | setup | incr, julday |
| risewind | comp | * |
| rlsmet | areas1, areas2, vols1, vols2, points1, points2, lines1, lines2 | zfind, windset, turbset, ptlaps |

| SUBROUTINE | CALLED BY | CALLS |
|---|---|---|
| rolldn | split, areas1, areas2, points1, points2, vols1, vols2, lines1, lines2, restarto | swap |
| rombtin | slugave | trapsl, polint |
| root2 | slgtlim, root3 | * |
| root3 | setline, slgtlim, prss | root2 |
| rotate | ctpar, ctrec | * |
| setcom | setup | * |
| setcsig | calcpf, pufrecs, calcsl, slgrecs, plgrecs, points1, points2, lines1, lines2, setpuf, setslg | * |
| setline | lines1, lines2 | root3 |
| setpuf | comp | setcsig, sigty, sigtz, heftran, ctadj2, walltrap |
| setslg | comp | setcsig, sigty, sigtz, heftran, ctadj2, walltrap |
| setup | main | met1, met2, met3, met4, rdhdem2, rdhdem3, rdhdem4, rdhdem5, chemi, datetm, comline, readcf, wrfiles, setcom, openot, emqa, rdtiem2, rdtiem3, rdtiem5, elevi, sigset, slugi, dryi, ctinit, numpr1, wrout1, tiblset, trelief, vwidth, restartq, mbalhdr, mflxhdr, mflxset, wrivl |
| setvar | readin | * |
| sigma | ctpar, lower, qrfac | sigty, sigtz |
| sigset | setup | * |
| sigty | pufrecs, slgrecs, plgrecs, heftran, recspec0, points1, points2, lines1, lines2, dwsigs, sigma, setpuf, setslg, calcpf | xvy |
| sigtz | pufrecs, slgrecs, plgrecs, heftran, recspec0, points1, points2, lines1, lines2, dwsigs, sigma, setpuf, setslg, calcpf | xvz |
| sigwv | turbset | * |
| slg2puf | comp | * |
| slgfrac | calcpf, pufrecs, plgrecs, slgrecs, slugct2, slugave, slugint, slugsnp | * |
| slgrecs | calcsl | setcsig, dwsigs, prss, grise, heftran, sigty, sigtz, stktip, ctadjslgfrac, slugct2 |
| slgtlim | slugave | root2, root3, finlini |
| slgxlim | calcsl | vecmax, vecmin |

| SUBROUTINE | CALLED BY | CALLS |
|---|---|---|
| slugave | calcsl, slgrecs | xerfdif, slugint, slgtlim, rombtin, erf, vcoup, slgfrac |
| slugct2 | slgrecs | slugfrac |
| slugi | setup | * |
| slugint | slugave | erf, erfdif, vcoup, asdf, slgfrac |
| slugsnp | trapsl | erf, vcoup, asdf, slgfrac, erfdif |
| snsq | snsqe | fdjac1, qrfac, qform, dogleg, r1updt, r1mpyq, enorm, r1mach, path0 |
| snsqe | path | snsq, xermsg |
| speed | ctpar, Flopuff | * |
| split | comp | rolldn, swap |
| sscb | prss | * |
| sscm | prss | * |
| sslatlon | chemi | * |
| stab2l | rdplm | * |
| stktip | pufrecs, slgrecs, plgrecs, points1, points2, calcpf | * |
| stprf | rdmet4 | * |
| sundata | comp | * |
| swap | split, areas1, areas2, points1, points2, vols1, vols2, lines1, lines2, rolldn | * |
| syarea | areas1, areas2 | * |
| teravg | trelief | * |
| tfac | fcty, fctz | * |
| tiblgro | comp | * |
| tiblon | comp | * |
| tiblset | setup | * |
| time | datetm | * |
| track | comp | * |
| trapsl | rombtin | slugsnp |
| trelief | setup | teravg |
| triarea | quadarea | * |
| trpf | chemeq | * |
| turbset | comp, rlsmet | sigwv, xtprf |
| under0 | main | * |
| unlump | numrise | * |
| upper | ctsg | qatr, flopuff, bi, bji, erf, erfdif, fcty, fctz |
| vcbar | dry | getelev, ctadj, vcoup |

| SUBROUTINE | CALLED BY | CALLS |
|------------|-----------|-------|
| vcoup | lsslint, calcpf, slugsnp, slugint, slugave, vcbar | * |
| vdcomp | dry | vdp |
| vdp | vdcomp | * |
| vdp1 | dryi | erf |
| vecmax | areaint, slgxlim | * |
| vecmin | areaint, slgxlim | * |
| vemfac | areas1, vols1, points1, lines1 | * |
| vmass | comp | * |
| vols1 | initpuf | rlsmet, rolldn, swap, inject, vemfac |
| vols2 | initpuf | rlsmet, rolldn, swap, inject |
| walltrap | setpuf, setslg | * |
| wet | comp | * |
| windset | comp, rlsmet | powlaw, xtprf |
| wrdat | wrout1, output, comprs | * |
| wrfiles | setup | * |
| wrint | wrout1, output | * |
| wrivl | readcf, setup | * |
| wrout1 | setup | julday, wrint, xtracti, wrdat |
| wrt | out, outsam | * |
| wrt2 | out, outsam | * |
| wrti1d | restarto | * |
| wrtr1d | restarto | * |
| wrtr2d | restarto | * |
| wrtr3d | restarto | * |
| xercnt | xermsg | * |
| xerfdif | lssint, slugave | erf |
| xerhlt | xermsg | * |
| xermsg | snsqe, r1mach, xsetf | xerprn, xerhlt, xersve, xercnt, fdump, j4save |
| xerprn | xermsg | xgetua |
| xersve | xermsg | xgetua |
| xgetua | xerprn, xersve | j4save |
| xintrp | ctpar | * |
| xsetf | path | xermsg, j4save |
| xtprf | advect, ptlaps, turbset, rdmet4, getprfp, windset | psim |
| xtract | output | * |
| xtracti | wrout1 | * |

