Atmospheric Sciences

Exponent®

CALPUFF Version 7
Users Guide Addendum

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Introduction

With the release by Exponent of CALPUFF Version 7[1], several new capabilities have been added to the CALPUFF modeling system. These include the ability to model flares, roadways and aerial spray sources. Each of these potential sources is included as a new source type within the CALPUFF model. The new source types are used to develop realistic emission profiles at the point of emission. All of the new source types fit within the existing dispersion frame work of CALPUFF.

The following sections detail the setup and use of the new source type modules. For all three source types, external variable emissions files can be used to define emissions. For the new Roadway source, constant emissions or emissions based on simple temporal profiles can alternatively be defined in the CALPUFF input file. Spray and Flare emissions and locations cannot be defined within the CALPUFF input file and require an external variable emission file.

The formats of the external variable emissions files are also detailed in the sections which follow. External variable emissions files are in ASCII format and can be generated by the user. For the Spray source type, recent versions of the AGDISP code distributed by the US Forest Service will produce many of the necessary input blocks for the external variable emissions files. Similarly, emissions files for the Flare source can be generated by external software including ABFLARE, which is available for download from Zelt PSI (http://www.zeltpsi.com/aertools.html).

This User's Guide Addendum serves as a supplement to the available CALPUFF Version 5 and Version 6 documentation. For additional information on the use and setup of CALPUFF Version 7, the reader is referred to the "CALPUFF Modeling System Version 6 User Instructions" (April 2011). Background information on CALPUFF model theory is

[1] CALPUFF modeling software, including EPA approved versions, is distributed by Exponent, Inc. to those that wish to apply the CALPUFF model for a particular situation. User's may download a copy of CALPUFF source code at the www.src.com website after their explicit acceptance of the CALPUFF End User License terms published on that website.

also available in the "Version 5 CALPUFF User Guide" (January 2000). All documentation is available on the CALPUFF website at www.src.com.

1 CALPUFF Flare Module

1.1 Introduction

The CALPUFF model has been enhanced with new modeling capabilities to model flares. The development work was sponsored by an Alberta Upstream Petroleum Research Fund (AUPRF) grant funded by the Petroleum Technology Alliance Canada (PTAC) under subcontract to Zelt Professional Services Inc (Zelt PSI). The CALPUFF model reads inputs computed by external programs including the ERCB Flare Spreadsheet and ABFLARE (available from Zelt PSI at http://www.zeltpsi.com/aertools.html).

The new developments include a new CALPUFF source-type, FLARE, which is a point source with all arbitrarily-varying emissions parameters, including (potentially) varying location and stack height. FLARE source specific processing flags can be turned on and off, independently of the general processing flags which apply to all other sources in a given CALPUFF simulation. Those FLARE-specific switches relate to the plume rise method and stack-tip downwash.

Exponent also created a series of new postprocessors to compute time-averages, maxima, n^{th} ranked and percentile concentrations (and deposition fluxes). Those new postprocessors are CALAVE, CALMAX and CALRANK. One of the applications for this new set of CALPUFF postprocessors is to meet emergency flaring impact assessment requirements in general and in the Province of Alberta (Canada) in particular. This new set of postprocessors streamlines the computation of the maximum (or n^{th} highest, or percentile) impact created by a short-lived event that can occur anytime during the year. This type of situation is typical for emergency events or upset conditions.

The new features are available when using CALPUFF v7.2.0 and METSERIES v7.0.0. The new postprocessors, CALAVE, CALMAX and CALRANK are distributed as new stand-alone FORTRAN codes.

1.2 CALPUFF System Flare Enhancements

1.2.1 CALPUFF

The developers of the CALPUFF modeling system (Scire et al., 2000a, 2000b) added a new flare source type to CALPUFF v7.2.0. In CALPUFF terms, a FLARE is a point source with arbitrarily-varying emissions parameters, including (potentially) varying location and stack height. FLARE source specific processing flags can be turned on and off, independently of the general processing flags which apply to all other sources in a given CALPUFF simulation. Those flare-specific flags are:

1) ***MRISE_FL***: determines the plume rise module for flare sources. Available selection is either Briggs plume rise (MRISE_FL=1) or CALPUFF numerical plume rise (MRISE_FL=2). The numerical plume rise model is recommended for flares and is set as the default. The CALPUFF numerical plume rise algorithm is recommended for flares because:

- Flares are very hot sources and the Boussinesq approximation, one of the Briggs plume rise assumptions, is not valid when the plume density is much smaller than the ambient air density.
- Flares generate highly buoyant plumes and the ambient air stratification and vertical wind shear above stack top should be taken into account during plume rise calculations (Briggs plume rise does not take either into account).

2) ***MTIP_FL***: determines whether stack-tip downwash is applied to FLARE sources in CALPUFF. Although stack tip downwash may affect flares, stack-tip downwash should be applied to flare sources in CALPUFF only if it has not been taken into account already when the effective flare source parameters were computed. In particular, if the flare effective parameters were computed with the Alberta Flare module (either ERCB Flare spreadsheet or ABFLARE), then stack-tip downwash is already taken into account when computing the flame length and effective stack height. In this case stack-tip downwash should be turned-off in CALPUFF to avoid double-counting its effect.

1.2.2 CALPUFF Input File

Input Group 0 of the updated CALPUFF input control file (CALPUFF.INP Version 7.0) includes variables to define the number and names of the external variable emissions files for FLARE sources (FLEMARB.DAT). More details on the format of the new external variable emissions files are included in Section 2.2.3 of this report. The updates to Input Group 0 are shown in Table 1-1.

The two new processing flags, MTIP_FL and MRISE_FL, are defined in Input Group 2 and the input format for these two new variables is shown in Table 1-2. As usual, all key information must be specified between exclamation point delimiters.

A new Input Group 17 has been added to the updated CALPUFF input control file. This allows the user to define the total number of Flare sources contained in the external variable emissions files. The format of Input Group 17 is shown in Table 1-3. Note that, unlike other source types (points, volumes, roads), Flare sources require the use of an external variable emissions file. Constant source parameters cannot be defined directly in the CALPUFF input file.

Table 1-1 New FLARE Variables in Input Group 0 of the CALPUFF.INP v7.0 Control File

```
INPUT GROUP: 0 -- Input and Output File Names
--------------

      …

     Number of FLARE source files (FLEMARB.DAT)
     with time-varying data (NFLDAT)
                                    Default: 0       ! NFLDAT   =  2 !

      …

-------------
Subgroup (0e) – FLEMARB.DAT files
-------------

  FLARE Source File Names
  The following FLEMARB.DAT filenames are processed if NFLDAT>0
  A total of NFLDAT lines is expected with one file name assigned per line
  Each line is treated as an input group and must terminate with END
  (surrounded by delimiters)
  (Each file contains emissions parameters for the entire period modeled
   for 1 or more sources)


Default Name  Type          File Name
------------  ----          ---------
 none         input       ! FLDAT=FLEMARB01.DAT   !   !END!
 none         input       ! FLDAT=FLEMARB02.DAT   !   !END!
```

Table 1-2 New FLARE Variables in Input Group 2 of the CALPUFF.INP v7.0 Control File

```
------------------------------------------------------------------------------

INPUT GROUP: 2 -- Technical options
---------------

…
     Apply stack-tip downwash to FLARE sources?
     (MTIP_FL)                          Default: 0     ! MTIP_FL  =  0 !
        0 = no  (no stack-tip downwash)
        1 = yes (apply stack-tip downwash)

     Plume rise module for FLARE sources
     (MRISE_FL)                         Default: 2     ! MRISE_FL =  2 !
        1 = Briggs module
        2 = Numerical rise module
…
```

Table 1-3 New FLARE Input Group 17 of the CALPUFF.INP v7.0 Control File

```
INPUT GROUP: 17  -- FLARE source control parameters (variable emissions file)
---------------
     Number of flare sources defined in FLEMARB.DAT file(s)
     (NFL2)                                Default: 0     !  NFL2    =  2 !

     (At least 1 FLEMARB.DAT file is needed if NFL2 > 0)

!END!
```

1.2.3 FLARE External Variable Emissions File (FLEMARB.DAT)

CALPUFF v7.2.0 accepts a new type of emission source suitable for emergency flare modeling, namely a point source for which all parameters can arbitrarily vary in time. This new format, dubbed FLEMARB.DAT, is an extension of the point-varying emission source format, PTEMARB.DAT.

FLARES are treated as arbitrarily-varying point sources with the added flexibility of time-varying location and height in order to track the location of the flame tip. No building downwash is allowed.

The file format is designed to be as general as possible in order to allow additional variables to be used by CALPUFF in the future without a change to the FLEMARB.DAT format. There are 8 time invariant variables defined for each source (labeled Var1 through Var8). Currently only Var1 is used. The remaining seven variables are retained for possible future use.

The variable Var1 allows alternative formats for the source data to be used. Setting Var1=1 specifies that source parameters will include values of exit temperature (T) and exit velocity (u,v,w). Note that though all three vector components of the exit velocity (u, v, w) have to be specified for each time record, only the vertical exit velocity (w) is currently used by the CALPUFF code. Setting Var1 to a value other than 1 allows for alternate data formats such as the use of buoyancy (F_b) and momentum (F_{mx}, F_{my}, F_{mz}), though these input options are not currently implemented in CALPUFF.

A FLEMARB.DAT file can contain multiple sources and species. The beginning and ending times of each record are specified in year, Julian day, hour and seconds, and can be of arbitrarily varying duration. However, the ending time of one record must be equal to the beginning time of the next record and periods of inactivity (zero emission) must be explicitly defined (zero emission rates), so that there are no time gaps in the FLEMARB.DAT file.

The FLEMARB.DAT record description and format are detailed in Table 1-4 through Table 1-7. Not all records in a FLEMARB.DAT file are “free reading” and attention must be paid to the length of each variable, type, and spacing in between them.

Table 1-4 Example FLARE Emissions File with Arbitrarily Varying Data (FLEMARB.DAT)

```
FLEMARB.DAT     1.0            Initial configuration
   9
Header records are a mix of formatted and free-format structures
Time-invariant data records are free-format
Time-invariant data records have 8 assignments per source (2-8 are not currently used)
     var1=1: stack inputs are T(K), U, V, W (m/s)
     var1=2: stack inputs are Fb, Fmx, Fmy, Fmz  (i.e., buoyancy and momentum fluxes)
Time-variable data records are free-format
Time-variable data records contain (if var1=1)
     X(km), Y(km), H(mAGL), Elev(mMSL), D(m), T(K), U, V, W, Sigy(m), Sigz(m), Q(g/s)...
Time-variant records contain (if var1=2) --- Not currently available!
UTM
  19N
NAS-C   02-21-2003
  KM
UTC-0500
1990 009  04  0000  1990 009  10 0000
   3   4
'SO2'   'NO'  'NO2'  'PM10'
      30.000      30.000      30.000      30.000
'Source 1'      1.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
'Source 2'      1.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
'Source 3'      1.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
   1990  009  04 0000    1990  009  05 0000
'Source 1'  340.011  4870.443    18.6  160.4  9.754  280.55 0.0   0.0   8.66  1.0   1.0    10.0  4.0  1.0  10.0
'Source 2'  340.486  4870.640    50.1  160.7  4.251  380.4  0.0   0.0   7.66  1.0   1.0    10.0  4.0  1.0  10.0
'Source 3'  341.051  4870.048   35.85  160.9  3.1    289.9  0.0   0.0   2.66  1.0   1.0    10.0  4.0  1.0  10.0
   1990  009  05 0000    1990  009  10 0000
'Source 1'  340.011  4870.443    18.6  160.4  9.754  280.55 0.0   0.0   8.66  1.0   1.0    10.0  4.0  1.0  10.0
'Source 2'  340.486  4870.640    50.1  160.7  4.251  380.4  0.0   0.0   7.66  1.0   1.0    10.0  4.0  1.0  10.0
'Source 3'  341.051  4870.048   35.85  160.9  3.1    289.9  0.0   0.0   2.66  1.0   1.0    10.0  4.0  1.0  10.0
```

Example header records for alternative map projection (either 2 or 3 records)
Sample file above shows UTM projection. Other options provided below:

Universal Transverse Mercator

```
UTM
  19N
```

Lambert Conformal Conic

```
LCC
40.5N           90.0W           30.0N           60.0N
0.00000000E+00 0.00000000E+00
```

Tangential Transverse Mercator

```
TTM
40.5N           90.0W
0.00000000E+00 0.00000000E+00
```

