CALPUFF Chemistry Updates:

User's Instructions for API Chemistry Options

October 25, 2010

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1.0 Introduction

Two chemical transformation module options were introduced into Version 5.8 of the CALPUFF modeling system (Scire et al., 2000a,b) by Karamchandani et al. (2008) in a study sponsored by the American Petroleum Institute (API). These modules include:

Modules 1 and 2

- Modification of the existing RIVAD chemical mechanism for the transformation of SO_2 to SO_4 and NO/NO_2 to HNO_3 and NO_3
- Replacement of the MESOPUFF-II CHEMEQ model with the ISORROPIA (Version 1.7) model for inorganic gas-particle equilibrium
- Addition of a new option for aqueous-phase transformation adapted from the RADM cloud implementation in CMAQ/SCICHEM

Module 2

- Addition of a new option for anthropogenic secondary organic aerosol (SOA) formation based on the CalTech SOA routines implemented in CMAQ-MADRID

TRC has implemented these modules as options into a new version of CALPUFF (Version 6.4). Module Option 1 is implemented as the 6th CALPUFF chemical transformation option (MCHEM = 6), and Module Option 2 is implemented as the 7th CALPUFF chemical transformation option (MCHEM = 7). However, one difference is that TRC has updated the gas-particle equilibrium model for nitrates from ISORROPIA v1.7 to ISORROPIA v2.1 (Nenes et al., 1998; Fountoukis and Nenes, 2007). ISORROPIA v2.1 is the only version of the model currently supported by the developers.

Both new module options use the ISORROPIA v2.1 model instead of the CHEMEQ gas-particle equilibrium model for nitrates used with the MCHEM=1, 3 options. Since total nitrate (TNO_3) is partitioned into the gas (HNO_3) and particulate (NO_3) phases based in part on the ammonia available after preferential scavenging by sulfate, the equilibrium should be determined using the total amount of sulfate and nitrate (due to all sources, background, etc.) present at a particular location and time. This is accomplished using the ammonia-limiting method (ALM) of the POSTUTIL postprocessor in the CALPUFF modeling system. Because POSTUTIL also employs the CHEMEQ model in the ALM, Karamchandani et al. (2009) replaced CHEMEQ with ISORROPIA v1.7 in POSTUTIL Version 1.56 in a hardwired way which prevented backward compatibility. TRC has implemented the current ISORROPIA v2.1 module into a new POSTUTIL Version 1.64 as an option which retains backward compatibility of the POSTUTIL code.

The ISORROPIA v2.1 model is documented and maintained by its developers, as described at the ISORROPIA home page (http://nenes.eas.gatech.edu/ISORROPIA). It is incorporated in this version of CALPUFF and POSTUTIL without modification, with permission from the model developers following the terms-of-use requirements.

2.0 Model Implementation

The FORTRAN codes introduced in the API-sponsored update to CALPUFF are made up of a number of subroutines and supporting include-files for declarations of parameters and variables stored in common. To facilitate future maintenance new subroutines other than those that are part of ISORROPIA are bundled in a single FORTRAN file (API_CHEM.FOR) that is separate from the CALPUFF file (CALPUFF.FOR), the code for ISORROPIA remains a separate file (ISORROPIA.FOR), and the included commons-files are retained without modification (aqueous.puf, newsoa.puf, soadat.puf, and isrpia.inc). Should any of these submodels be updated, CALPUFF can be immediately updated as well.

The file API_CHEM.FOR includes:

AER routines based on existing CALPUFF routines
- Subroutine CHEMRIV6
- Subroutine CHEMRIV7
- Subroutine CHMRIV6
- Subroutine CHMRIV7
- Subroutine SETBCKOC

ISORROPIA interface routine
- Subroutine ISODRIVER

CALTECH SOA routines
- Subroutine SOADRIVER
- Subroutine CALTECH_SOA
- Subroutine SOASUB

AQUEOUS-CHEMISTRY ROUTINES BASED ON RADM/CMAQ
- Subroutine AQRADM
- Function HLCONST
- Function INDEX1

Several modifications were made to these new modules. Options have been assigned either new user-selected modeling option variables (changed via the control file) or local logical operators that may be switched in an individual subroutine to restore the original logic. CALPUFF will need to be recompiled if a local logical variable is changed.

The following variable settings will restore the features and logic of the original API implementation (for testing):

Control File
- MLWC = 0 Do not read gridded cloud water from file
- MNH3 = 1 Read monthly ammonia vertical profiles
- MAVGNH3 = 0 Do not average NH_3 profiles within a puff

- RNITE1 = 0.0 Do not include heterogeneous SO_2 transformation

Local Logical in Subroutine

- L_KGPCM = .FALSE. CHEMRIV6, CHEMRIV7
- L_TNO3FLOOR = .FALSE. CHEMRIV6, CHEMRIV7
- L_RAINCLOUD = .FALSE. CHEMRIV6, CHEMRIV7
- L_SCAV6 = .FALSE. WET

More documentation about the local logical configuration is provided in the code.

