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ALM-step1
Repartitioning of NO3/HNO3
VISB 2001
---------- Run title (3 lines) ----------

POSTUTIL MODEL CONTROL FILE

INPUT GROUP: 0 -- Input and Output File Names

Subgroup (0a)

Output Files

File	Default File Name	
List File	POSTUTIL.LST	! UTLLST =PU_RODE_EDSI_01C.LST !
Data File	MODEL.DAT	! UTLDAT =PU_RODE_EDSI_01C.FLX !

Input Files

A time-varying file of "background" concentrations can be included
when the ammonia-limiting method (ALM) for setting the HNO3/NO3
concentration partition is accomplished in 1 step. This option
is selected by setting MNITRATE=3 in Input Group 1.
Species required in the "background" concentration file are:
SO4, NO3, HNO3 and TNH3 (total NH3).

File	Default File Name	
BCKG File	BCKGALM.DAT	* BCKGALM =BCKGALM.DAT *

A number of CALPUFF data files may be processed in this application.
The files may represent individual CALPUFF simulations that were made
for a specific set of species and/or sources. Specify the total number
of CALPUFF runs you wish to combine, and provide the filename for each
in subgroup 0b.

Number of CALPUFF data files (NFILES)
Default: 1 ! NFILES = 1 !

Meteorological data files are needed for the HNO3/NO3 partition option.
Three types of meteorological data files can be used:
METFM= 0 - CALMET.DAT

METFM= 1 - 1-D file with RH, Temp and Rhoair timeseries
METFM= 2 - 2-D files with either Rh, Temp or Rhoair in each
(3 2_D files are needed)
The default is to use CALMET.DAT files.

Default: 0 ! METFM = 0 !

Multiple meteorological data files may be used in sequence to span the processing period. Specify the number of time-period files (NMET) that you need to use, and provide a filename for each in subgroup 0b.
- NMET is 0 if no meteorological files are provided
- NMET is 1 if METFM=1 (multiple file feature is not available)
- NMET is 1 or more if METFM=0 or 2 (multiple CALMET files or 2DMET files)

Number of meteorological data file time-periods (NMET)
Default: 0 ! NMET = 36 !

All filenames will be converted to lower case if LCFILES = T
Otherwise, if LCFILES = F, filenames will be converted to UPPER CASE

Convert filenames to lower case? Default: T ! LCFILES = T !
T = lower case
F = UPPER CASE

!END!

NOTE: file/path names can be up to 70 characters in length

Subgroup (0b)

NMET CALMET Data Files (METFM=0):

Input File	Default File Name	
1	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met01a.met! !END!
2	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met01b.met! !END!
3	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met01c.met! !END!
4	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met02a.met! !END!
5	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met02b.met! !END!
6	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met02c.met! !END!
7	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met03a.met! !END!
8	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met03b.met! !END!
9	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met03c.met! !END!
10	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met04a.met! !END!
11	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met04b.met! !END!
12	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met04c.met! !END!
13	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met05a.met! !END!
14	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met05b.met! !END!
15	MET.DAT	! UTLMET=F:\Refined CENRAP\2001\01met05c.met! !END!

```
 16        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met06a.met!  !END!
 17        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met06b.met!  !END!
 18        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met06c.met!  !END!
 19        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met07a.met!  !END!
 20        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met07b.met!  !END!
 21        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met07c.met!  !END!
 22        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met08a.met!  !END!
 23        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met08b.met!  !END!
 24        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met08c.met!  !END!
 25        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met09a.met!  !END!
 26        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met09b.met!  !END!
 27        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met09c.met!  !END!
 28        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met10a.met!  !END!
 29        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met10b.met!  !END!
 30        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met10c.met!  !END!
 31        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met11a.met!  !END!
 32        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met11b.met!  !END!
 33        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met11c.met!  !END!
 34        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met12a.met!  !END!
 35        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met12b.met!  !END!
 36        MET.DAT        ! UTLMET=F:\Refined CENRAP\2001\01met12c.met!  !END!
```