Polar Stereographic

```
PS
40.5N           90.0W           30.0N
```

Equatorial Mercator

```
EM
0.0N            90.0W
```

Lambert Azimuthal Equal Area

```
LAZA
40.5N           90.0W
0.00000000E+00 0.00000000E+00
```

Table 1-5 FLARE Emissions File with Arbitrarily Varying Data (FLEMARB.DAT): Description of Header Variables

`FLEMARB.DAT 1.0 Initial configuration`	Dataset Name, Dataset Version, Dataset Message (char*16, char*16, char*64) **Format: (2a16,a64)**
`9`	Number of comment lines to follow (integer) **Free-Format**

`Header records are a mix of formatted and free-format structures`
`Time-invariant data records are free-format`
`Time-invariant data records have 8 assignments per source (2-8 not used)`
`var1=1: stack inputs are T(K), U, V, W (m/s)`
`var1=2: stack inputs are Fb, Fmx, Fmy, Fmz (not currently available)`
`Time-variable data records are free-format`
`Time-variable records(if var1=1) X,Y,H,Elev,D,T,U,V,W,Sigy,Sigz,Q(g/s)..`
`Time-variable records(if var1=2) --- var1=2 Not currently available!`
	Comment lines (80 characters per record are read)

`UTM`	**Map Projections (Select One)** - Map Projection (char*8) Format: (a8)
`19N`	- UTM Zone, Hemisphere (integer,char*1) **Format: (i4,a1)**
`LCC`	- Map Projection (char*8) **Format: (a8)**
`40.5N 90.0W 30.0N 60.0N` `0.00000000E+00 0.00000000E+00`	- Origin Latitude, Origin Longitude, and 2 matching parallels (char*16) **Format: (4a16)** - False Easting and Northing km (real) **Free-Format**
`TTM`	- Map Projection (char*8) **Format: (a8)**
`40.5N 90.0W` `0.00000000E+00 0.00000000E+00`	- Origin Latitude, Origin Longitude (char*16) **Format: (2a16)** - False Easting and Northing km (real) **Free-Format**
`PS`	- Map Projection (char*8) **Format: (a8)**
`40.5N 90.0W 30.0N`	- Origin Latitude, Origin Longitude, and 1 matching parallel (char*16) **Format: (3a16)**
`EM`	- Map Projection (char*8) **Format: (a8)**
`0.0N 90.0W`	- Origin Latitude, Origin Longitude (char*16) **Format: (2a16)**
`LAZA`	- Map Projection (char*8) **Format: (a8)**
`40.5N 90.0W` `0.00000000E+00 0.00000000E+00`	- Origin Latitude, Origin Longitude (char*16) **Format: (2a16)** - False Easting and Northing km (real) **Free-Format**
`NAS-C 02-21-2003`	DATUM code, date (char*8, char*12) **Format: (a8,a12)**
`KM`	Map units are KM (char*4) **Format: (a4)**
`UTC-0500`	Time Zone as (UTC+hhmm) (char*8) **Format: (a4)**
`1990 009 04 0000 1990 009 10 0000`	Start time and end time of data in file as Year, Julian Day, Hour, Second(0-3599) (integer) **Free-Format**
`3 4`	Number of sources, Number of species (integer) **Free-Format**
`'SO2' 'NO' 'NO2' 'PM10'`	Species names (char*16) **Free-Format** (quotes required)
`30.000 30.000 30.000 30.000`	Molecular weights for species (real) **Free-Format**

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Table 1-6 FLARE Emissions File with Arbitrarily Varying Data (FLEMARB.DAT): Description of Time-Invariant Data

```
'Source 1'      1.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
'Source 2'      1.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
'Source 3'      1.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
```

Source Name, Var1 - Var8 (char*16, real)
Free-Format (quotes required on Source Name)

Source Name	Var1	Var2	Var3	Var4	Var5	Var6	Var7	Var8

Time-invariant data must be assigned to each of the sources, which are identified by name.
In this example, there are 3 sources so there are 3 records.

Only the first variable (Var1) is currently defined for use, but all 8 variables must have values. Zeros are used for variables Var2-Var8.

The Variable Var1 defines the type of source characterization

Var1 = 1 : stack inputs are provided in this variable emissions file as T(K), U, V, W (m/s)
Var1 = 2 : stack inputs are provided in this variable emissions file as Fb, Fmx, Fmy, Fmz (i.e., buoyancy and momentum fluxes)

Table 1-7 FLARE Emissions File with Arbitrarily Varying Data (FLEMARB.DAT): Description of Time-Varying Data

```
   1990  009  04 0000    1990  009  05 0000
'Source 1'  340.011  4870.443    18.6  160.4  9.754  280.55 0.0   0.0   8.66  1.0   1.0    10.0  4.0  1.0  10.0
'Source 2'  340.486  4870.640    50.1  160.7  4.251  380.4  0.0   0.0   7.66  1.0   1.0    10.0  4.0  1.0  10.0
'Source 3'  341.051  4870.048   35.85  160.9  3.1    289.9  0.0   0.0   2.66  1.0   1.0    10.0  4.0  1.0  10.0
```

Source Name	X (KM)	Y (KM)	H (mAGL)	Elev (mMSL)	D (m)	T (K)	U (m/s)	V (m/s)	W (m/s)	Sigmay (m)	Sigmaz (m)	Q1 (g/s)	Q2 (g/s)	Q3 (g/s)	Q4 (4 species here) (g/s)

Time-varying data must be assigned to each of the sources, which are identified by name. These are matched to the names entered in the time-invariant data section. In this example, there are 3 sources and 4 records. The first record contains the start-time and end-time for the period in which the data are valid. The source data follow in the form determined by the value of Var1 entered in the time-invariant data section (current implementation recognizes Var1=1). This set of records is repeated for all time periods in the file.

Record 1: (8 variables)

Start Year, Julian Day, Hour, Second (0-3599), End Year, Julian Day, Hour, Second(0-3599) (integers) **Free-Format**

(Var1=1)
Record 2 through NSRC+1 (NSRC=number of sources):

Source Name, X, Y, H, Elev, D, T, U, V, W, Sigmay, Sigmaz, (Q(n), n=1,NSPEC) (char*16, reals) **Free-Format** (quotes required on Source Name)

- X,Y,H Flare-tip location
- Elev Elevation of the surface above sea level at the flare location
- D Effective flare diameter
- T Effective flare temperature
- U,V,W Effective initial flare velocity components (U along X, V along Y, W vertical)
- Sigmay Initial sigma-y for flare
- Sigmaz Initial sigma-z for flare
- Q(n) Emission rate for each species, in the order defined by the species names in the header

1.2.4 METSERIES V7.0.0

Modifications to METSERIES v1.81 Level 110308 allow the CALMET surface pressure to be written out in the TIMESERIES output file (TSF file). METSERIES Version 7.0.0, outputs the CALMET surface pressure along with the "OTHER" CALMET micrometeorological variables when the input parameter OTHER is set to 1 in the METSERIES.INP input file. The CALMET surface pressure is flagged by the symbol "SFC_PRESS", written in the last column of the TSF records, and expressed in millibar units. A TIMESERIES example is displayed in Table 1-8.

With this modification, all the variables that are needed by ABFLARE to compute the flame length, combustion efficiency and flare emissions can be extracted at the location of the flare stack and height of the flame by METSERIES, either from a CALMET dataset or from a MM5/WRF file (in M3D format).

Additionally, a bug in the prior versions of METSERIES has been fixed and will now avoid run termination when processing a SURF.DAT file with missing records.

Table 1-8 Example TIMESERIES.TSF file (with CALMET surface pressure output)

```
TIMESERIES.TSF  1.3             Full location/date/time documentation
 3      --- comment lines
Created by METSERIES (Version 1.81FL, Level 121201)
Time series from a CALMET.DAT file
NEUTRAL wind profiling method is used
 4      --- station information lines
(11)
CALMET.DAT: Nearest Grid Pt [(I,J)=(    7.000,    7.000)])][(X,Y)km=(   250.000,  4700.000) in MODEL Projection]
Input location:   (X,Y)km=(   250.000  4700.000) in UTM   Projection below
Nearest Grid Pt:  (X,Y)km=(   250.000  4700.000) in UTM   Projection below
UTM
  19N
NAS-C   02-21-2003
KM
UTC-0500
GREGORIAN_YMD
1988  7  7  5 0000 1988  7  7  9 0000    3600
   13     --- measure, units, mol.wt., missing,  Z_m,  X or LON,  Y or LAT
WDIR                DEGREES   -1.000    9999.000      10.000     250.000    4700.000
WSPEED              M/S               -1.000    9999.000      10.000     250.000    4700.000
TEMP                K                 -1.000    9999.000      10.000     250.000    4700.000
SHUMID              G/KG              -1.000    9999.000       1.000     250.000    4700.000
MIXHGT              METERS            -1.000    9999.000       0.000     250.000    4700.000
PRECIP_RATE         MM/HR             -1.000    9999.000       0.000     250.000    4700.000
USTAR                M/S              -1.000    9999.000       0.000     250.000    4700.000
MONIN_OB            METERS            -1.000    9999.000       0.000     250.000    4700.000
CONV_VEL_S           M/S              -1.000    9999.000       0.000     250.000    4700.000
SHORT_WAVE          W/M*2             -1.000    9999.000       0.000     250.000    4700.000
STAB_CLASS          CLASS             -1.000    9999.000       0.000     250.000    4700.000
RH_HUMIDITY         %                 -1.000    9999.000       2.000     250.000    4700.000
SFC_PRESS           MB                -1.000    9999.000       0.000     250.000    4700.000
 1988  7  7  5 0000 1988  7  7  6 0000   262.041     3.376   293.750    12.739   510.963  9999.000     0.599  -6.84096E+02     0.507   123.383         4        82   983.072
 1988  7  7  6 0000 1988  7  7  7 0000   263.098     4.115   295.240    12.960   524.072  9999.000     0.729  -7.50690E+02     0.661   159.348         4        76   983.411
 1988  7  7  7 0000 1988  7  7  8 0000   284.855     3.459   297.105    13.964   446.886  9999.000     0.629  -2.95951E+02     0.846   239.618         4        73   983.749
```

1.3 Post-Processing

1.3.1 Overview

Exponent created a series of new postprocessors to compute time-averages, maxima, n^{th} ranked and percentile concentrations (and deposition fluxes). One of the applications for this new set of CALPUFF postprocessors is to meet emergency flaring impact assessment requirements in general and in the Province of Alberta (Canada) in particular.

This new set of postprocessors streamlines the computation of the maximum (or n^{th} highest, or percentile) impact created by a short-lived event that can occur anytime during the year. This type of situation is typical for emergency events or upset conditions. In order to assess the potential impact of such an event, ideally 8,760 (8,784 in a leap year) simulations should be run, averages (if non-hourly averaging times are of interest e.g. daily averages) should be taken for each simulation, maxima should be identified, and then statistics (n^{th} highest, percentile) should be computed across all simulations. The suite of CALAVE-CALMAX-CALRANK postprocessors streamlines this approach as illustrated in Figure 1-1.

For short-lived events (couple of hours) and short-range impacts, it may not be necessary to run 8,760 (8,784) simulations. The number of simulations could for example be reduced to 24, with each simulation dealing with events starting at one of the 24 hours of the day, and repeating the event at this hour for each day of the year (Simulation 1 would model releases starting during the first hour of each day, Simulation 2 would model releases starting during the second hour of each day, etc.). Because the events and their impacts are short-lived, events on successive days are effectively independent of each other. This approach is often used for the assessment of emergency flaring and is illustrated in Figure 1-2. In any case, whether explicit simulations are run for each possible start time, or whether they are combined, the CALAVE-CALMAX-CALRANK suite can compute the necessary statistics.

Furthermore, any ranked-value or percentile can be computed with CALRANK, which thus extends the CALPOST n^{th} rank capability. Additionally, because specific percentile(s) can

be requested explicitly, the user does not have to convert the percentile into an n^{th} rank equivalent before conducting the post-processing.