3.0 CALPUFF

The new chemistry options in CALPUFF are accessed through control-file selections. Depending on the configuration, one or two new files may also be required. Most of the control-file selections are simple to characterize as few new settings are involved. These are detailed in Section 3.1.

When CALPUFF is used to calculate secondary aerosol (SOA) formation from the source emissions using the new mechanism (MCHEM = 7), species in addition to those used in the RIVAD mechanism are associated with the SOA treatment. These species include

- primary organic carbon
- precursor (emitted) volatile organic compounds (VOCs): toluene, xylene, long-chain alkanes, and polycyclic aromatic hydrocarbons
- condensable products from these species and their particle-phase counterparts

As with the other chemical transformation mechanisms, the species must use particular names and must be assigned in a particular order. Both must conform to the list in Table 3-1.

These species have been added to the species library of the CALPUFF GUI, and a "Quick-Start" option is available to select these species in the correct order. This feature should be used to construct the control file for this chemical transformation option.

Source emission rates for the SOA option will typically include emissions of the four VOC species and primary organic carbon emissions when available, although some sources may have zero emissions of some of these species. For example, if a given source only emits the aromatic VOCs TOL and XYL then all the other species can be designated as non-emitted species in the control file. Furthermore, fewer than 25 species may be used in a simulation if the omitted species are at the end of the list. For example, if PAH emissions are zero, then the first 20 species may be used. If both ALKH and PAH emissions are zero, then the first 17 species may be used.

Background organic carbon concentrations are also needed, and these are provided in the same way they are provided for MCHEM = 4, as monthly values of fine particulate concentration (BCKPMF) and the corresponding monthly fractions for the organic portion (OFRAC) of the fine particulate. See the control file Input Group 11 in Section 3.1.

Table 3-1
Species Names and Sequence

SPECIES NUMBER	SPECIES NAME	DESCRIPTION	PHASE
1	**SO2**	Sulfur Dioxide	Gas
2	SO4	Sulfate	Particle
3	**NO**	Nitrogen Oxide	Gas
4	**NO2**	Nitrogen Dioxide	Gas
5	HNO3	Nitrate	Gas
6	NO3	Nitrate	Particle
7	**POC**	Primary Organic Carbon	Particle
8	**TOL**	Toluene	Gas
9	TOLAER1	Condensable product from TOL	Gas
10	TOLAER2	Condensable product from TOL	Gas
11	ATOLA1	Condensable product from TOL	Particle
12	ATOLA2	Condensable product from TOL	Particle
13	**XYL**	Xylene	Gas
14	XYLAER1	Condensable product from XYL	Gas
15	XYLAER2	Condensable product from XYL	Gas
16	AXYLA1	Condensable product from XYL	Particle
17	AXYLA2	Condensable product from XYL	Particle
18	**ALKH**	Long-Chain Alkanes	Gas
19	ALKHAER	Condensable product from ALKH	Gas
20	AALKHA	Condensable product from ALKH	Particle
21	**PAH**	Polycyclic Aromatic Hydrocarbons	Gas
22	PAHAER1	Condensable product from PAH	Gas
23	PAHAER2	Condensable product from PAH	Gas
24	APAHA1	Condensable product from PAH	Particle
25	APAHA2	Condensable product from PAH	Particle
Notes: Species emitted from sources (primary) are in BOLD typeface			

3.1 CALPUFF Control File

Changes for selecting and configuring the new chemistry options are found in Input Groups 0, 2, and 11.

Input Group 0 provides the file-name information for the simulation. The new names are listed in the Other Files section, and are assigned to AUXEXT and NH3ZDAT:

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

-------------------------------------------------------------------------------
Other Files
-----------
OZONE.DAT     input    * OZDAT  =             *
VD.DAT        input    * VDDAT  =             *
CHEM.DAT      input    * CHEMDAT=             *
AUX           input    ! AUXEXT =  AUX        !
(Extension added to METDAT filename(s) for files
 with auxilliary 2D and 3D data)
H2O2.DAT      input    * H2O2DAT=             *
NH3Z.DAT      input    ! NH3ZDAT=NH3Z_07.DAT  !
HILL.DAT      input    * HILDAT=              *
HILLRCT.DAT   input    * RCTDAT=              *
COASTLN.DAT   input    * CSTDAT=              *
FLUXBDY.DAT   input    * BDYDAT=              *
BCON.DAT      input    * BCNDAT=              *
DEBUG.DAT     output   * DEBUG =              *
MASSFLX.DAT   output   * FLXDAT=              *
MASSBAL.DAT   output   ! BALDAT=CALPUFF.BAL   !
FOG.DAT       output   * FOGDAT=              *
RISE.DAT      output   * RISDAT=              *
-------------------------------------------------------------------------------
```

AUXEXT identifies auxiliary data files from a CALMET application. For the new chemistry options with aqueous-phase reactions, the auxiliary file may be used to provide a gridded field of liquid cloud water content. Data for this are processed within CALMET from the 3D.DAT mesoscale model fields to the CALMET modeling grid. Each auxiliary file retains the file name of the standard CALMET output file associated with it, but adds the extension assigned by AUXEXT. In the example above, the extension added to all output CALMET data files in the simulation is ".AUX".

NH3ZDAT identifies the name of a file of monthly average ammonia concentrations for each layer in the CALMET/CALPUFF simulation grid. This is used only if the new control variable MNH3 in Input Group 2 is set to 1.

Input Group 2 is used to configure the major technical options. New or augmented options are MCHEM, MAQCHEM, and MLWC:

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

     Chemical mechanism flag (MCHEM)       Default: 1     ! MCHEM =  6   !
        0 = chemical transformation not
            modeled
        1 = transformation rates computed
            internally (MESOPUFF II scheme)
        2 = user-specified transformation
            rates used
        3 = transformation rates computed
            internally (RIVAD/ARM3 scheme)
        4 = secondary organic aerosol formation
            computed (MESOPUFF II scheme for OH)
        5 = user-specified half-life with or
            without transfer to child species
        6 = transformation rates computed
            internally (Updated RIVAD scheme with
            ISORROPIA equilibrium)
        7 = transformation rates computed
            internally (Updated RIVAD scheme with
            ISORROPIA equilibrium and CalTech SOA)

     Aqueous phase transformation flag (MAQCHEM)
     (Used only if MCHEM = 6, or 7)        Default: 0     ! MAQCHEM =  0   !
        0 = aqueous phase transformation
            not modeled
        1 = transformation rates and wet
            scavenging coefficients adjusted
            for in-cloud aqueous phase reactions
            (adapted from RADM cloud model
             implementation in CMAQ/SCICHEM)

     Liquid Water Content flag (MLWC)
     (Used only if MAQCHEM = 1)            Default: 1     ! MLWC =  0   !
        0 = water content estimated from cloud cover
            and presence of precipitation
        1 = Gridded cloud water data read from CALMET
            water content output files (filenames are
            the CALMET.DAT names PLUS the extension
            AUXEXT provided in Input Group 0)
```

MCHEM selects the chemical transformation mechanism. The API modules appear as Options 6 and 7. They differ only in the addition of the SOA chemistry module in the latter.

MAQCHEM selects the RADM aqueous-phase transformation module, and is active only in combination with MCHEM Options 6 or 7. When selected, it requires information on the cloud liquid water content and the background H_2O_2 concentrations.

MLWC selects the method used to obtain cloud liquid water content. The cloud water originally used in the aqueous chemistry was set to 0.5 g/m^3 for precipitating (rain, not snow or ice) clouds and 0.1 g/m^3 for non-precipitating clouds in lieu of providing a pathway for obtaining more specific information. This method is used if MLWC = 0, and it requires cloud cover, temperature, and precipitation rate fields. Procedures have been implemented in CALMET to pass gridded cloud liquid water content from MM5/WRF to a new auxiliary output file which may be read by CALPUFF. These data currently allow CALPUFF to obtain a mean cloud water

mixing ratio (g/kg) that is vertically-averaged over the depth of the cloud layer, when present, at the current puff location. This method is used if MLWC = 1.