NMET 1-D Data Files (METFM=1):

```
Input File     Default File Name
----------     -----------------
  1          MET_1D.DAT        * MET1D   = MET_1D.DAT * *END*
```

NMET 2-D Data Files of Each Type (METFM=2):

```
Input File     Default File Name
----------     -----------------
  1          RHUMD.DAT         * M2DRHU  = RELHUM.DAT * *END*
  1          TEMP.DAT         * M2DTMP  = TEMP.DAT   * *END*
  1          RHOAIR.DAT        * M2DRHO  = RHOAIR.DAT * *END*
```

NFILES CALPUFF Data Files:

```
Input File     Default File Name
----------     -----------------
  1          CALPUFF.DAT       ! MODDAT =CP_RODE_EDSI_01C.DAT    ! !END!
```

Note: provide NMET lines of the form * UTLMET = name * *END*

or * MET1D = name * *END*

or * M2DRHU = name * *END*
(and) * M2DTMP = name * *END*
(and) * M2DRHO = name * *END*

and NFILES lines of the form * MODDAT = name * *END*

where the * should be replaced with an exclamation point,
the special delimiter character.

INPUT GROUP: 1 -- General run control parameters

```
Starting date:   Year  (ISYR) --   No default   ! ISYR  =  2001 !
                 Month (ISMO) --   No default   ! ISMO  = 1   !
                 Day   (ISDY) --   No default   ! ISDY  = 1   !
                 Hour  (ISHR) --   No default   ! ISHR  = 0   !

Number of periods to process
                 (NPER) -- No default   ! NPER  = 8752   !

Number of species to process from CALPUFF runs
                 (NSPECINP) -- No default   ! NSPECINP = 9 !

Number of species to write to output file
                 (NSPECOUT) -- No default   ! NSPECOUT = 9 !

Number of species to compute from those modeled
(must be no greater than NSPECOUT)
                 (NSPECCMP) -- No default   ! NSPECCMP = 0 !
```

When multiple files are used, a species name may appear in more than one file. Data for this species will be summed (appropriate if the CALPUFF runs use different source groups). If this summing is not appropriate, remove duplicate species from the file(s).

```
Stop run if duplicate species names
are found? (MDUPLCT)          Default: 0      ! MDUPLCT  =  1  !
  0 = no  (i.e., duplicate species are summed)
  1 = yes (i.e., run is halted)
```

Data for each species in a CALPUFF data file may also be scaled as they are read. This can be done to alter the emission rate of all sources that were modeled in a particular CALPUFF application. The scaling factor for each species is entered in Subgroup (2d), for each file for which scaling is requested.

```
Number of CALPUFF data files that will be scaled
(must be no greater than NFILES)
(NSCALED)                    Default: 0      ! NSCALED = 0 !
```

Ammonia-Limiting Method Option to recompute the HNO3/NO3 concentration partition prior to performing other actions is controlled by MNITRATE. This option will NOT alter any deposition fluxes contained in the CALPUFF file(s). Three partition selections are provided. The first two are typically used in sequence (POSTUTIL is run more than once). The first

selection (MNITRATE=1) computes the partition for the TOTAL (all sources) concentration fields (SO4, NO3, HNO3; NH3), and the second (MNITRATE=2) uses this partition (from the previous application of POSTUTIL) to compute the partition for individual source groups. The third selection (MNITRATE=3) can be used instead in a single POSTUTIL application if a file of background concentrations is provided (BCKGALM in Input Group 0).

Required information for MNITRATE=1 includes:
- species NO3, HNO3, and SO4
- NH3 concentration(s)
- met. data file for RH and T

Required information for MNITRATE=2 includes:
- species NO3 and HNO3 for a source group
- species NO3ALL and HNO3ALL for all source groups, properly partitioned

Required information for MNITRATE=3 includes:
- species NO3, HNO3, and SO4 for a source group
- species NO3, HNO3, SO4 and TNH3 from the background BCKGALM file
- If TNH3 is not in the background BCKGALM file, monthly TNH3 concentrations are used (BCKTNH3)

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

SOURCE OF AMMONIA:

Ammonia may be available as a modeled species in the CALPUFF files, and it may or may not be appropriate to use it for repartitioning NO3/HNO3 (in option MNITRATE=1 or MNITRATE=3). Its use is contolled by NH3TYP. When NH3 is listed as a processed species in Subgroup (2a), as one of the NSPECINP ASPECI entries, and the right option is chosen for NH3TYP, the NH3 modeled values from the CALPUFF concentration files will be used in the chemical equilibrium calculation.