| SUBROUTINE | CALLED BY | CALLS |
|---|---|---|
| xvy | sigty | * |
| xvz | sigtz | * |
| xy2uwcw | areaint | * |
| yr4 | rdhdoz, rdoz, met1, met2, met3, met4, rdmet, rdmet4, rdprof, rdisc, rdplm, rdhdem2, rdhdem3, rdhdem4, rdhdem5, rdem2, rdem3, rdem4, rdem5 | * |
| yr4c | fin, readcf | * |
| zfind | advwnd, comp, rlsmet | * |
| zmet | numrise | * |

# APPENDIX B

## Description of Each CALPUFF Subroutine and Function

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| ADVECT | Subr. | Obtains puff advection wind. |
| ADVWND | Subr. | Computes the vertically-averaged winds (U, V) through the layer ZBOT through ZTOP from CALMET winds. |
| ALLCAP | Subr. | Converts all lower case letters within a character string from a control file data record into upper case. |
| ALTONU | Subr. | Converts a character string from a control file data record into a real, integer, or logical variable. Computes the repetition factor for the variable. |
| AREAINT | Subr. | For a polygon area source, integrates the time-averaged concentration for the case of the unaged slug (i.e., IAGE=0) for a receptor at (X,Y). |
| AREAS1 | Subr. | Initializes newly released puff/slug variables for polygon area sources with constant emissions. |
| AREAS2 | Subr. | Initializes newly released puff/slug variables for buoyant polygon area sources specified in BAEMARB file. |
| ASDF | Funct. | Computes the Area Source Distribution Factor to account for the non-Gaussian cross-wind distribution near an area source. |
| AXIS | Subr. | Given a contour height above the grid-plane, the subroutine returns the major and minor axis lengths of the hill. |
| BI | Subr. | Computes the vertical distribution function for reflection of material from the mixing lid upwind of the hill (summation over i) for the special case in which sigma-z is virtually constant. |
| BJI | Subr. | Computes the vertical distribution function for reflection of material from the mixing lid upwind of the hill (summation over i) and over the hill (summation over j) for the subroutine UPPER. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| BJIL | Subr. | Computes the vertical distribution function for reflection of material from the mixing lid upwind of the hill (summation over i) and over the hill (summation over j) for the subroutine LOWER. |
| CALCPF | Subr. | For a given puff, performs the loop over all receptors for each species. Time-averaged coupling coefficients are used to compute concentration and wet and dry deposition fluxes. |
| CALCSL | Subr. | For a given slug, performs the loop over all receptors for each species. Time-averaged coupling coefficients are computed for each slug-receptor pair via the subroutine SLUGAVE. Also computes wet and dry deposition fluxes. |
| CHEM | Subr. | Computes chemical transformation rates for each species using the MESOPUFF II algorithm or user-specified diurnally varying values. Adjusts the pollutant mass in each layer to account for chemical transformation effects. |
| CHEMEQ | Subr. | Determines ammonium nitrate concentration from total nitrate concentration. |
| CHEMI | Subr. | Setup functions for the chemistry module. Reads user-specified conversion rates from CHEM.DAT. Reads header & time-invariant records of the hourly ozone data file (OZONE.DAT). Performs conversion of station coordinates and compute nearest ozone station to each grid point. |
| CHEMII | Subr. | Calculates the chemical transformation rates for the loss of $SO_2$ and $NO_x$ and formation of $SO_4$ and $HNO_3$. |
| CHEMRIV | Subr. | Sets up call to RIVAD chemical transformation subroutines, and passes results to calling program. |
| CHEMTF | Subr. | This routine adjusts the pollutant mass values to account for chemical transformations. |
| COMLINE | Subr. | Call compiler-specific system routines to pass back the command line argument after the text that executed the program. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| COMP | Subr. | Controls the computational phase of the CALPUFF run. Contains the basic time loop and calls all time-dependent computational routines. |
| COMPRS | Subr. | Compresses an array of concentrations, dry fluxes, or wet fluxes by replacing strings of zero values with a negative code indicating the number of zero values. |
| CPQROMB | Subr. | Performs Romberg integration of the polygon segment in the upwind distance domain (XLOWER,XUPPER) via calls to the slug line source routine LSSLINT. |
| CPTRAP | Subr. | Performs Trapezoidal integration of polygon segment in the upwind distance domain (XLOWER,XUPPER) via calls to the slug line source routine LSSLINT. |
| CTADJ | Subr. | Adjusts puff-height to simulate terrain effects when either the ISC terrain treatment (MCTADJ = 1) or the partial plume height correction (MCTADJ = 3) is used. |
| CTADJ2 | Subr. | Computes strain-induced adjustment factor for vertical dispersion, where the strain in the flow is approximately from the underlying gridded terrain field. This is used when MCTADJ=2. |
| CTINIT | Subr. | Transfers data that are needed for the subgrid-scale terrain option to common/CTPASS/, and initializes data passed in common/CONST/. |
| CTPAR | Subr. | Computes parameters for complex terrain option which depend only on specification of puff and hill data. |
| CTREC | Subr. | Computes receptor position in various coordinate systems and obtains travel times from regional bounds. |
| CTSG | Subr. | Main subroutine that controls computation of concentrations on sub-grid-scale terrain features. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| CWYVALS | Subr. | For an N-sided polygon area source with vertices at (upwind,cross-wind) coordinates (XY,YV), relative to the receptor at (0,0), determines the cross-wind Y VALS of the polygon boundary intercepted by the cross-wind line at upwind distance X. The min./max. values are computed and returned in YMIN/YMAX and the number of legitimate values returned in NHITS. |
| DATETM | Subr. | Gets the date and time from the system clock. Calls the system date and time routines. |
| DEBLNK | Subr. | Removes all blank characters from a character string within a pair of delimiters in a control file. |
| DELTT | Subr. | Computes the difference (in hours) between two dates and integer times (time 2 - time 1). |
| DOGLEG | Subr. | Given an M by N matrix A, an N by N nonsingular DIAGONAL matrix D, an M-vector B, and a positive number DELTA, this subroutine completes the solution of the problem to determine the convex combination X of the Gauss-Newton and scaled gradient directions that minimizes (A*X - B) in the least squares sense, subject to the restriction that the Euclidean norm of D*X be at most DELTA. |
| DRY | Subr. | Computes dry deposition velocities for each modeled species using a resistance model or user-specified diurnally varying values. Also computes mass removed during step. |
| DRYI | Subr. | Setup routine for dry deposition module. Initialization and time-invariant calculations performed. |
| DWSIGS | Subr. | Computes the dispersion coefficients, sigma-y and sigma-z due to building downwash effects. (Values returned are the max. obtained with or without building downwash.) |
| ELEVI | Subr. | Interpolates CALPUFF gridded terrain to array of gridded receptors. |