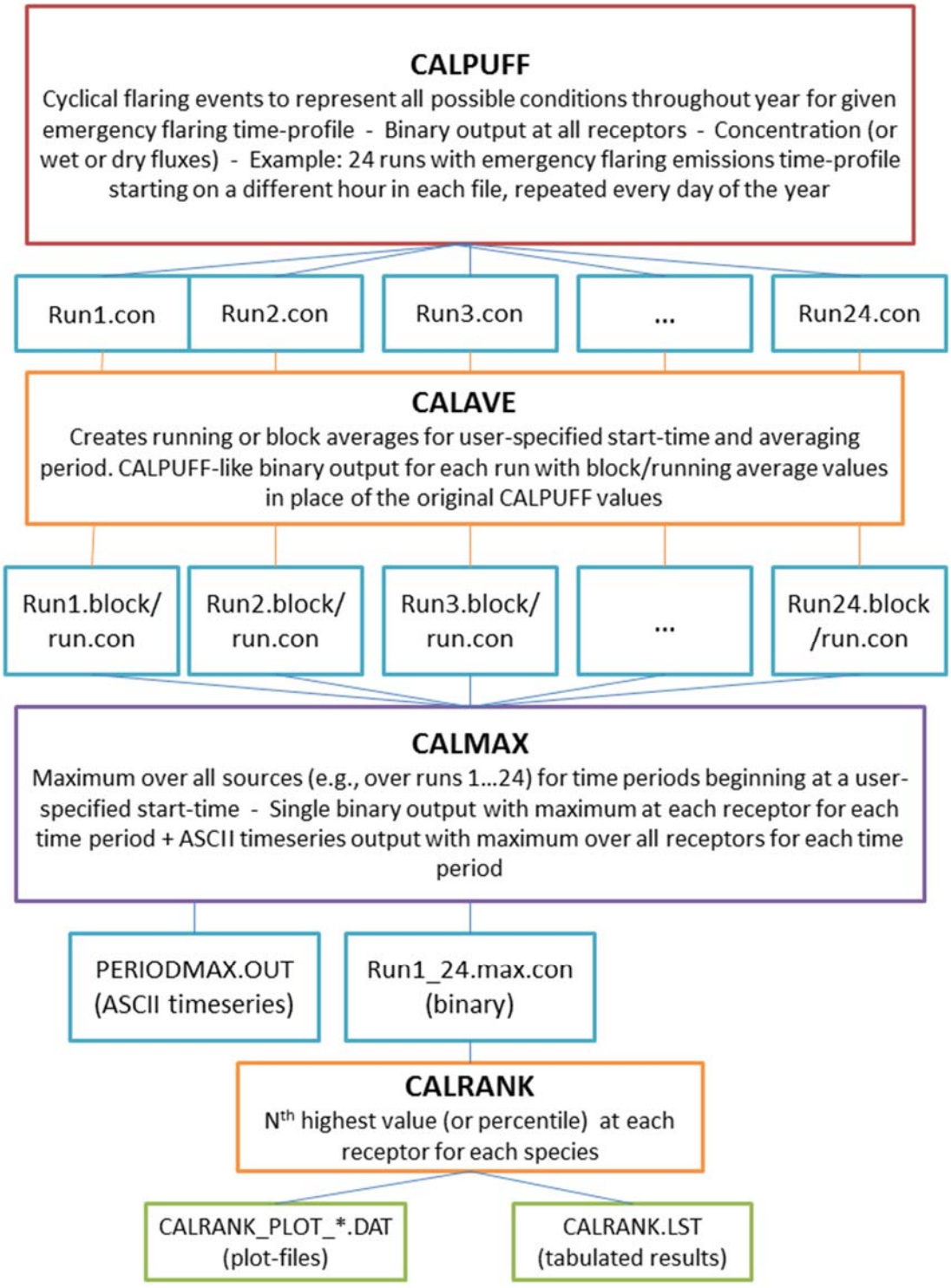

Figure 1-1 Post-Processing Flow

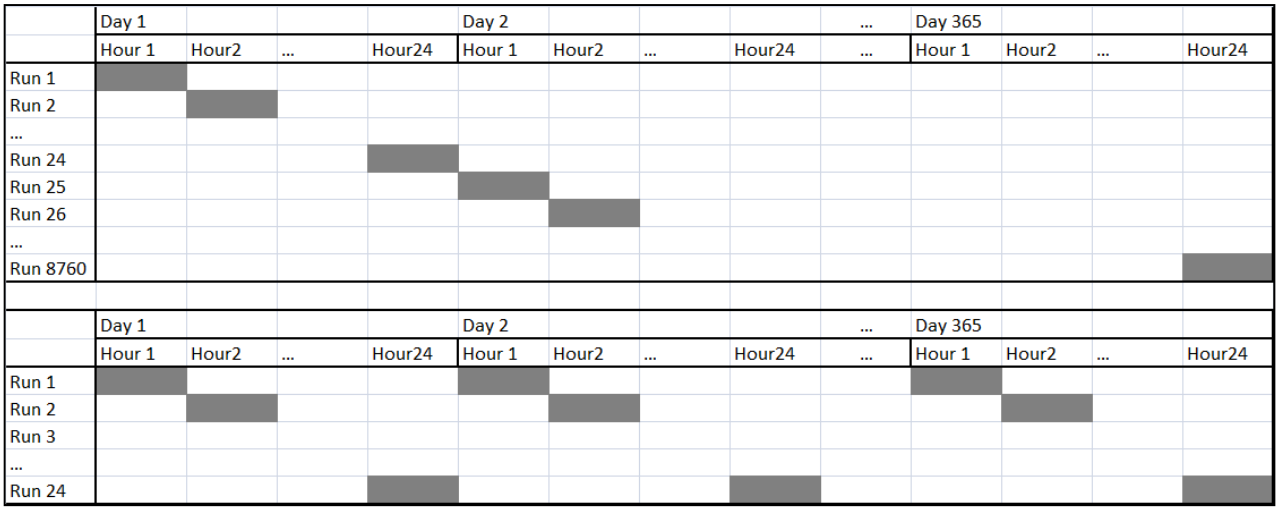

Figure 1-2 Simulation sequence for short-lived, short-range events which can occur any time of the year. Example illustrates 24 simulations with independent events starting every 24 hours in a cyclic fashion can be run instead of 8,760 individual runs (hour-long events are shown here).

1.3.2 CALAVE

CALAVE processes one or more CALPUFF binary output files (dataset v2.1 [CALPUFF output file created by CALPUFF prior to v6.41] or v2.2 [current output format with CALPUFF v6.42 and v7.2.0]) and computes either running-averages or block-averages of concentrations, dry deposition fluxes, or wet deposition fluxes for each file. The user instructs CALAVE when to start the averaging and what averaging time to use. A binary output file with a format similar to that of a binary CALPUFF output file is generated for each CALPUFF binary file that is being processed. When block averages are produced, the output file is the 'standard' CALPUFF file that can be processed by any of the postprocessors in the CALPUFF system. Running averages use the same format, but because begin and end-times for each average span a duration longer than the interval between the reported values, most of the postprocessors will not accept the running averages.

A sample CALAVE.INP file is included in Appendix A.

1.3.2.1 Mode 1: Running Averages

In Mode 1, CALAVE reads a CALPUFF output file (CONC, WET, DRY) and creates a running average of its contents. These averages are reported from a specified start-time and are written for each original data-period thereafter.

For example, if 24-hour averages starting at 10 a.m. (start time = 1000) are requested and the original CALPUFF output file contains half-hour values beginning at 0930 on March 13, the following averages will be computed:

1) First 24-hour average: 1000 (March 13) to 1000 (March 14)
2) Second 24-hour average: 1030 (March 13) to 1030 (March 14)
3) Third 24-hour average: 1100 (March 13) to 1100 (March 14)
4) The last 24-hour period will end at the end of the last 30-minute period in the file

1.3.2.2 Mode 2: Block Averages

In Mode 2, CALAVE reads a CALPUFF output file (CONC, WET, DRY) and creates a block average of its contents. These averages are reported from the specified start-time and are written end-to-end thereafter.

For example, if calendar-day 24-hour averages are requested (start time = 0000) and the original CALPUFF output file contains half-hour values beginning at 0930 on March 13, the following averages will be computed:

1) First 24-hour average: 0000 (March 14) to 0000 (March 15)
2) Second 24-hour average: 0000 (March 15) to 0000 (March 16)
3) Third 24-hour average: 0000 (March 16) to 0000 (March 17)
4) The last 24-hour period will end at the end of the last full day in the file

1.3.3 CALMAX

CALMAX reads a set of CALPUFF-type binary output files either created by CALPUFF directly or averaged with CALAVE, and selects the maximum value at each receptor for each

time period, for each species. The output time periods are contiguous blocks starting at a user-selected date and time, and the averaging time found in the data files determines the length of the block. All input data with a start-time within a block are associated with that block regardless of whether such data include times outside of the block. For example, a 3-hour running-average starting at 0700 covers the period 0700-1000. A CALMAX application with a start-time of 0000 will associate this running-average with the block from 0600-0900.

Many such files can be included without limit and CALMAX will cycle through all, selecting the maximum modeled value for each location and time. Since the main output file from CALMAX is also a CALPUFF-type binary file of "block-averages", CALMAX can be applied sequentially, using a mix of 'regular' CALPUFF files, CALAVE output files, and CALMAX files. The averaging time, receptors and species must be the same in all files.

A CALMAX application creates two output data files:

1. An ASCII time series file (PERIODMAX.OUT) of the maximum value over all receptors for each block of time for each species (one value per species per period).
2. A binary CALPUFF-format file of all maximum values (one maximum value at each receptor for each species and 'timestep').

A sample CALMAX input file and PERIODMAX.OUT output file is displayed in Appendix B.

1.3.4 CALRANK

CALRANK reads a CALPUFF-type concentration/flux output file (Dataset v2.1 or v2.2), ranks the time series for each species at each receptor for the entire application period, and identifies the n^{th}-highest values and the percentile values requested in the CALRANK.INP input file. More than one rank or percentile can be requested in a single run, and because of the overhead of ranking all of the values at each receptor, a single application with all desired ranks is normally prepared.

Individual plot-files are created for each requested rank/percentile, and include the location of each receptor, the value of the requested rank/percentile at that receptor, and the date and time at which that value occurred. If more than one species is in the file, this information is provided for each species. Additionally, the largest among all receptors is tabulated for each requested rank/percentile and species in the CALRANK.LST file.

Sample CALRANK.INP (input), CALRANK.LST (output) and CALRANK_PLOT_PCTL-75.00.DAT (75^{th} percentile output) files are displayed in Appendix C

1.3.5 EXAMPLE

Generate a 90^{th} percentile plot for hourly average impact of an unplanned two-hour long emergency flaring event

Step 1: CALPUFF

Run 24 CALPUFF annual simulations, with 24 FLEMARB.DAT emissions files starting on each hour of each day. Each emission profile lasts for 2 hours and is deemed independent and non-interacting with the next one in the same file (starting at the same hour on the following day). The emission profiles are generated with small timesteps and CALPUFF is run with 5 minute timesteps. The set up takes into account the fact that unplanned emergency flaring could start on any hour of the year and the set of meteorological conditions should be taken into account. The 24 CALPUFF simulations are run with the following FLEMARB.DAT emissions files and generate the following binary output files (CALPUFF_HH.CON):

1. FLEMARB_00.DAT (CALPUFF Emission starting at 0000 on Days 1, 2, 3 ….Day 365) → CALPUFF_00.CON

2. FLEMARB_01.DAT (CALPUFF Emission starting at 0100 on Days 1, 2, 3 ….Day 365) → CALPUFF_01.CON

   … (2 - 22 removed)

24. FLEMARB_23.DAT (CALPUFF Emission starting at 2300 on Days 1, 2, 3 ….Day 365) → CALPUFF_23.CON

Step 2: CALAVE

Run a single CALAVE simulation which will compute 1 hour block averages for each of the 24 annual CALPUFF simulations at each receptor, and create 24 annual CALPUFF binary output files with hourly timesteps (i.e. the 5 minute concentrations within every hour will be averaged to hourly values). CALAVE should be set up with:

- 24 CALPUFF_HH.CON files as input
- 1 hour averaging period (AVGPD_HH = 1 ; AVGPD_MM = 0)
- Mode =2 (block averages)
- Start time (00)
- → 24 output files:

  CALPUFF_00.CON.1BLOCK

  CALPUFF_01.CON.1BLOCK

  …

  CALPUFF_23.CON.1BLOCK

Step 3: CALMAX

Run a single CALMAX simulation to compute the maximum hourly concentrations at each receptor for each hour of the year. The maximum at each receptor is taken across the 24 CALPUF.CON.1BLOCK files generated by CALAVE.