Input Group 11 provides parameters used in the chemical transformation mechanisms. New parameters or existing parameters that are used with the API modules are MOZ, BCKO3, MNH3, MAVGNH3, BCKNH3, RNITE1, MH2O2, BCKH2O2, BCKPMF, and OFRAC:

```
INPUT GROUP: 11a, 11b -- Chemistry Parameters
---------------------

---------------
Subgroup (11a)
---------------

     Several parameters are needed for one or more of the chemical transformation
     mechanisms.  Those used for each mechanism are:
                                    M                   B
                                    A  B  R  R  R     C  B        N
                                 B  V  C  N  N  N  M  K  C  O     D
                                 C  M  G  K  I  I  I  H  H  K  F  V  E
                              M  K  N  N  N  T  T  T  2  2  P  R  C  C
                              O  O  H  H  H  E  E  E  O  O  M  A  N  A
     Mechanism (MCHEM)        Z  3  3  3  3  1  2  3  2  2  F  C  X  Y
     --------------------   ----------------------------------------------
     0 None                   .  .  .  .  .  .  .  .  .  .  .  .  .  .
     1 MESOPUFF II            X  X  .  .  X  X  X  X  .  .  .  .  .  .
     2 User Rates             .  .  .  .  .  .  .  .  .  .  .  .  .  .
     3 RIVAD                  X  X  .  .  X  .  .  .  .  .  .  .  .  .
     4 SOA                    X  X  .  .  .  .  .  .  .  .  X  X  X  .
     5 Radioactive Decay      .  .  .  .  .  .  .  .  .  .  .  .  .  X
     6 RIVAD/ISORRPIA         X  X  X  X  X  X  .  .  X  X  .  .  .  .
     7 RIVAD/ISORRPIA/SOA     X  X  X  X  X  X  .  .  X  X  X  X  .  .


     Ozone data input option (MOZ)     Default: 1            ! MOZ =  0   !
     (Used only if MCHEM = 1,3,4,6, or 7)
        0 = use a monthly background ozone value
        1 = read hourly ozone concentrations from
            the OZONE.DAT data file

     Monthly ozone concentrations in ppb (BCKO3)
     (Used only if MCHEM = 1,3,4,6, or 7 and either
        MOZ = 0, or
        MOZ = 1 and all hourly O3 data missing)
                                       Default: 12*80.
     !  BCKO3 = 30.00, 30.00, 30.00, 30.00, 30.00, 30.00,
                30.00, 30.00, 30.00, 30.00, 30.00, 30.00 !

     Ammonia data option (MNH3)        Default: 1            ! MNH3 =  0   !
     (Used only if MCHEM = 6 or 7)
        0 = use a single monthly background ammonia value for all layers
        1 = read monthly background ammonia values for each layer from
            the NH3Z.DAT data file

     Ammonia vertical averaging option (MAVGNH3)
     (Used only if MCHEM = 6 or 7, and MNH3 = 1)
        0 = use NH3 at puff center height (no averaging is done)
        1 = average NH3 values over vertical extent of puff
                                       Default: 1            ! MAVGNH3 =  0   !
```

```
    Monthly ammonia concentrations in ppb (BCKNH3)
    (Used only if MCHEM = 1 or 3, or
               if MCHEM = 6 or 7, and MNH3 = 0)
                                    Default: 12*10.
    !  BCKNH3 = 1.00, 1.00, 1.00, 1.00, 1.00, 1.00,
                1.00, 1.00, 1.00, 1.00, 1.00, 1.00 !

    Nighttime SO2 loss rate in %/hour (RNITE1)
    (Used only if MCHEM = 1, 6 or 7)
    This rate is used only at night for MCHEM=1
    and is added to the computed rate both day
    and night for MCHEM=6,7 (heterogeneous reactions)
                                    Default: 0.2          ! RNITE1 = .2 !

    Nighttime NOx loss rate in %/hour (RNITE2)
    (Used only if MCHEM = 1)
                                    Default: 2.0          ! RNITE2 = 2.0 !

    Nighttime HNO3 formation rate in %/hour (RNITE3)
    (Used only if MCHEM = 1)
                                    Default: 2.0          ! RNITE3 = 2.0 !

    H2O2 data input option (MH2O2)    Default: 1          ! MH2O2 =  1   !
    (Used only if MCHEM = 6 or 7, and MAQCHEM = 1)
       0 = use a monthly background H2O2 value
       1 = read hourly H2O2 concentrations from
           the H2O2.DAT data file

    Monthly H2O2 concentrations in ppb (BCKH2O2)
    (Used only if MQACHEM = 1 and either
       MH2O2 = 0 or
       MH2O2 = 1 and all hourly H2O2 data missing)
                                    Default: 12*1.
    !  BCKH2O2 = 1.00, 1.00, 1.00, 1.00, 1.00, 1.00,
                 1.00, 1.00, 1.00, 1.00, 1.00, 1.00 !

--- Data for SECONDARY ORGANIC AEROSOL (SOA) Options
    (used only if MCHEM = 4 or 7)

    The MCHEM = 4 SOA module uses monthly values of:
         Fine particulate concentration in ug/m^3 (BCKPMF)
         Organic fraction of fine particulate     (OFRAC)
         VOC / NOX ratio (after reaction)         (VCNX)

    The MCHEM = 7 SOA module uses monthly values of:
         Fine particulate concentration in ug/m^3 (BCKPMF)
         Organic fraction of fine particulate     (OFRAC)

    These characterize the air mass when computing
    the formation of SOA from VOC emissions.
```

MOZ selects the source of the background ozone data, and functions as before.

BCKO3 provides monthly ozone concentrations to be used as indicated by MOZ.

MNH3 selects the source of the monthly background ammonia data when chemical transformation mechanism MCHEM = 6 or 7 is selected. It provides the option to use either monthly concentrations entered in this control file or to read monthly ammonia profiles (a concentration for each layer for each month) from the NH3Z.DAT input file.

MAVGNH3 selects the way vertical ammonia profiles are used. The background ammonia concentration for a particular puff and time step may be either taken from the layer that contains the puff-center, or averaged from values in the layers that the puff overlaps.

BCKNH3 provides monthly ammonia concentrations to be used as indicated by MNH3 for chemical transformation mechanisms MCHEM = 6 and 7. These values are always used for chemical transformation mechanisms MCHEM = 1 and 3.

RNITE1 assigns the nighttime SO_2 loss rate for the MESOPUFF-II (MCHEM = 1) chemical mechanism, and it assigns the SO_2 loss rate due to heterogeneous reactions (day and night) for the API modules (MCHEM = 6, 7). Its default value is 0.2%/hr.