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| EMQA | Subr. | Performs QA checks on data from emissions files by checking for consistency with the control file inputs. Computes cross-referencing arrays relating species ordering in the emissions files to that of the main concentration array. |
| ENORM | Funct. | Given an N-vector X, this function calculates the Euclidean norm of X. |
| ERF | Funct. | Computes the error function, erf(x). This is the Quick medium accuracy error function from NBS 55. Using an approximation due to Hastings; absolute error about 3e-7. |
| ERFC | Funct. | Computes the complementary error function, 1-erf(x). This is the Quick medium accuracy COMP. error function from NBS 55. Using an approximation due to Hastings; absolute error about 3e-7. Asymptotic expression added for large x to reduce percent error. |
| ERFDIF | Funct. | Computes the difference: erfdif = erf(x1) - erf(x2). Various methods are used to avoid roundoff errors depending on the values of the two arguments. |
| ETIME | Subr. | CPU time routine for SUN system. |
| EXMET | Subr. | Finds the closest non-missing value of air temperature, short-wave radiation, relative humidity, and air density to a particular grid point. |
| EXTREME | Subr. | For an N element array of values, XV, determines the min./max. values and returns as XMIN, XMAX. |
| FCTY | Funct. | Computes value of integrand function denoted as fcty, at time t. |
| FCTZ | Funct. | Computes value of integrand function denoted as fctz, at time t. |
| FDJAC1 | Subr. | This subroutine computes a forward-difference approximation to the N by N Jacobian matrix associated with a specified problem of N functions in N-variables. If the Jacobian has a banded form, then function evaluations are saved by only approximating the nonzero terms. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| FDUMP | Subr. | Produces a symbolic dump which prints subprogram nesting list. |
| FILCASE | Subr. | Converts all filenames to upper or lower case. |
| FIN | Subr. | Main routine for the termination phase of the CALPUFF run. Computes run time, writes termination messages. |
| FINDI | Subr. | Finds the closest station to a specified (X,Y) coordinate that has non-missing data and passes the integer variable at that station back to the calling routine. |
| FINDR | Subr. | Finds the closest station to a specified (X,Y) coordinate that has non-missing data and passes the real variable at that station back to the calling routine. |
| FINLINI | Subr. | Checks real roots for finite line intercept. For a specific time T, this routine computes the point on the line segment where the intersection with the receptor perimeter (circle or square) occurs. If that intercept yields an S such that $0 < S < 1$, then the intersection falls on the finite portion of the line and is of interest. If S is outside this domain, RETURN without altering TMIN,TMAX integration limits. |
| FLOPUFF | Subr. | Computes the perturbation winds up,vp,wp at (X,Y,Z) and computes the vertical and lateral deflections (ETA,DEL) of the streamline that passes through the point (X,Y,Z) above the surface of a rotated gaussian hill. This code computes IDYY and IXXDYY to compute T-factors. |
| GETELEV | Subr. | Employs bilinear interpolation to obtain terrain elevation at a point within the MET grid. |
| GETOZ | Subr. | Determine the appropriate value of ozone concentration to use in the chemical transformation routine: use constant background value if MOZ = 0; read hourly values if MOZ = 1 |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| GETPRFM | Subr. | Passes vertical profiles of wind speed and the Brunt-Vaisala frequency into common for use by CTSG-related routines. Uses MET arrays. |
| GETPRFP | Subr. | Passes vertical profiles of wind speed and the Brunt-Vaisala frequency into common for use by CTSG-related routines. Uses PROFILE.DAT arrays. |
| GRDAY | Subr. | Computes the Gregorian date (month, day) from Julian day and year. |
| GRISE | Subr. | Calculates the height of gradual plume rise at position X. |
| HDUN | Subr. | Computes the dividing-streamline height ($H_d$) and U/N above $H_d$. |
| HEFTRAN | Subr. | Defines sigmas and corresponding virtual times at which transition to the Heffter time-based sigma functions is made. |
| HILHGT | Funct. | Computes the fractional hill height at the position (X,Y) for a rotated gaussian hill. |
| HILROT | Subr. | Computes the needed length scales lx and ly and the factor gam for a gaussian hill having major axis AH, minor axis BH, and rotated CCW by an angle PSI. When PSI=0 the minor axis is oriented along the X-axis (or flow direction) and the major axis lies along the Y-axis. |
| I1MACH | Funct. | Used to obtain machine-dependent parameters for the local machine environment. |
| INCR | Subr. | Increment the time and date by a specified number of hours. |
| INITAI | Subr. | Initializes an integer array with a constant value. |
| INITAR | Subr. | Initializes a real array with a constant value. |
| INITI2D | Subr. | Initializes a two dimensional integer array with a constant value. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| INITPUF | Subr. | Invokes routines that initialize newly released puff/slug variables from each source. |
| INITR2D | Subr. | Initializes all or a portion of a REAL 2-D array with a constant value. |
| INJECT | Subr. | Injects emissions into proper layer (above/below mixing ht.). |
| INPREC | Subr. | This routine is responsible for reading the receptor data. |
| INPTER | Subr. | This routine is responsible for reading the terrain information for each hill. |
| IREG | Funct. | Determines position of a point relative to boundaries of the CTSG modeling regions. |
| J4SAVE | Funct. | Saves and recalls several global variables needed by the library error handling routines. |
| JULDAY | Subr. | Computes the Julian day number from the Gregorian date (month, day). |
| KLOSE | Funct. | This function returns the position of the data value in array XA which is nearest to the value X but less than X. |
| LINES1 | Subr. | Initialize newly released puff/slug variables for line sources with constant emissions. |
| LINES2 | Subr. | Initialize newly released puff/slug variables for line sources with variable release parameters. |
| LN2FILL | Subr. | Fill common /LN2/ for LINE SOURCES with variable parameters. |
| LOWER | Subr. | Computes concentrations due to puff material in segment of the flow (below $H_d$). |