- Input files: CALPUFF_01.CON.1BLOCK, … CALPUFF_23.CON.1BLOCK
- Output file: CALMAX_1hr.CON

Step 4: CALRANK

Run a single CALRANK simulation requesting the 90^{th} percentile (90^{th} percentile at each receptor for each species, date and time at which it occurred)

- Input file: CALMAX_1hr.CON
- Statistic parameter: PERCENTILE = 90 (specified in CALRANK.INP)
- Output plot file: PLOT_PCTL-90.000.DAT

2 Roadway

2.1 Introduction

Emissions from roadways are typically characterized by a distribution of sources located along each road. Commonly applied methods use strings of closely-spaced point/volume sources distributed along the roads. For large or complex road networks that can incur significant computational expense due to the large number of sources required, CALPUFF Version 7 introduces the capability of modeling the transport and dispersion of roadway emissions more efficiently than was previously possible.

The new approach simulates line sources such as roadways using the concept of rod-like puffs, or simply "rods". Emitting rods follow the same rules as emitting horizontally symmetric Gaussian puffs, but far fewer rods aligned with road segments are needed to emulate the uniform distribution of emissions along a road segment. Furthermore, the notion of a rod release can be applied to individual intermittent roadway sources, with a representative temporal pattern specified through the use of the module's variable emissions input file.

A rod represents a special case of the CALPUFF slug formulation in which all properties are uniformly distributed along its axis. This allows all transport and dispersion after release to be accomplished using the slug algorithms already in place. Reduced simulation times for larger domains are expected while maintaining the near-field details embodied in the initial effective source distributions. Near-field "hot spots" can be resolved as well as the drift of pollutants to sensitive areas further away.

2.2 Modeling Procedures

Each roadway link in a simulation is treated as a discrete, named source and is defined as a section of the road for which emissions (g/m/s) are uniform. Link properties include the effective height above ground, the initial concentration distribution width (σ_y) and height (σ_z) perpendicular to the link axis, and the emission rate for all emitted species. Links with constant properties for the simulation period can be described in the model control file. Some variability

in emission rates may be included using emission factors for selected links and species. These factors can be specified by time-of-day, day-of-week, month, temperature, etc., so simple emissions profiles can be accommodated. Much more variation can be obtained using external variable emissions (RDEMARB.DAT) files which can include sub-hourly updates that do not need to be uniform in time.

A link is located by a series of two or more coordinate triples (x,y,z) that describe its path, where the vertical coordinate is the road elevation above mean sea level. A long, winding isolated road might be characterized by a single link made up of many coordinate triples. These points should be sufficient to resolve curves, but need not have uniform spacing. For example, a straight flat segment can be defined by 2 points, regardless of the distance covered. All line segments are automatically divided further within the model into segments that are limited by the modeling grid-cell boundaries (no segment may extend across multiple meteorological grid cells). One emission rate for each species is used for the entire link. Near a congested intersection, many short links may be required to resolve the spatial and temporal distribution of emissions.

Individual segments of a link emit rod-like puffs with the long axis aligned with the segment. Like symmetric puffs, many discrete rods are emitted sequentially in time and concentrations are obtained at receptors by integrating their impact during a sampling period as they are transported by the wind. A rod has a uniform mass distribution along its length and a single Gaussian lateral (σ_y) and vertical (σ_z) distribution across it and at each end. The ends of the rod have identical properties, as there is no difference in "age". Unlike slugs emitted from point sources, rods do not elongate in the transport direction during the emission time step, and so they have no young and old ends. Otherwise, they are treated just like slugs in the sampling routines. As the σ_y at the ends of a rod grow with time and become large compared to its length, the elongation of the rod becomes imperceptible and each eventually converts to a symmetric puff. Because puffs are sampled more quickly than slugs, this improves the overall efficiency of the simulation.

2.3 Road Emission File (RDEMARB.DAT)

This CALPUFF emissions file characterizes the distribution of one or more pollutants resulting from activities that are distributed along a network of roads or similar line-segments. Each segment generates an elongated puff or 'tube', which is described by the location and height of the endpoints of the segment and the effective vertical and horizontal cross-segment distribution sigmas at these points. Mass emissions per unit length along the segment are provided for all species modeled.

Roads are described by a sequence of coordinates provided for each road-link. Each link is entered as a discrete, named source and is defined as a section of the road for which emissions are uniform. A long, winding isolated road might be characterized by a single link made up of many coordinate triples (x,y,z) that describe its pathway. These points should be sufficient to resolve curves, but need not have uniform spacing. For example, a straight flat segment can be defined by two points, regardless of the distance covered. Long line segments are automatically divided further within the model into segments that are limited by the grid-cell boundaries (no segment may extend across multiple cells). One emission rate (in grams per second per meter) for each species is used for the entire road-link. Near a congested intersection, many short links might be required to resolve the spatial and temporal distribution of emissions. Each is entered and modeled as a discrete source.

The sequence of coordinates (x,y,z) that defines each link appears in the header, and so is constant for the simulation. The sequence may be specified in a coordinate system other than that used in the dispersion model, and will be transformed within the model. Time-varying properties are provided in the data records that follow the header, and include the height above ground, the initial distribution parameters (σ_y and σ_z,) and the emission rate for all emitted species.

The beginning and ending times of each data record are specified as year, Julian-day, hour and seconds, and can be of arbitrarily varying duration. However, as for all other arbitrarily-varying emissions files, the ending time of one record must be equal to the beginning time of the next

record and periods of inactivity (zero emission) must be explicitly defined with zero emission rates.

The RDEMARB.DAT record description and format are detailed in Table 2-1 through Table 2-5. As some records in the RDEMARB.DAT file are processed via a formatted read in CALPUFF, attention must be paid to the length, type, and spacing in between each variable when preparing the RDEMARB.DAT file.

Table 2-1 Example Road Emissions File with Arbitrarily Varying Data (RDEMARB.DAT)

```
RDEMARB.DAT     1.0             Initial configuration
   3
Comment Line 1
Comment Line 2
Comment Line 3
UTM
  19N
NAS-C   02-21-2003
  KM
UTC-0500
2002 009  00  0000  2002 009  20 0000
   2   1
'SO2'
      30.000
'MAIN_ST_32'      8
    1.      340.000  4875.500    101.000        0.000   0.000   0.000   0.000
    2.      342.087  4875.492    100.500        0.000   0.000   0.000   0.000
    3.      344.171  4872.470    103.000        0.000   0.000   0.000   0.000
    4.      344.250  4871.433    105.000        0.000   0.000   0.000   0.000
    5.      345.321  4868.383    101.000        0.000   0.000   0.000   0.000
    6.      343.383  4865.321    105.000        0.000   0.000   0.000   0.000
    7.      341.433  4860.250    110.040        0.000   0.000   0.000   0.000
    8.      340.470  4861.171    108.600        0.000   0.000   0.000   0.000
'CENTRAL'         4
    1.      339.000  4879.500     96.000        0.000   0.000   0.000   0.000
    2.      334.021  4876.600    101.000        0.000   0.000   0.000   0.000
    3.      336.370  4876.400    108.000        0.000   0.000   0.000   0.000
    4.      338.750  4877.503    113.000        0.000   0.000   0.000   0.000
   2002  009  00 0000    2002  009  05 0000
'MAIN_ST_32'  2.0  4.2   3.0     .040
'CENTRAL'     1.0  3.5   1.5     .020
   2002  009  05 0000    2002  009  06 0000
'MAIN_ST_32'  2.0  4.2   3.0     .050
'CENTRAL'     1.0  3.5   1.5     .021
   2002  009  06 0000    2002  009  20 0000
'MAIN_ST_32'  2.2  4.2   3.5     .060
'CENTRAL'     1.1  3.5   1.6     .025
```

Table 2-2 RDEMARB.DAT Header Record Variables

`RDEMARB.DAT 1.0 Initial configuration`	Dataset Name, Dataset Version, Dataset Message (char*16, char*16, char*64) **Format: (2a16,a64)**
`3`	Number of comment lines to follow (integer) **Free-Format**

`Comment Line 1`
`Comment Line 2`
`Comment Line 3`
	Comment lines (80 characters per record are read)

`UTM` **`19N`**	Map Projection Type (char*8) **Format: (a8)** UTM Zone, Hemisphere (integer,char*1) **Format: (i4,a1)** *[See Table 3-5 for alternate map projection records]*
`NAS-C 02-21-2003`	DATUM code and date (char*8, char*12) **Format: (a8,a12)**
`KM`	Map units are kilometers (char*4) **Format: (a4)**
`UTC-0500`	Time Zone as (UTC+hhmm) (char*8) **Format: (a4)**
`2002 009 00 0000 2002 009 20 0000`	Start time and end time of data in file as Year, Julian Day, Hour, Second (0-3599) (integer) **Free-Format**
`2 1`	Number of sources, Number of species (integer) **Free-Format**
`'SO2'`	Species names (char*16) **Free-Format (single quotes required)**
`30.000`	Molecular weights for species (real) **Free-Format**

Table 2-3 RDEMARB.DAT Time-Invariant Data Records

```
'MAIN_ST_32'      8
    1.      340.000  4875.500    101.000        0.000   0.000   0.000   0.000
    2.      342.087  4875.492    100.500        0.000   0.000   0.000   0.000
    3.      344.171  4872.470    103.000        0.000   0.000   0.000   0.000
    4.      344.250  4871.433    105.000        0.000   0.000   0.000   0.000
    5.      345.321  4868.383    101.000        0.000   0.000   0.000   0.000
    6.      343.383  4865.321    105.000        0.000   0.000   0.000   0.000
    7.      341.433  4860.250    110.040        0.000   0.000   0.000   0.000
    8.      340.470  4861.171    108.600        0.000   0.000   0.000   0.000
'CENTRAL'         4
    1.      339.000  4879.500     96.000        0.000   0.000   0.000   0.000
    2.      334.021  4876.600    101.000        0.000   0.000   0.000   0.000
    3.      336.370  4876.400    108.000        0.000   0.000   0.000   0.000
    4.      338.750  4877.503    113.000        0.000   0.000   0.000   0.000
```

Source 1 to N (number of sources):
- Name and number of points (char*16, integer)
  - **Free-Format**
  - (single quotes required around Source Name)
- Coordinates with elevation for each point (reals)
  - Point number, X(km), Y(km), Z(m MSL), NULL(4)
  - **Free-Format**

- Time-invariant data must be assigned to each of the sources (identified by Source Name). In the example above, there are two sources (`'MAIN_ST_32'` and `'CENTRAL'`) with a corresponding block of time-invariant data records for each.
- Coordinates are in the map projection defined in the header (see CALPUFF documentation for supported projection and datum codes).
- The NULL variables are currently placeholders and should be entered with zero values as shown above.

Table 2-4 RDEMARB.DAT Time-Varying Data Records

```
   2002  009  00 0000    2002  009  05 0000
'MAIN_ST_32'  2.0  4.2   3.0     .040
'CENTRAL'     1.0  3.5   1.5     .020
   2002  009  05 0000    2002  009  06 0000
'MAIN_ST_32'  2.0  4.2   3.0     .050
'CENTRAL'     1.0  3.5   1.5     .021
   2002  009  06 0000    2002  009  20 0000
'MAIN_ST_32'  2.2  4.2   3.5     .060
'CENTRAL'     1.1  3.5   1.6     .025
```

Time Period 1 to N (spanning start to end time in file):
- Period start and end times (integers)
  - Start Year, Julian Day, Hour, Second(0-3599),
  - End Year, Julian Day, Hour, Second(0-3599)
  - **Free-Format**

- Time-varying data (***repeated for Source 1 to N***)
  - Name (char*16; single quotes required)
  - Height above ground of initial distribution (real)
    - (meters above ground level)
  - Initial sigma-y (across the 'tube') (real)
    - (meters)
  - Initial sigma-z (real)
    - (meters)
  - Emission rate (***repeated for each species in the order defined by the species names in the header***) (real)
    - (grams per second per meter)
  - **Free-Format**

- Time-varying data must be entered for each source matching the source names entered in the time-invariant data section.
- In the example above, there are three time periods (spanning the start to end times of the data in the file) with a corresponding block of time-varying data for each of the two sources (`'MAIN_ST_32'` and `'CENTRAL'`) below each.