Both the MESOPUFF-II and the RIVAD (MCHEM = 3) transformation options in CALPUFF include an SO_2-to-SO_4 transformation rate due to heterogeneous reactions. These are not important during the day when gas reactions dominate, but remain active at night. The default transformation rate is 0.2%/hour for this pathway. RIVAD adds this rate to all other SO_2 transformation rates calculated both day and night. MESOPUFF-II uses 0.2%/hour as a minimum for heterogeneous reactions during the day and it uses RNITE1 at night. Karamchandani et al. (2008) do not explicitly include heterogeneous SO_2-to-SO_4 reactions in their implementation for API, so the SO_2-to-SO_4 transformation rate at night in the absence of aqueous-phase reactions is identically zero, which is equivalent to setting RNITE1 = 0.0.

3.2 Monthly Ammonia Concentration File

The control-file variable MNH3 selects the source of the monthly background ammonia data when chemical transformation mechanism MCHEM = 6 or 7 is selected. It provides the option to use monthly vertical profiles of ammonia (a concentration for each layer for each month) from the NH3Z.DAT input file.

The header of the NH3Z.DAT file provides the concentration units, the number of layers, and the row-order of the data. The row-order currently accepted places data for one month on a single line in which the data progress from Layer 1 to the top-most CALPUFF layer. Therefore there are 12 data records, one for each month. The first entry of each line is the name of the month so there is no ambiguity. An example file is listed in Table 3-2, and the variables are defined in Table 3-3 and Table 3-4. Note that Record 2 of the file identifies the number of comment records that follow. These comment records should provide important information on the source of the ammonia data and the methods and assumptions used to prepare the file. There is no limit on the number of these records.

Table 3-2
Example NH3Z.DAT Input Data File

```
NH3Z.DAT       1.0            Monthly NH3 for each model layer
2
Example file for illustration only.
Application-specific ammonia concentration profiles must be developed.
PPB
MONTH_LAYER
10
JANUARY    : 0.2186 0.2186 0.2125 0.2054 0.1918 0.1645 0.1460 0.1228 0.0993 0.0903
FEBRUARY   : 0.2186 0.2186 0.2125 0.2054 0.1918 0.1645 0.1460 0.1228 0.0993 0.0903
MARCH      : 0.5416 0.5416 0.5394 0.5394 0.5348 0.4955 0.4431 0.3636 0.2412 0.1847
APRIL      : 0.5416 0.5416 0.5394 0.5394 0.5348 0.4955 0.4431 0.3636 0.2412 0.1847
MAY        : 0.5416 0.5416 0.5394 0.5394 0.5348 0.4955 0.4431 0.3636 0.2412 0.1847
JUNE       : 0.6458 0.6458 0.6378 0.6339 0.6139 0.5699 0.5287 0.4508 0.3354 0.2660
JULY       : 0.6458 0.6458 0.6378 0.6339 0.6139 0.5699 0.5287 0.4508 0.3354 0.2660
AUGUST     : 0.6458 0.6458 0.6378 0.6339 0.6139 0.5699 0.5287 0.4508 0.3354 0.2660
SEPTEMBER  : 0.5107 0.5107 0.4986 0.4869 0.4691 0.4334 0.3763 0.2981 0.1921 0.1400
OCTOBER    : 0.5107 0.5107 0.4986 0.4869 0.4691 0.4334 0.3763 0.2981 0.1921 0.1400
NOVEMBER   : 0.5107 0.5107 0.4986 0.4869 0.4691 0.4334 0.3763 0.2981 0.1921 0.1400
DECEMBER   : 0.2186 0.2186 0.2125 0.2054 0.1918 0.1645 0.1460 0.1228 0.0993 0.0903
```

Table 3-3
NH3Z.DAT - Header Records - General Data

Record	Variable	Type	Description
1	DATASET	character*16	Dataset name (NH3Z.DAT)
1	DATAVER	character*16	Dataset version (1.0)
1	DATAMOD	character*64	Dataset message field
2	NCOM	integer	Number of comment records to follow
NEXT NCOM Lines	COMMENT1	character *132	Documentation for QA (up to 132 characters/line)
NCOM+3	CUNITS	character*16	Concentration units (must be PPB)
NCOM+4	CFORMAT	character*16	Format of data records (must be MONTH_LAYER)
NCOM+5	NZFILE	integer	Number of layers (must match modeling grid)

Table 3-4
NH3Z.DAT - Data Records
(Repeated for each month for MONTH-LAYER format)

Data Record No.	Variable No.	Variable	Type	Description
1	1	CMONTH	C*10	Month name (upper case, left-justified)
1	2	(Delimiter)	C*1	':' delimiter separates month name from data
1	3	BCKNH3ZM (imo,1)	real	Background ammonia concentration for month in model Layer 1
1	4	BCKNH3ZM (imo,2)	real	Background ammonia concentration for month in model Layer 2
1	5	BCKNH3ZM (imo,3)	real	Background ammonia concentration for month in model Layer 3
1	2+iz	BCKNH3ZM (imo,iz)	real	Background ammonia concentration for month in model Layer iz
1	2+ NZFILE	BCKNH3ZM (imo,nzfile)	real	Background ammonia concentration for month in model Layer nzfile (top layer in grid)

NOTES:

1. Record length is limited to 264 characters
2. BCKNH3ZM values are read free-format and must be separated by 1 or more spaces.