## APPENDIX B
## CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| LSSLINT | Subr. | Computes the time-average coupling coefficients (s/m**3) at the downwind distance RHOA for the time period T to T+DT for a cross-wind line source. |
| LSTAB | Funct. | Calculates a PG stability class given the Monin-Obukhov length and the surface roughness from Golder's 1972 curves. |
| LUMP | Subr. | Calculate the lumped variables. |
| MARCHING | Subr. | Marches numerical rise equations one step, either PREDICTOR or CORRECTOR. |
| MBALHDR | Subr. | Writes header records to the mass balance file (MASSBAL.DAT). |
| MBALINI | Subr. | Initializes data arrays for mass balance output. |
| MBALOUT | Subr. | Writes mass balance for hours to output file (MASSBAL.DAT). |
| MBALSUM | Subr. | Updates mass balance totals for current puff, for current step. |
| MET1 | Subr. | Reads the 14 header records of the CALMETmeteorological data file. |
| MET2 | Subr. | Creates the header information normally contained in the CALMET file (using ISCMET file).  Also, sets the wind profile power-law exponents if not provided in control file. |
| MET3 | Subr. | Sets the header records normally contained in the CALMET file (using PLMMET data file).  Also, sets the wind profile power-law exponents if not provided in control file. |
| MET4 | Subr. | Creates the header information normally contained in the CALMET file (using CTDMPLUS PROFILE file). |
| METQA | Subr. | Performs consistency checks of data read from the CALMET header records with control file inputs. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| MFLXCMP | Subr. | Updates mass flux totals for current puff, for current step. |
| MFLXGRP | Subr. | Sums mass flux results for individual species into output groups. |
| MFLXHDR | Subr. | Writes header records to the mass flux file (MASSFLX.DAT). |
| MFLXINI | Subr. | Initializes data arrays for mass flux output. |
| MFLXOUT | Subr. | Writes selected mass fluxes for hours to output file (MASSFLX.DAT). |
| MFLXSET | Subr. | Processes boundary information for the mass flux module. |
| MUNU | Subr. | Computes the elliptical coordinates of a point that is referenced to the system centered on the ellipse, with x-axis along the major axis. |
| NEXTFIL | Subr. | Prepares next CALMET.DAT file when multiple files are used. |
| NUMMET | Subr. | Prepares meteorological data for numerical plume rise. |
| NUMPR1 | Subr. | Initializes the variables used by the numerical plume rise algorithm. |
| NUMRISE | Subr. | Computes plume rise using a numerical solution to the non-Boussinesq conservation laws.  Model allows: |

      (1) arbitrary ambient temperature stratifications
      (2) arbitrary uni-directional wind stratification
      (3) any size of finite emission source
      (4) is free of the Boussinesq approximation
      (5) radiative heat loss