Table 2-5 RDEMARB.DAT Map Projection Records

UTM **19N**	**Universal Transverse Mercator** Map Projection Type (char*8) **Format: (a8)** UTM Zone, Hemisphere (integer,char*1) **Format: (i4,a1)**
LCC **40.5N 90.0W 30.0N 60.0N** **0.00000000E+00 0.00000000E+00**	**Lambert Conformal Conic** Map Projection Type (char*8) **Format: (a8)** Origin Latitude, Origin Longitude, and two matching parallels (char*16) **Format: (4a16)** False Easting and Northing km (real) **Free-Format**
TTM **40.5N 90.0W** **0.00000000E+00 0.00000000E+00**	**Tangential Transverse Mercator** Map Projection Type (char*8) **Format: (a8)** Origin Latitude, Origin Longitude (char*16) **Format: (2a16)** False Easting and Northing km (real) **Free-Format**
PS **40.5N 90.0W 30.0N**	**Polar Stereographic** Map Projection Type (char*8) **Format: (a8)** Origin Latitude, Origin Longitude, and 1 matching parallel (char*16) **Format: (3a16)**
EM **0.0N 90.0W**	**Equatorial Mercator** Map Projection Type (char*8) **Format: (a8)** Origin Latitude, Origin Longitude (char*16) **Format: (2a16)**
LAZA **40.5N 90.0W** **0.00000000E+00 0.00000000E+00**	**Lambert Azimuthal Equal Area** Map Projection Type (char*8) **Format: (a8)** Origin Latitude, Origin Longitude (char*16) **Format: (2a16)** False Easting and Northing km (real) **Free-Format**

3 Spray

3.1 Introduction

Exponent was retained by the U.S. Department of Agriculture (USDA) Forest Service to update the CALPUFF model in order to accommodate emissions produced during aerial spraying activities. The emissions input to the CALPUFF model are produced by the model AGDISP which predicts the motion of spray material released from aircraft, including evaporation and turbulent dispersion within the aircraft wake. The hand-off to CALPUFF will be executed at a time after release when all turbulent vortices have died down and evaporation of the droplet volatile fraction is complete. AGDISP will export the position, elevation, final droplet diameter and emissions associated with the range of particle sizes released from each aircraft nozzle. These values will be accepted by CALPUFF version 7.3.0 and used to define sources for the purpose of predicting further down-wind dispersion and deposition.

3.2 CALPUFF Code Updates

The CALPUFF version 7.3 code was updated to include a new SPRAY source type. This source type has been developed in order to represent the distribution of liquid droplets which are generated by aerial spraying applications or similar activities. Conceptually, this new source corresponds to a set of line-sources or 'tubes', which are described by the location and height of the endpoints of the flight track and an effective initial vertical and horizontal cross-track distribution (σ_x and σ_y) at these points. The concentration distribution for each tube is essentially equivalent to the distribution which would be achieved through the use of a large number of adjacent volume sources and is similar to the configuration used for the ROAD source introduced in CALPUFF version 7.2. Mass emissions per unit length per second along the track are provided for all species modeled. Each 'tube' will contain droplets of a single diameter size and all species are modeled as being contained within the common droplets. Multiple 'tubes' in the same spray-track can be used to represent the distribution of different droplet diameters.

The SPRAY source and CALPUFF code have been designed conceptually to allow the evaporation calculations present in the AGDISP model to be continued in the CALPUFF simulation after hand-off. At the present time, the values necessary to perform these calculations have been included in an updated CALPUFF control file and external variable emissions file, but the evaporation option is not active. It is anticipated that for the initial situation under consideration, evaporation will be complete within a reasonably short period after the release, so that further evaporation in CALPUFF is not presently required.

In order to implement this new SPRAY source type, updates have been made to the CALPUFF input control file and a new variable emissions file for SPRAY sources (SPEMARB.DAT) has been created. The sections below detail the changes and updates which have been made.

3.3 Control File Updates

The CALPUFF version 7.0 control file has been updated to version 7.01 in order to accept parameters necessary to model the SPRAY source. The following additions were made to the control file structure.

Input Group 0 (*Added parameter*):

```
Number of SPRAY source files (SPEMARB.DAT)
with time-varying data (NSPDAT)
                                Default: 0       ! NSPDAT   =  1 !
```

The value of NSPDAT reflects the number of external time varying emissions files which will be provided. The external time varying emissions files follow a format which will be explained in section 4.

Input Group 0g (*Added field*)

```
------------
Subgroup (0g) – SPEMARB.DAT files
-------------

  SPRAY Source File Names
  The following SPEMARB.DAT filenames are processed if NRDDAT>0
  A total of NSPDAT lines is expected with one file name assigned per line
  Each line is treated as an input group and must terminate with END
  (surrounded by delimiters)
  (Each file contains emissions parameters for the entire period modeled
   for 1 or more sources)

Default Name  Type          File Name
------------  ----          ---------
 none         input       ! SPDAT= SPEMARB.DAT   !   !END!
```

The name and path (if required) of each time varying emissions file is provided in input group 0g.

Input Group 2 (*Added parameter*)

```
     Evaporation modeled ? (MEVAP)           Default: 0    ! MEVAP =  0   !
        0 = no
        1 = yes  (evaporation rates specified -[not currently available])
        2 = yes  (evaporation rates internally calculated -[not currently
available])
```

The parameter MEVAP has been added to the control file structure in order to allow for future implementation of evaporation within the CALPUFF model. The option is not presently implemented and use of any value other than 0 will result in a warning message and termination of the run.

Input Group 3a (*Table format modified*)

```
                                                                      OUTPUT GROUP
    SPECIES       MODELED       EMITTED     DEPOSITED          DROPLETS         NUMBER
     NAME      (0=NO, 1=YES) (0=NO, 1=YES) (0=NO,             (0=NO, 1=YES)    (0=NONE,
   (Limit: 12                              1=COMPUTED-GAS                      1=1st CGRUP,
    Characters                             2=COMPUTED-PARTICLE                 2=2nd CGRUP,
    in length)                             3=USER-SPECIFIED)                   3= etc.)
!        ACT1  =      1,          1,           2,                  1,             0   !
!        ADD1  =      1,          1,           2,                  1,             0   !
```

The table in Input Group 3a has been modified to include a column (column 5) noting which species will be modeled as droplets. Species which are modeled as droplets will all have a common diameter defined by the diameter of the droplet. Any modification to the droplet

diameter will affect all species contained within it. Presently droplets can only be emitted from SPRAY sources and a run which includes droplets cannot contain other non-droplet species.

Input Group 8 (*Modified Documentation*)

```
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.

     For DROPLET species, the GEOMETRIC MASS MEAN DIAMETER is included
     in the external variable emissions file.  Values should not be
     reported here for droplet species

      SPECIES      GEOMETRIC MASS MEAN        GEOMETRIC STANDARD
       NAME             DIAMETER                 DEVIATION
                        (microns)                (microns)
      -------      ------------------        ------------------

!END!
```

Input Group 8 provides for the input of size parameters for dry deposition of particles. Droplets are modeled as particles, but size parameters are not entered in this input group for species included in droplets. For these species, the size parameters will be provided in the external variable emissions file. Documentation has been added in this section to clarify use when modeling droplets.

Input Group 10b (*New Input Group*)

```
---------------
Subgroup (10b)
---------------

     Scavenging Coefficient for droplet species
     All species contained in a drop will have
     common scavenging coefficients based on the
     droplet.
     (SCSPRAY)

                      Scavenging Coefficient -- Units: (sec)**(-1)

                      Liquid Precip.       Frozen Precip.
                      --------------       --------------
!      SCSPRAY =         1.0E-04,             3.0E-5 !


!END!
```

Input Group 10b provides wet deposition scavenging coefficients for species modeled as droplets. For non-droplet species, these parameters are provided for each species in Input Group 10a (which in previous input file formats was labeled as Input Group 10). Droplet species will all have common values.

Input Group 11c (*New Input Group*)

```
--------------
Subgroup (11c)
--------------

     Each species modeled as evaporating in Input Group 3a
     should have an evaporation rate set here.  (Current code does
     not include evaporation. – Option is not Active)

                      Evaporation Rates -- Units: (um2/deg C/sec)

       Pollutant      Evaporation Rate
       ---------      --------------
!          H2O =         84.76  !
! END !
```

Input Group 11c was implemented to accept an evaporation rate consistent with the evaporation calculations made in AGDISP. The option to calculate evaporation is not presently active in CALPUFF so this value is not used in the current version of the code.

Input Group 19 (*New Input Group*)

```
---------------
Subgroup (19)
---------------

     Emissions from spray lines are generated from individual line segments
     defined by a sequence of coordinates provided for each spray-link.  Each
     link is entered as a discrete source and is defined as a section of the
     spray line for which emissions are uniform.

     Long spray line segments are automatically
     divided further within the model into segments that are limited by the
     grid-cell boundaries (no segment may extend across multiple cells).
     One emission rate (g/m/s) for each species is used for the entire line.

     Number of spray-lines with arbitrarily time-varying
     emission parameters (NSP2)          No default      !  NSP2 =  2   !
     (If NSP2 > 0, ALL variable road data
     are read from the file: SPEMARB.DAT)

!END!
```

Input Group 19 is a new input group to accept the SPRAY emission source. The variable NSP2 denotes the number of spray-lines which will be included in the external variable emissions file (SPEMARB.DAT).

3.4 External Variable Emissions SPRAY File (SPEMARB.DAT)

The CALPUFF external variable spray emissions file characterizes the distribution of air-born droplets or particulates resulting from spraying operations carried out from a moving platform (e.g., aircraft, truck, etc.) where the speed of the spray-craft dominates the geometry of the emitted trail.

The tracks locations, droplet diameters and mass emission rates are specified in SPEMARB.DAT. Coordinate projection parameters and time zones are defined in the header and so may be independent of the map projection and time zone selected for the CALPUFF simulations.

The beginning and ending times of each record are specified as year, Julian-day, hour and seconds, and can be of arbitrarily varying duration. However, as for all other arbitrarily-varying emissions files, the ending time of one record must be equal to the beginning time of the next record and periods of inactivity (zero emission) must be explicitly defined with zero emission rates.

The SPEMARB.DAT record description and format are detailed in Table 3-1 through Table 3-4. Not all records in a SPEMARB.DAT file are “free reading” and attention must be paid to the length of each variable, type, and spacing in between them.

Table 3-1 Example SPRAY Emissions File with Arbitrarily Varying Data (SPEMARB.DAT)

```
SPEMARB.DAT     1.0            Initial configuration
   6
Header records are a mix of formatted and free-format structures
Time-invariant data records are free-format
Time-invariant data records allow 3 assignments per source (none are currently used)
Time-variable data records are free-format
Time-variable data records contain
  X1(km),Y1(km),Z1(mASL),H1(mAGL),Sigy1(m),Sigz1(m),X2(km),Y2(km),Z2(mASL),H2(mAGL),Sigy2(m),Sigz2(m),
Pdiam(um),Dcut(um),Q(g/m/s)...
UTM
  19N
NAS-C   02-21-2003
  KM
UTC-0500
1990 009  04  0000  1990 009  10 0000
   3   2
'NONVOLATILE' 'ACTIVE1'
      30.00   30.000
'Source 1'       0.0    0.0    0.0
'Source 2'       0.0    0.0    0.0
'Source 3'       0.0    0.0    0.0
   1990  009  04 0000     1990  009  04 0001
'Source 1'  340.486  4870.640 10.0 9.4 5.1 5.1 341.051  4870.048 10.0 9.4 5.1 5.1  3.0  2.0  .10 .05
'Source 2'  340.486  4870.640 10.0 6.9 5.8 5.8 341.051  4870.048 10.0 6.9 5.8 5.8  3.0  2.0  .10 .05
'Source 3'  340.486  4870.640 10.0 5.9 5.9 5.9 341.051  4870.048 10.0 5.9 5.9 5.9  3.0  2.0  .10 .05
   1990  009  04 0001     1990  009  04 1835
'Source 1'  340.486  4870.640 10.0 9.4 5.1 5.1 341.051  4870.048 10.0 9.4 5.1 5.1  3.0  2.0  .00 .00
'Source 2'  340.486  4870.640 10.0 6.9 5.8 5.8 341.051  4870.048 10.0 6.9 5.8 5.8  3.0  2.0  .00 .00
'Source 3'  340.486  4870.640 10.0 5.9 5.9 5.9 341.051  4870.048 10.0 5.9 5.9 5.9  3.0  2.0  .00 .00
   1990  009  04 1835     1990  009  10 1836
'Source 1'  341.486  4871.640 10.0 9.4 5.1 5.1 342.051  4871.048 10.0 9.4 5.1 5.1  3.0  2.0  .10 .05
'Source 2'  341.486  4871.640 10.0 6.9 5.8 5.8 342.051  4871.048 10.0 6.9 5.8 5.8  3.0  2.0  .10 .05
'Source 3'  341.486  4871.640 10.0 5.9 5.9 5.9 342.051  4871.048 10.0 5.9 5.9 5.9  3.0  2.0  .10 .05
   1990  009  04 1836     1990  009  10 0000
'Source 1'  341.486  4871.640 10.0 9.4 5.1 5.1 342.051  4871.048 10.0 9.4 5.1 5.1  3.0  2.0  .00 .00
'Source 2'  341.486  4871.640 10.0 6.9 5.8 5.8 342.051  4871.048 10.0 6.9 5.8 5.8  3.0  2.0  .00 .00
'Source 3'  341.486  4871.640 10.0 5.9 5.9 5.9 342.051  4871.048 10.0 5.9 5.9 5.9  3.0  2.0  .00 .00
```