3.3 CALMET Auxiliary Data File (CALMET.AUX)

Gridded cloud liquid water data from MM5/WRF can be passed through CALMET via the 3D.DAT input file and then output as one of the variables written to a CALMET auxiliary data file (CALMET.AUX). The content of this file is flexible in that any number of 2-dimensional (2-D) and 3-dimensional (3-D) variables can be accommodated. All 2-D and 3-D data arrays are defined on the CALMET modeling grid.

The CALMET.AUX file header records contain file identification labels, descriptive titles of the CALMET run (including a complete image of the CALMET control file) as comment records, and information about the horizontal and vertical grid systems of the meteorological grid. A description of each variable in the header records is provided in Table 3-5.

Sample FORTRAN write statements for the CALMET.AUX header records are:

```
c --- Record #1 - File Declaration -- 24 words
      write(ioaux) dataset,dataver,datamod

c --- Record #2 - Number of comment lines -- 1 word
      write(ioaux) ncom

c --- Record #3 to NCOM+2 (Comment record section) -- 33 words each
c --- Loop over records
      do i=1,ncom
         write(ioaux) comment
      enddo

c --- record #NCOM+3 - run control parameters -- 36 words
      write(ioaux) ibyrn,ibmon,ibdyn,ibhrn,ibsecn,
     1 ieyrn,iemon,iedyn,iehrn,iesecn,axtz,irlg,
     2 nx, ny, nz, dgrid, xorigr, yorigr,
     3 pmap,datum,daten,feast,fnorth,utmhem,iutmzn,
     4 rnlat0,relon0,xlat1,xlat2,naux2d,naux3d

c --- record #NCOM+4 - cell face heights (NZ + 1 words)
      clabel='ZFACE'
      write(ioaux)clabel,idum,idum,idum,idum,zface

c --- record #NCOM+5 - Names, units and types of 2D variables
c ---                                  (2+naux2d*5 words)
      clabel='2D_VARS'
      write(ioaux) clabel,(auxnam2d(k),k=1,naux2d),
     &                    (auxunit2d(k),k=1,naux2d),
     &                    (auxtyp2d(k),k=1,naux2d)

c --- record #NCOM+6 - Names, units and types of 3D variables
c ---                                  (2+naux3d*5 words)
      clabel='3D_VARS'
      write(ioaux) clabel,(auxnam3d(k),k=1,naux3d),
     &                    (auxunit3d(k),k=1,naux3d),
     &                    (auxtyp3d(k),k=1,naux3d)
```

The following declarations apply:

```
      real ZFACEM(nz+1)
      character*132 COMMENT(ncom)
      character*64 DATAMOD
```

```
 character*16 DATASET,DATAVER
 character*12 DATEN
 character*8 PMAP,DATUM
 character*8 CLABEL
 character*4 UTMHEM
character*8 AUXNAM2D(naux2d), auxnam3d(naux3d)
character*8 AUXUNIT2D(naux2d), auxunit3d(naux3d)
character*4 AUXTYP2D(naux2d), auxtyp3d(naux3d)
```

The CALMET.AUX file data records contain time-varying fields of the gridded meteorological variables named in the header. For each time period, data for the 2-D variables are written first, followed by data for the 3-D variables. A description of each variable in the data records is provided in Table 3-6.

Sample FORTRAN write statements for the CALMET.AUX data records are:

```
c --- Write the 2D variables
      Loop over NAUX2D 2D variables, k
         (for integer*4 variables …)
         write(ioaux)AUXNAME2D(k),NDATHRB,IBSEC,NDATHRE,IESEC,I2DVAR
         (OR, for real*4 variables …)
         write(ioaux)AUXNAME2D(k),NDATHRB,IBSEC,NDATHRE,IESEC,R2DVAR
      End loop over 2D variables

c --- Write the 3D variables
      Loop over NAUX3D 3D variables, k
         Loop over NZFILE layers, n
            clabel=AUXNAME3D(k)
            write(clabel(6:8),'(i3.3)') n
            (for integer*4 variables …)
            write(ioaux)clabel,NDATHRB,IBSEC,NDATHRE,IESEC,((I3DVAR(i,j,k),i=1,nx),j=1,ny)
            (OR, for real*4 variables …)
            write(ioaux)clabel,NDATHRB,IBSEC,NDATHRE,IESEC,((R3DVAR(i,j,k),i=1,nx),j=1,ny)
         End loop over layers
      End loop over 3D variables
```

The following declarations apply:

```
 real R2DVAR(nx,ny), R3DVAR(nx,ny,nzfile)
 integer I2DVAR(nx,ny), I3DVAR(nx,ny,nzfile)
 character*8 CLABEL
```