| | | |
|---|---|---|
| OPENAB | Subr. | Open existing input file after determining if file is ASCII or Binary format |
| OPENOT | Subr. | Opens all input / output files (other than the control file and list file), based on the values in the control file inputs. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| OUT | Subr. | Prints a gridded 2-D field of real or integer numbers to a specified number of digits. Internally computes a scaling factor for printing the field based on the maximum value within the grid. |
| OUTPUT | Subr. | Outputs concentration, dry & wet deposition flux fields. |
| OUTSAM | Subr. | Writes a gridded field of real or integer numbers. Array dimensions sized for SAMPLING grid. |
| PATH | Subr. | Computes the position of the streamline that passes through point at (-INFINITY,YI,ZI) for any X assuming a Gaussian hill function H(a,b)=HH*EXP(-(a/AH)**2-(b/BH)**2). Local deformation factors Th,Tl,Tu are computed at (X,Y,Z). |
| PATH0 | Subr. | Computes difference between actual upstream location of streamline in the y-z plane, and corresponding position of approximated streamline. |
| PDFPATH | Subr. | Computes the vertical distribution factor for the combined direct and indirect path of the PDF formulation. |
| PDFVARS | Subr. | Computes variables associated with the PDF formulation for the convective boundary layer (CBL). |
| PFSAMP | Subr. | For a given puff and receptor, computes the time-averaged coupling coefficients used to compute concentration and wet and dry deposition fluxes. |
| PFSCRN | Subr. | For a given puff and receptor, uses the puff radius at the end of the step and the trajectory to screen out cases with zero contribution. |
| PLGRECS | Subr. | Computes the receptor-specific sigmas y and z, and finds receptor-specific puff height (gradual rise) with terrain adjustments for PLUGS. PLUGS are puff-like segments of a slug . |
| POINTS1 | Subr. | Initializes newly released puff/slug variables for point sources with constant emissions. |

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| POINTS2 | Subr. | Initializes newly released puff/slug variables for point sources with variable emissions. |
| POLINT | Subr. | Computes Y(X) as Interpolation of XA, YA. |
| POWLAW | Subr. | Extrapolates wind speed to specified height using a power law profile adjustment factor. |
| PRB | Subr. | Calculates transitional buoyant plume rise (excluding building downwash effects). This routine is used for both neutral/unstable and stable conditions. |
| PRBL | Subr. | Calculates distance-dependent plume rise for buoyant line sources from precalculated tabulation. |
| PRFIN | Subr. | Calculates the distance to final plume rise and height of final plume rise. |
| PRFINSH | Subr. | Calculates final buoyant plume rise using plume rise equations with wind shear effects. |
| PRFPP | Subr. | Revise height of final rise due to partial penetration of an elevated inversion. Used for buoyant rise in convective mixed layer. |
| PRM | Subr. | Calculates transitional momentum plume rise (excluding building downwash effects). This routine is used for both neutral/unstable and stable conditions. |
| PRSHEAR | Subr. | Calculates transitional buoyant plume rise using plume rise equations with wind shear effects. |
| PRSS | Subr. | Calculates distance-dependent plume rise for Schulman-Scire downwash algorithm, as coded in ISC2. |
| PRTAB | Subr. | Calculates distance-dependent plume rise by interpolating plume height table. |

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| PSIM | Funct. | Computes the Businger-Dyer surface layer PSI function for momentum. |
| PTLAPS | Subr. | Calculates the potential temperature lapse rate (deg. K/m) in a layer "DELZ" meters deep above the a specified height, using either the temperature data from the MET file, or the PROFILE.DAT file. |
| PUFFC | Subr. | Computes concentrations for those receptors that are modeled as a "receptor-on-a-pole" (including cases in which terrain effects are negligible). |
| PUFFCT2 | Subr. | Compute receptor-specific puff height for the MCTADJ=2 terrain treatment option, for puff sampling. |
| PUFFDZ | Subr. | Computes the top and bottom of the puff/slug for use in obtaining the advection wind. |
| PUFRECS | Subr. | Computes the receptor-specific sigmas y and z, and finds receptor-specific puff height (gradual rise) with terrain adjustments for puffs. |
| QAINP | Subr. | Checks selected input data provided in control file. |
| QATR | Subr. | Integration routine adapted from the IBM SSP program DQATR. Modified for single precision. |
| QAYR4 | Subr. | Defines century for converting 2-digit years into 4-digit years. |
| QCHECK | Subr. | Checks number species, species names against control file inputs, molecular weights. Sets up cross-referencing table. |
| QFORM | Subr. | This subroutine proceeds from the computed QR factorization of an M by N matrix A to accumulate the M by M orthogonal matrix Q from its factored form. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| QRFAC | Subr. | This subroutine uses Householder transformations with column pivoting (optional) to compute a QR factorization of the M by N matrix A. That is, QRFAC determines an orthogonal matrix Q, a permutation matrix P, and an upper trapezoidal matrix R with diagonal elements of nonincreasing magnitude, such that A*P = Q*R. |
| QUADAREA | Subr. | Computes the area of a quadrilateral polygon. The shape must be regular in the sense that no line that drawn through it may cross more than 2 sides. |
| R1MACH | Funct. | Used to obtain machine-dependent parameters for the local machine environment. |
| R1MPYQ | Subr. | Given an M by N matrix A, this subroutine computes A*Q where Q is the product of 2*(N - 1) transformations: GV(N-1)*...*GV(1)*GW(1)*...*GW(N-1) and GV(I), GW(I) are Givens rotations in the (I,N) plane which eliminate elements in the I-th and N-th planes, respectively. |
| R1UPDT | Subr. | Given an M by N lower trapezoidal matrix S, an M-vector U, and an N-vector V, the problem is to determine an orthogonal matrix Q such that: $(S + U*V^T )*Q$ is again lower trapezoidal. |
| RATE | Subr. | Computes the right-hand side of the numerical rise equations. |
| RDCHEM | Subr. | Reads a file containing a diurnal cycle of 24 hourly chemical transformation rates (in percent/hour). |
| RDEM2 | Subr. | Reads the time-varying records of the PTEMARB point source emissions file (arbitrarily-varying emissions). |
| RDEM3 | Subr. | Reads the time-varying records of the BAEMARB buoyant area source data file (arbitrarily-varying emissions). |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| RDEM4 | Subr. | Reads a set of data records from the VOLUME source gridded emissions file (VOLEM). |
| RDEM5 | Subr. | Reads the time-varying records of the LNEMARB buoyant line source emissions file (arbitrarily-varying emissions). |
| RDEMREC | Subr. | Reads NX * NY words of a 2-D real emissions data record. |
| RDHDEM2 | Subr. | Reads the header records from the PTEMARB point source emissions file (arbitrarily-varying emissions). |
| RDHDEM3 | Subr. | Reads the header records from the BAEMARB buoyant area source file (arbitrarily-varying location & emissions). |
| RDHDEM4 | Subr. | Reads the header records from the VOLEM volume source gridded emissions file. |
| RDHDEM5 | Subr. | Reads the header records from the LNEMARB buoyant line source emissions file (arbitrarily-varying emissions). |
| RDHDOZ | Subr. | Reads the header records from the OZONE.DAT data file. |
| RDI1D | Subr. | Reads "NWORDS" of a one-dimensional integer array. |
| RDI2D | Subr. | Reads NX * NY words of a 2-D integer array. |
| RDISC | Subr. | Reads ISCMET.DAT meteorological data for one hour. |
| RDMET | Subr. | Reads CALMET meteorological data for one hour. |
| RDMET4 | Subr. | Reads meteorological data for one hour from CTDMPLUS PROFILE and SURFACE files. |
| RDOZ | Subr. | Reads the time-varying records of the OZONE data file. |