Example header records for each map projection (either 2 or 3 records):

Universal Transverse Mercator

```
UTM
  19N
```

Lambert Conformal Conic

```
LCC
40.5N           90.0W           30.0N           60.0N
0.00000000E+00 0.00000000E+00
```

Tangential Transverse Mercator

```
TTM
40.5N           90.0W
0.00000000E+00 0.00000000E+00
```

Polar Stereographic

```
PS
40.5N           90.0W           30.0N
```

Equatorial Mercator

```
EM
0.0N            90.0W
```

Lambert Azimuthal Equal Area

```
LAZA
40.5N           90.0W
0.00000000E+00 0.00000000E+00
```

Table 3-2 SPRAY Emissions File With Arbitrarily Varying Data (SPEMARB.DAT): Description of Header Variables

SPEMARB.DAT 1.0 Initial configuration	Dataset Name, Dataset Version, Dataset Message (char*16, char*16, char*64) **Format: (2a16,a64)**
6	Number of comment lines to follow (integer) **Free-Format**
Header records are a mix of formatted and free-format structures Time-invariant data records are free-format Time-invariant data records allow 3 assignments per source (none are currently used) Time-variable data records are free-format Time-variable data records contain X1(km),Y1(km),Z1(mASL),H1(mAGL),Sigy1(m),Sigz1(m),X2(km),Y2(km),Z2(mASL),H2(mAGL),Sigy2(m),Sigz2(m), Pdiam(um),Dcut(um),Q(g/m/s)...	Comment lines (80 characters per record are read) These should provide any information related to the model application. Here, the comments provide some documentation on the file structure.
UTM **19N**	- Map Projection (char*8) Format: (a8) - UTM Zone, Hemisphere (integer,char*1) **Format: (i4,a1)**
LCC **40.5N 90.0W 30.0N 60.0N** **0.00000000E+00 0.00000000E+00**	- Map Projection (char*8) **Format: (a8)** - Origin Latitude, Origin Longitude, and 2 matching parallels (char*16) **Format: (4a16)** - False Easting and Northing km (real) **Free-Format**
TTM **40.5N 90.0W** **0.00000000E+00 0.00000000E+00**	- Map Projection (char*8) **Format: (a8)** - Origin Latitude, Origin Longitude (char*16) **Format: (2a16)** - False Easting and Northing km (real) **Free-Format**
PS **40.5N 90.0W 30.0N**	- Map Projection (char*8) **Format: (a8)** - Origin Latitude, Origin Longitude, and 1 matching parallel (char*16) **Format: (3a16)**
EM **0.0N 90.0W**	- Map Projection (char*8) **Format: (a8)** - Origin Latitude, Origin Longitude (char*16) **Format: (2a16)**
LAZA **40.5N 90.0W** **0.00000000E+00 0.00000000E+00**	- Map Projection (char*8) **Format: (a8)** - Origin Latitude, Origin Longitude (char*16) **Format: (2a16)** - False Easting and Northing km (real) **Free-Format**
NAS-C 02-21-2003	DATUM code, date (char*8, char*12) **Format: (a8,a12)**
KM	Map units are KM (char*4) **Format: (a4)**
UTC-0500	Time Zone as (UTC+hhmm) (char*8) **Format: (a4)**
1990 009 04 0000 1990 009 10 0000	Start time and end time of data in file as Year, Julian Day, Hour, Second(0-3599) (integer) **Free-Format**
3 2	Number of sources, Number of species (integer) **Free-Format**
'NONVOLATILE' 'ACTIVE1'	Species names (char*16) **Free-Format** (quotes required)
30.000 30.000	Molecular weights for species (real) **Free-Format**

Table 3-3 SPRAY Emissions File With Arbitrarily Varying Data (SPEMARB.DAT): Description of Time-Invariant Data

`'Source 1'  0.0  0.0  0.0`
`'Source 2'  0.0  0.0  0.0`
`'Source 3'  0.0  0.0  0.0`
	Source Name, Var1 - Var3 (char*16, real)
	Free-Format (quotes required on Source Name)

Time-invariant data must be assigned to each of the sources, which are identified by name. In this example, there are 3 sources so there are 3 records. None of "Var" values are currently defined for use, but all 3 columns must have values (zeros).	

Table 3-4 SPRAY Emissions File With Arbitrarily Varying Data (SPEMARB.DAT): Description of Time-Varying Data

```
   1990  009  04 0000     1990  009  04 0001
'Source 1'  340.486  4870.640 10.0 9.4 5.1 5.1 341.051  4870.048 10.0 9.4 5.1 5.1  3.0  2.0  .10 .05
'Source 2'  340.486  4870.640 10.0 6.9 5.8 5.8 341.051  4870.048 10.0 6.9 5.8 5.8  3.0  2.0  .10 .05
'Source 3'  340.486  4870.640 10.0 5.9 5.9 5.9 341.051  4870.048 10.0 5.9 5.9 5.9  3.0  2.0  .10 .05
```

Source Name	X1 (KM)	Y1 (KM)	Z1 (mASL)	H1 (mAGL)	Sigmay1 (m)	Sigmaz1 (m)	X2 (KM)	Y2 (KM)	Z2 (mASL)	H2 (mAGL)	Sigmay2 (m)	Sigmaz2 (m)	Pdiam (um)	Dcut (um)	Q… (g/m/s)

Time-varying data must be assigned to each of the sources, which are identified by name. These are matched to the names entered in the time-invariant data section. In this example, there are 3 sources and 4 records. The first record contains the start-time and end-time for the period in which the data are valid. The entries when the source is emitting are 1 second long which is used to represent an instantaneous release. The source data follow. This set of records is repeated for all time periods in the file.

Record 1: (5 variables)

Year, Julian Day, Hour, Second(0-3599), Number of Active Sources for this Release (integers) **Free-Format**

Record 2 through NSRC+1 (NSRC=number of sources):

Source Name, X1, Y1, Z1,Sigmay1,Sigmaz1, H1, X2, Y2, Z2, H2, Sigmay2, Sigmaz2, Pdiam, Dcut, (Q(n), n=1,NSPEC) (char*16, reals)
Free-Format (quotes required on Source Name)

- X1,Y1,Z1,H1 Location of end 1 of track (X1,Y1,Z1 coordinate and H1 Height above ground)
- Sigmay1, Sigmaz1 Initial sigma-y across the 'tube' and initial sigma-z at end 1
- X2,Y2,Z1,H2 Location of end 2 of track (X1,Y1,Z1 coordinate and H1 Height above ground)
- Sigmay2, Sigmaz2 Initial sigma-y across the 'tube' and initial sigma-z at end 2
- Pdiam Aerodynamic particle size (um)
- Dcut Minimum diameter for evaporation (um)
- Q(n) Instantaneous Emission rate for each species (g/m/s), in the order defined by the species names in the header

3.5 Preparation of External Variable Emissions Files from AGDISP Output.

Coupling between AGDISP and CALPUFF is accomplished through an output file generated by AGDISP which can be used to produce a SPRAY External Variable Emissions file (SPEMARB.DAT) readable by CALPUFF. In AGDISP, an option must be selected under "Advanced Settings" specifying that the model should "Save CALPUFF data". After completion of the AGDISP run, the user can then select the menu option to "Export CALPUFF Data" which will open a screen for data input. The "Export CALPUFF Data" screen will allow input of 5 values:

- SPRAY Line Beginning X Coordinate (km)
- SPRAY Line Beginning Y Coordinate (km)
- Base Z Elevation (m)
- Spray Line Length (km)
- Flight Direction (0 deg = North) (deg)

Values for the SPRAY Line Beginning X and Y coordinates should be entered in a coordinate system consistent with the configuration of the CALPUFF run. Base Z Elevation represents a single base elevation representative of the field being sprayed. It will be used as the base elevation for all sources produced by AGDISP. The SPRAY Line Length and Flight Direction define the length and direction of the spray line relative to the beginning point.

The output file generated by AGDISP does not represent a complete SPRAY External Variable Emissions file (SPEMARB.DAT). Additional user editing is necessary to configure the data file for use in CALPUFF. A SPEMARB.DAT file consists of 3 main sections: Header Records (described in Table 3-2), Time Invariant Records (described in Table 3-3) and Time Varying Records (described in Table 3-4). The following sections describe generation of each of these record sections for a simple CALPUFF application using AGDISP output.

3.5.1 Header Records

The header records must be generated by the user and, consistent with Table 3-2, contain the following fields:

- A user defined number of comment lines
- Geographic projection information which should be consistent with the coordinates entered in the AGDISP "Export CALPUFF Data" screen
- Time zone and time period which should cover the full length of the desired CALPUFF simulation
- The number of sources and number of species. The number of sources can be determined based on the numbered sources listed in the AGDISP output file. The number of species will always be 2 for runs using an AGDISP output file. The two species produced by AGDISP are the Nonvolatile and Active portions of the spray. Those two species should be listed here
- The Species name, which must be consistent with the species name used in the CALPUFF input control file
- The Species molecular weight (a parameter not presently used in any CALPUFF calculations, but which must be present)

3.5.2 Time Invariant Records

The time invariant records contain a list of the modeled sources and their format is summarized in Table 3-3. No user editing is required in this section. Time invariant data is provided in the first portion of the output file generated by AGDISP. Each line contains a source name in quotes, followed by 3 numerical fields, each containing a value of 0.0. The numerical fields are not presently used by the CALPUFF code, but must be present. The number of lines of data defined in this section should match the number of sources listed in the Header Records.

3.5.3 Time Varying Records

Time varying records must be provided to cover the entire period of the CALPUFF run. Each time varying record includes a line containing a time beginning and time ending stamp for the emissions data. It then includes emissions data for each modeled source. The format is documented in Table 3-4. Data must be provided both for the time when the spray is released and the periods of time between spraying releases. The periods of time between releases include records for all sources, but emissions are zero for every source.

The output file generated by AGDISP provides blocks of time varying data required to define the source and emissions for multiple aerial passes. It includes records both for the spray emission periods, and the times between spray emissions. The user is required to edit the time beginning and ending fields, as described on the next page. Each time varying data record will contain multiple rod sources with differing locations and/or droplet diameters. The source and emissions data represent the values at the handoff time between AGDISP and CALPUFF. The fields contained in the AGDISP output file include:

- X coordinate for beginning of rod – X1 (km)
- Y coordinate for beginning of rod – Y1 (km)
- Base elevation for beginning of rod – Z1 (m)
- Height above ground for beginning of rod – H1 (m)
- sigma y for beginning of rod – σy1 (m)
- sigma z for beginning of rod – σz1 (m)
- X coordinate for ending of rod – X2 (km)
- Y coordinate for ending of rod – Y2 (km)
- Base elevation for ending of rod – Z2 (m)
- Height above ground for ending of rod – H2 (m)
- σ_y for ending of rod – σy2 (m)
- σ_z for ending of rod – σz2 (m)
- Droplet diameter (μm)
- Cut-off diameter for evaporation (μm)
- Nonvolatile emissions for this droplet diameter and position (g/m)
- Active emissions for this droplet diameter and position (g/m)

Note that the emissions provided by AGDISP are in units of g/m. In order to ensure that these units are consistent with the CALPUFF units of g/m/s, the length of the timestep when the spray is emitting will need to be defined to be 1 second long (See Table 3-1 for an example).

Each block of time varying data output by AGDISP begins with a place-holder string of text which reads “YYYY DDD HH SSSS YYYY DDD HH SSSS”. These fields must be replaced by the user with the year, Julian day, hour, and second representing the beginning and ending time of the represented period. For periods when a spray is emitted, the total length of time between the beginning and ending time must be 1 second. For example, to represent a spray release which occurs at 10 am on July 1st (Julian Day 182), 2010 the following beginning and ending time stamps should be used.

```
2010 182 10 0000     2010 182 10 0001
```

Time varying records must also be supplied for periods between spray releases. AGDISP will produce a second time varying block of data for this period with zero emissions for all sources. This block of data will again include a place-holder string of text which must be updated by the user. The time stamps used for this section should represent the period of time between the end of the last spray release and the beginning of the next release. For example, if spray releases are spaced 30 seconds apart, the time varying record representing the period between releases (with zero emissions) should use the following beginning and ending time stamps.

```
2010 182 10 0001     2010 182 10 0030
```

The time stamps for the next emitting spray line with a period of 1 second would be:

```
2010 182 10 0030     2010 182 10 0031
```

If AGDISP is configured to model multiple aerial passes, the output file will contain multiple sets of emitting and non-emitting time varying records. Each record will require the user to provide time stamps which follow the above pattern. The final non-emitting time varying record should cover the full time from the end of the last emitting spray to the end of the CALPUFF run.