Table 3-5
CALMET.AUX - Header Records

Header Record No.	Variable No.	Variable	Type[a]	Description
1	1	DATASET	char*16	Dataset name (CALMET.AUX)
1	2	DATAVER	char*16	Dataset version
1	3	DATAMOD	char*64	Dataset message field
2	1	NCOM	integer	Number of comment records to follow
3 to NCOM+2	1	COMMENT	char*132	Comment record (repeated NCOM times), each containing an image of one line of the CALMET control file, or other information
NCOM+3	1	IBYR	integer	Starting year of CALMET run
NCOM+3	2	IBMO	integer	Starting month
NCOM+3	3	IBDY	integer	Starting day
NCOM+3	4	IBHR	integer	Starting time (hour at start)
NCOM+3	5	IBSEC	integer	Starting time (seconds at start, 0-3600)
NCOM+3	6	IEYR	integer	Ending year of CALMET run
NCOM+3	7	IEMO	integer	Ending month
NCOM+3	8	IEDY	integer	Ending day
NCOM+3	9	IEHR	integer	Ending time (hour at end)
NCOM+3	10	IESEC	integer	Ending time (seconds at end, 0-3600)
NCOM+3	11	ABTZ	char*8	Base time zone (e.g., UTC-0500 = EST in USA)
NCOM+3	12	IRLG	integer	Run length
NCOM+3	13	NX	integer	Number of grid cells in the X direction
NCOM+3	14	NY	integer	Number of grid cells in the Y direction
NCOM+3	15	NZ	integer	Number of vertical layers
NCOM+3	16	DGRID	real	Grid spacing (m)
NCOM+3	17	XORIGR	real	X coordinate (m) of southwest corner of grid cell (1,1)
NCOM+3	18	YORIGR	real	Y coordinate (m) of southwest corner of grid cell (1,1)

[a]char*N = Character*N

Table 3-5 (Continued)
CALMET.AUX - Header Records

Header Record No.	Variable No.	Variable	Type[a]	Description
NCOM+3	19	PMAP[b]	char*8	Map projection[b] UTM : Universal Transverse Mercator TTM : Tangential Transverse Mercator LCC : Lambert Conformal Conic PS : Polar Stereographic EM : Equatorial Mercator LAZA : Lambert Azimuthal Equal Area
NCOM+3	20	DATUM	char*8	DATUM Code for grid coordinates
NCOM+3	21	DATEN	char*12	NIMA date (MM-DD-YYYY) for datum definitions
NCOM+3	22	FEAST	real	False Easting (km) for PMAP = TTM, LCC, or LAZA
NCOM+3	23	FNORTH	real	False Northing (km) for PMAP = TTM, LCC, or LAZA
NCOM+3	24	UTMHEM	char*4	Hemisphere for UTM projection (N or S)
NCOM+3	25	IUTMZN	integer	UTM zone for PMAP = UTM
NCOM+3	26	RNLAT0	real	North latitude (degrees) for projection origin (for PMAP= TTM, LCC, PS, EM, or LAZA)
NCOM+3	27	RELON0	real	East longitude (degrees) for projection origin (for PMAP= TTM, LCC, PS, EM, or LAZA)
NCOM+3	28	XLAT1	real	North latitude (degrees) of matching parallel #1 for map projection PMAP= LCC or PS
NCOM+3	29	XLAT2	real	North latitude (degrees) of matching parallel #2 for map projection PMAP= LCC
NCOM+3	30	NAUX2D	integer	Number of 2D variables
NCOM+3	31	NAUX3D	integer	Number of 3D variables

[a] char*N = Character*N
[b] PMAP = EM, PS, and LAZA are not currently available in CALMET

Table 3-5 (Concluded)
CALMET.AUX - Header Records

Header Record No.	Variable No.	Variable	Type[a]	Description
NCOM+4	1	CLABEL	char*8	Variable label ('ZFACE')
NCOM+4	2-5	IDUM	integer	Variable not used
NCOM+4	6	ZFACE	real array	Heights (m) of cell faces (NZ + 1 values)
NCOM+5	1-NAUX2D	AUXNAM2D	char*8 array	Names of 2D variables in file
NCOM+5	NAUX2D +1 to 2*NAUX2D	AUXUNIT2D	char*8 array	Units for 2D variables in file (e.g. M, KG/M3, G/KG, etc.)
NCOM+5	2*NAUX2D +1 to 3*NAUX2D	AUXTYP2D	char*4 array	Data type for 2D variables in file (R_4 for real*4, I_4 for integer*4, etc.)
NCOM+6	1-NAUX3D	AUXNAM3D	char*8 array	Names of 3D variables in file
NCOM+6	NAUX3D +1 to 2*NAUX3D	AUXUNIT3D	char*8 array	Units for 3D variables in file (e.g. M, KG/M3, G/KG, etc.)
NCOM+6	2*NAUX3D +1 to 3*NAUX3D	AUXTYP3D	char*4 array	Data type for 3D variables in file (R_4 for real*4, I_4 for integer*4, etc.)