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| RDPLM | Subr. | Reads PLMMET.DAT meteorological data for one hour. |
| RDPROF | Subr. | Reads meteorological data for one hour from CTDM PROFILE file. |
| RDR1D | Subr. | Reads "NWORDS" of a one-dimensional real array. |
| RDR2D | Subr. | Reads NX * NY words of a 2-D real array. |
| RDTIEM2 | Subr. | Reads the time-invariant records of the PTEMARB point source emissions file (arbitrarily-varying emissions). |
| RDTIEM3 | Subr. | Reads the time-invariant records of the BAEMARB buoyant area source data file (arbitrarily-varying emissions). |
| RDTIEM5 | Subr. | Reads the time-invariant records of the LNEMARB buoyant line source data file (arbitrarily-varying emissions). |
| RDTIOZ | Subr. | Reads the time-invariant records of the OZONE data file. |
| RDTVW | Subr. | Reads the time-varying records of the SIGMA data file. |
| RDVD | Subr. | Reads a file containing a diurnal cycle of 24 hourly deposition velocities (m/s) for selected species. |
| READCF | Subr. | Controls the reading of the control file.  Calls subroutine READIN for each input group. |
| READFN | Subr. | Reads the file containing the path and filename of the model's input and output files. |
| READIN | Subr. | Reads one input group of a free formatted control data file. |
| RECSPEC0 | Subr. | Computes the receptor-specific sigmas y and z, and receptor-specific slug height (gradual rise) with terrain adjustments, for the special case of the unaged slug (IAGE = 0) from either an area source or a line source. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| RESTARTI | Subr. | Input puff array data from a restart file, written at the end of a previous run, needed to restart CALPUFF with current puffs in the domain. |
| RESTARTO | Subr. | Output puff array data to a restart file that is needed to restart CALPUFF with current puffs in the domain. |
| RESTARTQ | Subr. | Read and check (QA) header record of the restart file. |
| RISEWIND | Subr. | Compute the mean wind components for advecting a puff during the transitional rise range. |
| RLSMET | Subr. | Obtains release height wind speed & other met. variables. |
| ROLLDN | Subr. | Identifies inactive puff/slug indices, and "rolls down" arrays to free space for new puffs/slugs. |
| ROMBTIN | Subr. | Performs Romberg time integration of the sequence of slug snapshots over the interval (TLOWER,TUPPER) via calls to the slug quardrture routine TRAPSL. |
| ROOT2 | Subr. | Solves for NR multiple roots RT(I) of the quadradic: $$AA2 * Z**2 + AA1 * Z + AA0 = 0$$ |
| ROOT3 | Subr. | Solves for NR multiple roots RT(I) of the cubic equation: $$AA3 * Z**3 + AA2 * Z**2 + AA1 * Z + AA0 = 0$$ |
| ROTATE | Subr. | Rotates coordinate system through angle "ang" to map point (x,y) into point (xp,yp). |
| SETCOM | Subr. | Computes miscellaneous common block variables in the setup phase of the run. |
| SETCSIG | Subr. | Sets selected parameters for calls to sigma routines, and place in /CSIGMA/. |