Appendix A

Sample CALAVE.INP

CALAVE.INP

```
CALAVE.INP      1.0             Test Configuration
--------------------------------------------------------------------------------

                    CALAVE Processor CONTROL FILE
                    -----------------------------
PURPOSE
-------

Mode 1:  Running averages

This utility reads a CALPUFF output file (CONC, WET, DRY) and creates a running
average of its contents.  These averages are reported from a specified start-time
and are written for each data period thereafter.

For example, if 24-hour averages starting at 10AM (start time = 10:00) are
requested and the original CALPUFF output file contains half-hour values
beginning at 0930 on March 13:

  First  24-hour average:  1000 (March 13) to 1000 (March 14)
  Second 24-hour average:  1030 (March 13) to 1030 (March 14)
  Third  24-hour average:  1100 (March 13) to 1100 (March 14)

The last 24-hour period will end at the end of the last 30-minute period in the file.

Mode 2:  Block averages

This utility reads a CALPUFF output file (CONC, WET, DRY) and creates a blocked
average of its contents.  These averages are reported from a specified start-time
and are written end-to-end thereafter.

For example, if calendar-day 24-hour averages are requested (start time = 00:00)
and the original CALPUFF output file contains half-hour values beginning at 0930
on March 13:

  First  24-hour average:  0000 (March 14) to 0000 (March 15)
  Second 24-hour average:  0000 (March 15) to 0000 (March 16)
  Third  24-hour average:  0000 (March 16) to 0000 (March 17)

The last 24-hour period will end at the end of the last full day in the file.

--------------------------------------------------------------------------------

 Processing Options
-------------------

     Define the output averaging period in hours and minutes.  Typically, the
     hours will be zero when minutes are non-zero, and minutes will be zero
     when hours are non-zero.

     Averaging Period (hours)             Default: 0     ! AVGPD_HH =   3  !
     Averaging Period (minutes)           Default: 0     ! AVGPD_MM =   0  !


     Mode                                 No Default     ! MODE =  1  !
         1 = Running averages
         2 = Block averages

     Starting time (HHMM)                 Default: 0000  ! START_HHMM =  0000  !




Output Files
------------

   Output files are named by adding characters to the end of the input filenames
   in the form of a new extension.  For example, if an extension '.24_running'
   is entered, the output associated with the first file above would be named
   'source1.dat.24_running'.  Enter the extension, including any punctuation
```

```
   (must resolve to a legal file name) between delimiters:

     Output data file extension            Default: .ave  ! OUT_EXT = .24run !


   Name of output list file for run:

     List-file name               Default: CALAVE.LST     ! LSTFILE = calave.lst !



All file names will be converted to either lower or upper case
         T = lower case       (LCFILES)    Default: F     ! LCFILES = F !
         F = UPPER CASE


Input Files
-----------

   Provide one or more filenames for CALPUFF files to process
   (place assignments between delimiters):

      ! INPFILE = source1.dat !
      ! INPFILE = source2.dat !
      ! INPFILE = source3.dat !
      ! INPFILE = source4.dat !
      ! INPFILE = source5.dat !
      ! INPFILE = source6.dat !
```

Appendix B

Sample CALMAX.INP and PERIODMAX.OUT

CALMAX.INP

```
CALMAX.INP      1.0             Test Configuration
--------------------------------------------------------------------------------

                    CALMAX Processor CONTROL FILE
                    -----------------------------
PURPOSE
-------

This utility reads a set of CALPUFF-format output files (CONC, WET, or DRY)
and selects the maximum value at each receptor for each block of time.  These
time-blocks start at the beginning of the processing period defined below,
and the length of each block is equal to the averaging time of the data in the
input files (averaging time in all input files must match).  The input data
may consist of block-averages or running-averages.  The start of each average
may be different among the set of input files.  All averages with a start-time
that falls within an output time-block are compared when selecting the maximum
for the time-block.  If the period of data in a file begins later or ends
earlier than the processing period, CALMAX assumes that those data are zero at
these times.

Example:

Time         File 1            File2         Output Block
           (3-hr Avg)        (3-hr Avg)       (3-hr Avg)
-----------------------------------------------------
0000           x                 x               1 (start)
0100           x                 1 (start)       |   File2(1)
0200           x                 |               |
-----------------------------------------------------
0300           x                 |               2
0400           x                 2               |   File2(2)
0500           x                 |               |
-----------------------------------------------------
0600           1 (start)         |               3
0700           |                 3               |   MAX(File1(1),File2(3))
0800           |                 |               |
-----------------------------------------------------
0900           2                 |               4
1000           |                 4               |   MAX(File1(2),File2(4))
1100           |                 |               |
-----------------------------------------------------
1200           3                 |               5
1300           |                 x               |   File1(3)
1200           |                 x               |
-----------------------------------------------------

Many CALPUFF output files can be included without limit and CALMAX will cycle
through all.  Receptors and species must be the same in all files.

CALMAX creates a binary CALPUFF-format file of maximum values for each
species and each receptor for each time-block, which can be processed like any
standard CALPUFF file.  It also creates an ASCII timeseries file of the maximum
across all receptors for each time-block and each species.
--------------------------------------------------------------------------------

 Processing Period
-------------------

     Starting date:    Year     (S_YEAR)  --   No default   ! S_YEAR  =  1995  !
                       Month    (S_MONTH) --   No default   ! S_MONTH =  6  !
                       Day      (S_DAY)   --   No default   ! S_DAY   =  30 !
     Starting time:    HH:MM:SS (S_TIME)  --   No default   ! S_TIME  =  16:00:00  !

     Ending date:      Year     (E_YEAR)  --   No default   ! E_YEAR  =  1995  !
                       Month    (E_MONTH) --   No default   ! E_MONTH =  7  !
                       Day      (E_DAY)   --   No default   ! E_DAY   =  31 !
     Ending time:      HH:MM:SS (E_TIME)  --   No default   ! E_TIME  =  20:00:00  !


Output Files
```

```
------------

   ASCII file of Time-Block-Maximum values:

     File name                    No Default              ! PERFILE = calmax_period_blk_s.con !


   Binary CALPUFF-format file of all maximum values:

     File name                    No Default              ! BINFILE = calmax_test_blk_s.bin !


   Name of output list file for run:

     List-file name               Default: CALAVE.LST     ! LSTFILE = calmax_test_blk_s.lst !



All file names will be converted to either lower or upper case
         T = lower case       (LCFILES)    Default: F     ! LCFILES = F !
         F = UPPER CASE


Input Files
-----------

   Provide two or more filenames for CALPUFF files to process
   (place assignments between delimiters):

      ! INPFILE = flare.con.01-03blk !
      ! INPFILE = flare.con.02-03blk !
      ! INPFILE = flare.con.03-03blk !
      ! INPFILE = flare.con.04-03blk !
      ! INPFILE = flare.con.05-03blk !
      ! INPFILE = flare.con.06-03blk !
      ! INPFILE = flare.con.07-03blk !
      ! INPFILE = flare.con.08-03blk !
      ! INPFILE = flare.con.09-03blk !
      ! INPFILE = flare.con.10-03blk !
      ! INPFILE = flare.con.11-03blk !
      ! INPFILE = flare.con.12-03blk !
      ! INPFILE = flare.con.13-03blk !
      ! INPFILE = flare.con.14-03blk !
      ! INPFILE = flare.con.15-03blk !
      ! INPFILE = flare.con.16-03blk !
      ! INPFILE = flare.con.17-03blk !
      ! INPFILE = flare.con.18-03blk !
      ! INPFILE = flare.con.19-03blk !
      ! INPFILE = flare.con.20-03blk !
      ! INPFILE = flare.con.21-03blk !
      ! INPFILE = flare.con.22-03blk !
      ! INPFILE = flare.con.23-03blk !
      ! INPFILE = flare.con.24-03blk !
```

PERIODMAX.OUT

```
PERIODMAX.OUT   1.0
  8
------------------------------------------------------------------------
Prepared by CALMAX Version 1.1          Level 120915
Maxima from a set of CALPUFF output files; information about first is:
Processed by CALAVE Version 1.1          Level 120915
Original CALPUFF output is averaged to    3-hour,  0-minute periods
Averaging Method for Output:  RUNNING
CALPUFF      Version 6.42         Level 110325
------------------------------------------------------------------------
START(YYYYJJJHHSSSS) =       1995181160000
END  (YYYYJJJHHSSSS) =       1995212190000
NUMBER_PERIODS       =   249
NUMBER_SPECIES       =     2
'SO2           1'    'g/m3           '
'SO4           1'    'g/m3           '
 1995181160000 1995181190000      0.0000000E+00  0.0000000E+00
 1995181190000 1995181220000      0.1236652E-06  0.4296419E-06
 1995181220000 1995182010000      0.1620922E-06  0.4367350E-06
 1995182010000 1995182040000      0.1920760E-06  0.5641223E-06
 1995182040000 1995182070000      0.2449551E-06  0.6999548E-06
 1995182070000 1995182100000      0.2414128E-06  0.7225233E-06
 1995182100000 1995182130000      0.2257391E-06  0.8143888E-06
 1995182130000 1995182160000      0.2091050E-06  0.7982892E-06
 1995182160000 1995182190000      0.1993398E-06  0.7821818E-06
 1995182190000 1995182220000      0.1405862E-06  0.8824974E-06
 1995182220000 1995183010000      0.1541312E-06  0.7509557E-06
 1995183010000 1995183040000      0.1941535E-06  0.7105132E-06
 1995183040000 1995183070000      0.2419434E-06  0.7160419E-06
 1995183070000 1995183100000      0.2379932E-06  0.7245426E-06
 1995183100000 1995183130000      0.2252482E-06  0.7410509E-06
 1995183130000 1995183160000      0.2118052E-06  0.7659141E-06
 1995183160000 1995183190000      0.2213503E-06  0.6943087E-06
 1995183190000 1995183220000      0.2206614E-06  0.7885833E-06
 1995183220000 1995184010000      0.1754233E-06  0.6280415E-06
  . . .  (records removed)
 1995211040000 1995211070000      0.2389819E-06  0.9125792E-06
 1995211070000 1995211100000      0.2448705E-06  0.9817674E-06
 1995211100000 1995211130000      0.2148565E-06  0.9891634E-06
 1995211130000 1995211160000      0.2138693E-06  0.8830513E-06
 1995211160000 1995211190000      0.2050581E-06  0.8602494E-06
 1995211190000 1995211220000      0.1671577E-06  0.8617992E-06
 1995211220000 1995212010000      0.1653654E-06  0.7678133E-06
 1995212010000 1995212040000      0.1733464E-06  0.7147995E-06
 1995212040000 1995212070000      0.2328687E-06  0.7122401E-06
 1995212070000 1995212100000      0.2320222E-06  0.4438733E-06
 1995212100000 1995212130000      0.2211245E-06  0.4894759E-06
 1995212130000 1995212160000      0.2021380E-06  0.5094999E-06
 1995212160000 1995212190000      0.1918380E-06  0.5112856E-06
```

Appendix C

Sample CALRANK.INP, CALRANK.LST, and CALRANK_PLOT_PCTL.DAT

CALRANK.INP

```
CALRANK.INP     1.0             Test Configuration
------------------------------------------------------------------------------

                    CALRANK Processor CONTROL FILE
                    ------------------------------
PURPOSE
-------

This utility reads a CALPUFF-type concentration/flux output file (dataset v2.1
or v2.2), ranks the timeseries for each species at each receptor, and identifies
the nth-highest values and the percentile values requested below.
Plot-files are created for each requested rank/percentile, and the largest among
all receptors is tabulated for each rank/percentile and species.
------------------------------------------------------------------------------


Input File
----------

   File of modeled data (include path if desired):

     File name          No Default             ! DATFILE = CALMAX_TEST_BLK.BIN !


Results File
------------

   Name of output list file of results for run (include path if desired):

     File name          Default: CALRANK.LST    ! LSTFILE = calrank_test_blk.lst !


Plot Files
----------

Plot files are created for each rank/percentile requested, reporting the ranked value
of each species for each receptor with records containing x,y,v(1),v(2),...,v(nspec).
The filenames have a default structure composed of the results file name [LSTFILE]
with the rank or percentile appended.

Nth-Rank Plot File         [LSTFILE]_PLOT_RANK-nnnn.DAT
Pth-Percentile Plot File   [LSTFILE]_PLOT_PCTL-pp.ppp.DAT

All file names will be converted to either lower or upper case
         T = lower case       (LCFILES)    Default: F     ! LCFILES = F !
         F = UPPER CASE
```

Processing Options

Report values corresponding to the following Nth-highest and percentile values.
Enter specific ranks using either NTH_HIGHEST or PERCENTILE within
delimiters (exclamation point), placing one assignment per line

```
! NTH_HIGHEST  =   2  !
! NTH_HIGHEST  =   8  !
! NTH_HIGHEST  =   12 !


! PERCENTILE   =  98  !
! PERCENTILE   =  95  !
! PERCENTILE   =  90  !
! PERCENTILE   =  75  !
```

Reported mass units

(MASS_UNIT) Default: 1 ! MASS_UNIT = 3 !