[a] char*N = Character*N

Table 3-6
CALMET.AUX - Data Records

Record Type	Variable No.	Variable Name	Type[a]	Description
2D integer	1	CLABEL	char*8	Variable label equal to corresponding AUXNAM2D in header
2D integer	2,3	NDATHRB, IBSEC	integer	Year, Julian day and hour (YYYYJJJHH) and seconds (SSSS) -- begin
2D integer	4,5	NDATHRE, IESEC	integer	Year, Julian day and hour (YYYYJJJHH) and seconds (SSSS) -- end
2D integer	6	I2DVAR	integer array	Value of integer variable at each grid point
2D real	1	CLABEL	char*8	Variable label equal to corresponding AUXNAM2D in header
2D real	2,3	NDATHRB, IBSEC	integer	Year, Julian day and hour (YYYYJJJHH) and seconds (SSSS) -- begin
2D real	4,5	NDATHRE, IESEC	integer	Year, Julian day and hour (YYYYJJJHH) and seconds (SSSS) -- end
2D real	6	R2DVAR	real array	Value of real variable at each grid point
3D integer	1	CLABEL	char*8	Variable label AUXNAM3D in header with characters 6,7,8 replaced with the layer number (001, 002, etc.)
3D integer	2,3	NDATHRB, NSECB	integer	Year, Julian day and hour (YYYYJJJHH) and seconds (SSSS)
3D integer	4,5	NDATHRE, NSECB	integer	Year, Julian day and hour (YYYYJJJHH) and seconds (SSSS)
3D integer	6	I3DVAR	integer array	Value of integer variable at each grid point in the current layer
3D real	1	CLABEL	char*8	Variable label AUXNAM3D in header with characters 6,7,8 replaced with the layer number (001, 002, etc.)
3D real	2,3	NDATHRB, NSECB	integer	Year, Julian day and hour (YYYYJJJHH) and seconds (SSSS)
3D real	4,5	NDATHRE, NSECB	integer	Year, Julian day and hour (YYYYJJJHH) and seconds (SSSS)
3D real	6	R3DVAR	real array	Value of real variable at each grid point in the current layer

(3D record type is repeated NZFILE times (once per layer))

[a] char*8 = Character*8

4.0 POSTUTIL

Since total nitrate (TNO_3) is partitioned into the gas (HNO_3) and particulate (NO_3) phases based in part on the ammonia available after preferential scavenging by sulfate, the equilibrium should be determined using the total amount of sulfate and nitrate (due to all sources, background, etc.) present at a particular location and time. This is accomplished using the ammonia-limiting method (ALM) in POSTUTIL. TRC has implemented the ISORROPIA (Version 2.1) model as an option which retains backward compatibility of the POSTUTIL code.

The option to use the ISORROPIA model for inorganic gas-particle equilibrium in place of the MESOPUFF-II CHEMEQ model is controlled by one new POSTUTIL control-file variable, MEQPHASE. This is located in Input Group 1:

```
Recompute the HNO3/NO3 partition for concentrations?
(MNITRATE)                    Default: 0       ! MNITRATE  =  1  !
   0 = no
   1 = yes, for all sources combined
   2 = yes, for a source group
   3 = yes, ALM application in one step

Gas-Particulate Phase Equilibrium Model used?
(MEQPHASE)                    Default: 1       ! MEQPHASE  =  1  !
   1 = MESOPUFF-II CHEMEQ
   2 = ISORROPIA
```

No other changes are required.

5.0 References

Karamchandani, P., S.-Y. Chen and C. Seigneur, 2008. *CALPUFF Chemistry Upgrade,* AER Final Report CP277-07-01 prepared for API, Washington, DC, February 2008.

Karamchandani, P., S.-Y. Chen and R. Balmori, 2009. *Evaluation of Original and Improved Versions of CALPUFF using the 1995 SWWYTAF Data Base,* AER Report CP281-09-01 prepared for API, Washington, DC, October 2009.

Fountoukis, C. and Nenes, A., 2007: ISORROPIA II: A Computationally Efficient Aerosol Thermodynamic Equilibrium Model for K+, Ca2+, Mg2+, NH4+, Na+, SO42-, NO3-, Cl-, H2O Aerosols, Atmos.Chem.Phys., **7**, 4639–4659.

Nenes A, Pandis SN, Pilinis C. ISORROPIA, 1998: A new thermodynamic equilibrium model for multiphase multicomponent inorganic aerosols, *Aquat.Geoch.*, **4**, 123-152.

Scire, J.S., F.R. Robe, M.E. Fernau and R.J. Yamartino, 2000a: A User's Guide for the CALMET Meteorological Model. (Version 5.0). Earth Tech., Inc. Concord, MA. (Available from http://www.src.com).

Scire, J.S., D.G. Strimaitis and R.J. Yamartino, 2000b: A User's Guide for the CALPUFF Dispersion Model. (Version 5.0). Earth Tech, Inc., Concord, MA. (Available from http://www.src.com).