APPENDIX B
CALPUFF Subroutines and Functions

| **ROUTINE NAME** | **TYPE** | **PURPOSE** |
| --- | --- | --- |
| SETLINE | Subr. | Performs initial processing for buoyant line sources for current meteorology, and compute rise table. |
| SETPUF | Subr. | Sets distances/times for puff, and update stored puff data. |
| SETSLG | Subr. | Sets the coordinates, sigmas, and plume height variables for the "current" slug in common block /CURRENT/ for use by the slug sampling routine. |
| SETUP | Subr. | Controls the setup phase of the CALPUFF model. Calls all initialization and one-time setup routines. |
| SETVAR | Subr. | Fills a variable or array with the value read from a control file data record. |
| SIGMA | Funct. | Computes a value of sigma for a given travel-time, using the CALPUFF sigma subroutines, starting from the nearest of three known values. The effect of buoyancy-induced growth is treated as a virtual time, as in CTDMPLUS. |
| SIGSET | Subr. | Computes several /CSIGMA/ common block variables during the setup phase. |
| SIGTY | Subr. | For a given dispersion option, IDOPT, and a given initial lateral plume standard deviation, SIGY0, computes the plume standard deviation for a given downwind distance or time increment, consistent with the dispersion regime, and returns this value, SIGY (meters), for use as the puff's or slug's lateral sigma. |
| SIGTZ | Subr. | For a given dispersion option, IDOPT, and a given initial vertical plume standard deviation, SIGZ0, computes the plume standard deviation for a given downwind distance or time increment, consistent with the dispersion regime, and returns this value, SIGZ (meters), for use as the puff's or slug's vertical sigma. |
| SIGWV | Subr. | For dispersion option IDOPT=2 computes the standard deviation of vertical velocity (sigw) and the horizontal cross-wind velocity (sigv) based on micrometeorological parameters. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| SLGFRAC | Subr. | Compute along-slug and cross-slug distances from the younger end (x2,y2) to a reference point (x,y), the spatial interpolation factor for the scaled along-slug position, and the slug length. |
| SLG2PUF | Subr. | Subroutine determines the number of puffs required to simulate GLC's due to a slug (prepares for CTSG call). Assumes that separation between puffs is fixed, and is set by a mean sigma-y along the slug. |
| SLGRECS | Subr. | Computes the receptor-specific sigmas y and z, and receptor-specific slug height (gradual rise) with terrain adjustments for SLUGS. |
| SLGTLIM | Subr. | For a given slug and receptor combination for which a numerical dose integration is about to be done, determines the dimensionless time integration limits, $0.0 < TSTART, TEND < 1.0$ , which will capture the major part of the integrand's contribution. |
| SLGXLIM | Subr. | For a given slug's initial and final positions, computes the window of receptor space which should be examined. This version computes such a window for both grided and non-gridded receptors. |
| SLUGAVE | Subr. | Computes the time-average coupling coefficients (s/m**3) at the point (x,y,z) over the time period T to T+DT (where DT is a time step and TDDT is the fraction of DT that is elapsed). |
| SLUGCT2 | Subr. | Compute receptor-specific puff height for the MCTADJ=2 terrain treatment option, for slug sampling. |
| SLUGI | Subr. | Initializes the variables defining the sampling grid in common block /RECGRD/. This common is used by the slug sampling function. |
| SLUGINT | Subr. | Computes the time-average coupling coefficients (s/m**3) at the point (x,y,z) over the time period T to T+DT (where DT is a time step and TDDT is the fraction of DT that is elapsed). |
| SLUGSNP | Subr. | Computes the instantaneous coupling coefficient (s/m**3) at the point (x,y,z) at the time T + TDDT*DT (where DT is a time step and TDDT is the fraction of DT that is elapsed). |