1:	g/m**3	or	g/m**2/s	grams	
2:	mg/m**3	or	mg/m**2/s	milligrams	(1.0e-03 g)
3:	ug/m**3	or	ug/m**2/s	micrograms	(1.0e-06 g)
4:	ng/m**3	or	ng/m**2/s	nanograms	(1.0e-09 g)
5:	pg/m**3	or	pg/m**2/s	picograms	(1.0e-12 g)

Peak values that are ranked may be restricted to no more than 1 per calendar day (e.g., the calendar-day maximum). The day in which a value is placed is determined by its start-time.

Report as Calendar-Day maximums?

(ICDAY) Default: 0 ! ICDAY = 0 !

0 = No : all values at each receptor are ranked
(more than 1 rank may be in same day)
1 = Yes : peak value in calendar day at each receptor is ranked

CALRANK.LST

```
                    CALRANK RESULTS SUMMARY
                VERSION:1.1           LEVEL:120915


 File Processed: CALMAX_TEST_BLK.BIN

 Selected Header Information From File:
--------------------------------------------------------------------------------
Processed by CALMAX Version 1.0          Level 120915
Maxima from the set of CALPUFF output files is obtained
Processed by CALAVE Version 1.0          Level 120915
Original CALPUFF output is averaged to    3-hour,  0-minute periods
Averaging Method for Output:  BLOCK
Produced by CALPUFF Version: 6.42    Level: 110325
--------------------------------------------------------------------------------
 Information about data in file

 Averages (DAY,HH,MM,SS) =   0 3 0 0
 Type of Averaging       =  BLOCK
 Number of averages/day  =  8
 Number of days          =  32
 Number of receptors     =  20
 Number of species       =  6
 First day (YYYYJJJ)     =  1995181     UTC-0700
 Last day (YYYYJJJ)      =  1995212     UTC-0700


 Model data for each receptor are ranked over all times based on magnitude and
 the requested Nth-Highest and/or Percentile values are reported for each receptor
 in the output files:

 CALRANK_TEST_BLK_UG.LST_PLOT_RANK-0002.DAT
 CALRANK_TEST_BLK_UG.LST_PLOT_RANK-0008.DAT
 CALRANK_TEST_BLK_UG.LST_PLOT_RANK-0012.DAT
 CALRANK_TEST_BLK_UG.LST_PLOT_PCTL-98.000.DAT
 CALRANK_TEST_BLK_UG.LST_PLOT_PCTL-95.000.DAT
 CALRANK_TEST_BLK_UG.LST_PLOT_PCTL-90.000.DAT
 CALRANK_TEST_BLK_UG.LST_PLOT_PCTL-75.000.DAT
```

The largest of these for each rank are tabulated below with the location and time

Tabulation for Requested Nth-Highest Values
Results for the Maximum Receptor
All Values in Each Day are Included

N	Percentile	Species - Level	Modeled	Units	Location X (KM)	Location Y (KM)	Starting UTC-0700 Date (YYYY_JJJ)	Starting UTC-0700 Time (HH:MM:SS)
2	99.414	SO2 1	6.4238036E-01	ug/m3	-45.636	17.249	1995_210	09:00:00
8	97.070	SO2 1	5.7844645E-01	ug/m3	-45.636	17.249	1995_190	15:00:00
12	95.508	SO2 1	5.4899251E-01	ug/m3	-22.266	-5.743	1995_190	06:00:00
2	99.414	SO4 1	2.0132611E+00	ug/m3	-49.056	20.559	1995_192	09:00:00
8	97.070	SO4 1	1.3413306E+00	ug/m3	-23.587	19.800	1995_187	21:00:00
12	95.508	SO4 1	1.2776209E+00	ug/m3	-22.266	-5.743	1995_188	00:00:00
2	99.414	NO 1	2.4241890E-01	ug/m3	-86.380	90.776	1995_186	06:00:00
8	97.070	NO 1	2.1577983E-01	ug/m3	-86.380	90.776	1995_205	06:00:00
12	95.508	NO 1	1.7484842E-01	ug/m3	-86.380	90.776	1995_201	06:00:00
2	99.414	NO2 1	5.8553219E-01	ug/m3	-86.380	90.776	1995_208	00:00:00
8	97.070	NO2 1	5.5068791E-01	ug/m3	-86.380	90.776	1995_208	03:00:00
12	95.508	NO2 1	5.4399544E-01	ug/m3	-86.380	90.776	1995_204	00:00:00
2	99.414	HNO3 1	1.6972790E+00	ug/m3	-73.181	19.414	1995_187	15:00:00
8	97.070	HNO3 1	1.5065962E+00	ug/m3	-23.587	19.800	1995_191	15:00:00
12	95.508	HNO3 1	1.4168251E+00	ug/m3	-45.636	17.249	1995_193	15:00:00
2	99.414	NO3 1	2.4409448E-01	ug/m3	-23.587	19.800	1995_200	15:00:00
8	97.070	NO3 1	9.6489988E-02	ug/m3	-36.765	7.793	1995_193	00:00:00
12	95.508	NO3 1	7.0543371E-02	ug/m3	-95.958	46.149	1995_183	00:00:00

Note: number of times in period = 256

Tabulation for Requested Percentile Values
Results for the Maximum Receptor
All Values in Each Day are Included

N	Percentile	Species - Level	Modeled	Units	Location X (KM)	Location Y (KM)	Starting UTC-0700 Date (YYYY_JJJ)	Starting UTC-0700 Time (HH:MM:SS)
6	98.000	SO2 1	6.0360593E-01	ug/m3	-22.266	-5.743	1995_193	09:00:00
14	95.000	SO2 1	5.3457832E-01	ug/m3	-22.266	-5.743	1995_193	12:00:00
27	90.000	SO2 1	4.5703641E-01	ug/m3	-23.587	19.800	1995_191	12:00:00
65	75.000	SO2 1	2.2311690E-01	ug/m3	-45.636	17.249	1995_182	06:00:00
6	98.000	SO4 1	1.3920479E+00	ug/m3	-82.802	31.563	1995_191	03:00:00
14	95.000	SO4 1	1.2384740E+00	ug/m3	-23.587	19.800	1995_190	06:00:00
27	90.000	SO4 1	1.0732707E+00	ug/m3	-56.449	16.810	1995_188	00:00:00
65	75.000	SO4 1	7.2078431E-01	ug/m3	-45.636	17.249	1995_197	09:00:00
6	98.000	NO 1	2.2316346E-01	ug/m3	-86.380	90.776	1995_204	06:00:00
14	95.000	NO 1	1.5821451E-01	ug/m3	-86.380	90.776	1995_198	09:00:00
27	90.000	NO 1	1.3154908E-01	ug/m3	-86.380	90.776	1995_205	09:00:00
65	75.000	NO 1	8.1808403E-02	ug/m3	-86.380	90.776	1995_195	09:00:00
6	98.000	NO2 1	5.5393910E-01	ug/m3	-86.380	90.776	1995_185	21:00:00
14	95.000	NO2 1	5.3284913E-01	ug/m3	-86.380	90.776	1995_210	21:00:00
27	90.000	NO2 1	4.9811035E-01	ug/m3	-86.380	90.776	1995_185	03:00:00
65	75.000	NO2 1	3.8550305E-01	ug/m3	-86.380	90.776	1995_194	03:00:00
6	98.000	HNO3 1	1.5779656E+00	ug/m3	-45.636	17.249	1995_191	15:00:00
14	95.000	HNO3 1	1.3985200E+00	ug/m3	-22.266	-5.743	1995_190	06:00:00
27	90.000	HNO3 1	1.2455554E+00	ug/m3	-22.266	-5.743	1995_193	09:00:00
65	75.000	HNO3 1	1.0136856E+00	ug/m3	-22.266	-5.743	1995_183	09:00:00
6	98.000	NO3 1	1.3482775E-01	ug/m3	-95.958	46.149	1995_193	21:00:00
14	95.000	NO3 1	6.2677436E-02	ug/m3	-56.449	16.810	1995_203	03:00:00
27	90.000	NO3 1	3.5989128E-02	ug/m3	-95.958	46.149	1995_192	12:00:00
65	75.000	NO3 1	2.1382032E-03	ug/m3	-56.449	16.810	1995_197	21:00:00

Note: number of times in period = 256

CALRANK_PLOT_PCTL.DAT

```
-------------------------------------------
Requested Values for Percentile (%) =  75.000
Corresponding Nth-Highest N         =      65
All Values in Each Day are Included
Number of times in period           =     256
-------------------------------------------
```

Model data for each receptor are ranked over all times based on magnitude and
the requested Nth-Highest and/or Percentile values are reported for each receptor

Location X (KM)	Location Y (KM)	Species - Level SO2 1 ug/m3	Starting UTC-0700 Date (YYYY_JJJ)	Starting UTC-0700 Time (HH:MM:SS)	Species - Level SO4 1 ug/m3	Starting UTC-0700 Date (YYYY_JJJ)	Starting UTC-0700 Time (HH:MM:SS)
-112.534	73.569	2.1135101E-01	1995_208	12:00:00	6.5649730E-01	1995_206	12:00:00
-96.928	42.265	2.1820070E-01	1995_196	09:00:00	6.7459333E-01	1995_198	15:00:00
-22.266	-5.743	2.2265026E-01	1995_187	09:00:00	7.0490843E-01	1995_187	00:00:00
-23.587	19.800	2.1413609E-01	1995_195	09:00:00	6.9981647E-01	1995_194	12:00:00
-86.380	90.776	2.2001354E-01	1995_208	15:00:00	6.5835202E-01	1995_210	03:00:00
-87.952	52.945	2.1083651E-01	1995_183	15:00:00	6.7068070E-01	1995_194	15:00:00
-49.056	20.559	2.1864684E-01	1995_196	09:00:00	7.0782602E-01	1995_211	00:00:00
-48.990	18.439	2.1931919E-01	1995_187	06:00:00	6.8925285E-01	1995_209	12:00:00
-35.131	7.998	2.1881981E-01	1995_194	09:00:00	6.9019318E-01	1995_211	15:00:00
-86.481	69.038	2.1725047E-01	1995_183	15:00:00	6.5713358E-01	1995_206	12:00:00
-61.098	34.721	2.1867444E-01	1995_210	12:00:00	6.8315142E-01	1995_192	00:00:00
-45.636	17.249	2.2311690E-01	1995_182	06:00:00	7.2078431E-01	1995_197	09:00:00
-36.765	7.793	2.1968804E-01	1995_194	09:00:00	6.9777107E-01	1995_206	00:00:00
-100.509	80.586	2.1060951E-01	1995_194	09:00:00	6.5706438E-01	1995_195	15:00:00
-108.462	60.535	2.1599288E-01	1995_208	15:00:00	6.6985178E-01	1995_189	15:00:00
-56.449	16.810	2.1571998E-01	1995_182	06:00:00	7.0858204E-01	1995_211	18:00:00
-82.802	31.563	2.2208786E-01	1995_189	09:00:00	6.7448241E-01	1995_197	15:00:00
-73.181	19.414	2.2289866E-01	1995_183	09:00:00	7.1023667E-01	1995_183	18:00:00
-38.410	4.943	2.1189842E-01	1995_188	03:00:00	6.8579751E-01	1995_209	12:00:00
-95.958	46.149	2.1288925E-01	1995_183	15:00:00	6.7593855E-01	1995_201	12:00:00