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| SNSQ | Subr. | Finds a zero of a system of a N nonlinear functions in N variables by a modification of the Powell hybrid method. |
| SNSQE | Subr. | Finds a zero of a system of N nonlinear functions in N variables by a modification of the Powell hybrid method. |
| SPEED | Funct. | Computes wind speed at the height provided. |
| SPLIT | Subr. | Creates "new" puffs/slugs by splitting old puffs/slugs in the vertical when appropriate for tracking effects of wind shear. |
| SSCB | Subr. | Calculates C coefficient for BUOYANT rise used in Schulman-Scire downwash algorithm, as coded in ISC2. |
| SSCM | Subr. | Calculates C coefficient for MOMENTUM rise used in Schulman-Scire downwash algorithm, as coded in ISC2. |
| SSLATLON | Subr. | Compute N. Latitude and W. Longitude for the surface meteorological stations (from CALMET file). |
| STAB2L | Subr. | Calculates a Monin-Obukhov length given the PG class and the surface roughness from Golder's 1972 curves. |
| STKTIP | Subr. | Calculates the plume height adjustment to account for stack-tip downwash effects. |
| STPRF | Subr. | Sorts arrays of PROFILE data. |
| SUNDATA | Subr. | Computes cloud cover and cosine of solar zenith angle at each surface met station. |
| SWAP | Subr. | Transfers puff/slug array elements from index "J" to index "I". If J=0, array elements are initialized to ZERO. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| SYAREA | Subr. | For a polygon area source, determines the effective initial sigma-y based on the projection of the source in the cross-wind direction for this met period. |
| TERAVG | Subr. | Compute average elevation of a strip of cells containing cell (i,j), which lie across a 45 degree sector centered on the direction from cell (i0,j0) to cell (i,j). |
| TIBLGRO | Subr. | Grow an existing TIBL along the path of a puff, using current land use. |
| TIBLON | Subr. | Screen coastline segments to determine if puff trajectory can encounter a TIBL, and compute initial TIBL properties if it does. |
| TIBLSET | Subr. | Setup the sub-grid TIBL module by: reading user-supplied coast line(s) (COASTLN.DAT); identifying met. grid cells with coast segments; identifying nearest land and water met. grif cells for each point stored for each coast line; and computing the slope/intercept for coastline segments. |
| TFAC | Subr. | Interpolates flow distortion factors at position X along the trajectory of the puff. |
| TRACK | Subr. | Writes selected puff/slug data to a file to track evolution in time. |
| TRAPSL | Subr. | Performs trapezoidal integration of polygon segment in the upwind distance domain (TLOWER,TUPPER) via calls to the slug snapshot routine SLUGSNP. |
| TRELIEF | Subr. | Compute local relief of the terrain for each cell in the meteorological grid, and also the peak elevation associated with this relief. The relief height and peak terrain elevation are used for terrain treatment option MCTADJ = 2. |
| TRIAREA | Funct. | Computes the area of a triangle. |
| TRPF | Funct. | TRPF is a linear interpolator. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| TURBSET | Subr. | Determines turbulence velocities and associated dispersion options (backup if needed). |
| UNDER0 | Subr. | Lahey® F77 compiler routine used to set underflows. |
| UNLUMP | Subr. | Calculates physical variables from lumped variables in numerical rise. |
| UPPER | Subr. | Computes concentrations due to puff material in the upper segment of the flow (above Hd). |
| VCBAR | Funct. | Computes the space- and time-averaged vertical coupling coefficient, via calls to VCOUP. A slug is sampled at each end, both at the start and end of the step. A puff is sampled at the start, mid-pt, and end of the step. |
| VCOUP | Funct. | Computes the vertical coupling coefficient for a source at height ZS, to a receptor at height ZR given a plume with sigma-z of SZ and including reflections from the ground and lid at height HLID. |
| VDCOMP | Subr. | Computes deposition velocities for each species deposited for a single grid cell. |
| VDP | Subr. | Computes a mass-weighted particle deposition velocity for a single size distribution. |
| VDP1 | Subr. | Setup routine for particle dry deposition. Initialization and time-invariant calculations are performed. |
| VECMAX | Funct. | For an N element array of values, XV, determines the maximum value. |
| VECMIN | Funct. | For an N element array of values, XV, determines the minimum value. |
| VEMFAC | Funct. | Provides a scaling factor for the emission rate from values provided in the control file. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| VMASS | Subr. | Assigns vertical distribution of puff/slug for current sampling step (puff code, mass). |
| VOLS1 | Subr. | Initializes newly released puff/slug variables for discrete volume sources with constant emissions. |
| VOLS2 | Subr. | Initialize newly released puff/slug variables gridded volume sources with variable emissions. |
| VWIDTH | Subr. | Compute local valley width in met. grid cell units as a function of height at each cell (used for terrain treatment option MCTADJ = 2). |
| WALLTRAP | Subr. | Compute local valley width at height "z" above cell elevation for puff position at beginning and end of step; then limit growth of sigma-y during step if valley width is small enough (used for terrain treatment option MCTADJ = 2). |
| WET | Subr. | Computes the scavenging ratios as a function of species for wet removal. |
| WINDSET | Subr. | Obtains wind at height HT. |
| WRDAT | Subr. | Writes a gridded concentration or dry/wet flux data record (one 15-character identifier and a 2-D data array). |
| WRFILES | Subr. | Writes a table to the list file with the name and path of input and output files used in the current run. |
| WRINT | Subr. | Writes a gridded field of integers to binary file (one 15-character identifier and a 2-D data array). |
| WRIVL | Subr. | Writes identification label (model, version, level). |
| WROUT1 | Subr. | Writes the header records to the concentration, dry flux, wet flux, and visibility output files. |

## APPENDIX B
## CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| WRT | Subr. | Writes one Y row of formatted gridded data (in conjunction with subroutine OUT) |
| WRT2 | Subr. | Writes a line labeling the X coordinates of a row of gridded data (in conjunction with subroutines OUT). |
| XERCNT | Subr. | Allows user control over handling of errors. |
| XERFDIF | Subr. | Computes the integral of $X^{**N} * ERF(X)$ from XL to XU. For N = 0 the quantity X0ERF is computed and for N = 1 the quantity X1ERF is computed. |
| XERHLT | Subr. | Aborts program execution and prints error message. |
| XERMSG | Subr. | Processes a diagnostic message in a manner determined by the value of level and the current value of the library error control flag. |
| XERPRN | Subr. | This routine sends one or more lines to each of the (up to five) logical units to which error messages are to be sent. |
| XERSVE | Subr. | Record that this error occurred and possibly dump and clear the tables. |
| XGETUA | Subr. | Called to determine the unit number or numbers to which error messages are being sent. |
| XINTRP | Funct. | Linearly interpolates between two points (Y1,Y2) given three other points (X1,X2,X) where X1 and X2 are endpoints and X is between X1 and X2. |
| XSETF | Subr. | Sets the error control flag. |
| XTPRF | Subr. | Extracts value from PROFILE at a specified height, using CTDM profiling constructs when needed. |
| XTRACT | Subr. | Extracts the active portion of a 2-D array. |

APPENDIX B
CALPUFF Subroutines and Functions

| ROUTINE NAME | TYPE | PURPOSE |
|---|---|---|
| XTRACTI | Subr. | Extracts the active portion of a 2-D integer array. |
| XVY | Funct. | XVY calculates the virtual distance necessary to account for the initial cross-wind dispersion based on Briggs urban dispersion coeffcients. |
| XVZ | Funct. | XVZ calculates the virtual distance necessary to account for the initial vertical dispersion based on Briggs urban dispersion coeffcients. |
| XY2UWCW | Subr. | Transforms the NSIDE vertex coordinates (XVERT,YVERT) relative to the receptor coordinates (X,Y), into upwind/cross-wind frame vectors (XV,YV). Also compute upwind distance from receptor to the upwind corner of the block of line sources (if modeled). |
| YR4 | Subr. | Checks for 2-digit year and converts to 4-digit year if required. |
| YR4C | Subr. | Converts 2-digit year returned from system (current date) to 4-digit year. |
| ZFIND | Subr. | Finds the vertical layer containing height Z. |
| ZMET | Subr. | Obtains ambient met parameters at height Z by interpolation of gridded values. |