NH3TYP also controls when monthly background ammonia values are used. Both gaseous (NH3) and total (TNH3) ammonia can be provided monthly as BCKNH3/BCKTNH3.

What is the input source of Ammonia?
(NH3TYP) No Default ! NH3TYP = 3 !
- 0 = No background will be used.
  ONLY NH3 from the concentration files listed in Subgroup (2a) as a processed species will be used.
  (Cannot be used with MNITRATE=3)

- 1 = NH3 Monthly averaged background (BCKNH3) listed below will be added to NH3 from concentration files listed in Subgroup (2a)

2 = NH3 from background concentration file BCKGALM
will be added to NH3 from concentration files
listed in Subgroup (2a)
(ONLY possible for MNITRATE=3)

3 = NH3 Monthly averaged background (BCKNH3)
listed below will be used alone.

4 = NH3 from background concentration file BCKGALM
will be used alone
(ONLY possible for MNITRATE=3)

NH3TYP	NH3 CONC	NH3 FROM BCKNH3	NH3 FROM BCKGALM
0	X	0	0
1	X	X	0
2	X	0	X
3	0	X	0
4	0	0	X

Default monthly (12 values) background ammonia concentration (ppb)
used for HNO3/NO3 partition:

Gaseous NH3 (BCKNH3) Default: -999
! BCKNH3 = 3., 3., 3., 3., 3., 3., 3., 3., 4*3. !

Total TNH3 (BCKTNH3) Default: -999
* BCKTNH3 = 1., 1., 1., 1.1, 1.4, 1.3, 1.3, 1.2, 4*1. *

If a single value is entered, this is used for all 12 months.
Month 1 is JANUARY, Month 12 is DECEMBER.

!END!

INPUT GROUP: 2 -- Species Processing Information

Subgroup (2a)

The following NSPECINP species will be processed:

! ASPECI = SO2 ! !END!
! ASPECI = SO4 ! !END!
! ASPECI = NOX ! !END!
! ASPECI = HNO3 ! !END!
! ASPECI = NO3 ! !END!

```
! ASPECI =        PMC !        !END!
! ASPECI =        PMF !        !END!
! ASPECI =         EC !        !END!
! ASPECI =        SOA !        !END!
```

Subgroup (2b)

The following NSPECOUT species will be written:

```
! ASPECO =        SO2 !        !END!
! ASPECO =        SO4 !        !END!
! ASPECO =        NOX !        !END!
! ASPECO =       HNO3 !        !END!
! ASPECO =        NO3 !        !END!
! ASPECO =        PMC !        !END!
! ASPECO =        PMF !        !END!
! ASPECO =         EC !        !END!
! ASPECO =        SOA !        !END!
```

Subgroup (2c)

The following NSPECCMP species will be computed by scaling and summing one or more of the processed input species. Identify the name(s) of the computed species and provide the scaling factors for each of the NSPECINP input species (NSPECCMP groups of NSPECINP+1 lines each):

Subgroup (2d)

Each species in NSCALED CALPUFF data files may be scaled before being processed (e.g., to change the emission rate for all sources modeled in the run that produced a data file). For each file, identify the file name and then provide the name(s) of the scaled species and the corresponding scaling factors (A,B where x' = Ax+B).

```
            A(Default=1.0)      B(Default=0.0)
            --------------      --------------

* MODDAT =NOFILES.DAT    *
*    SO2  =     1.1,              0.0   *
*    SO4  =     1.5,              0.0   *
*   HNO3  =     0.8,              0.0   *
*    NO3  =     0.1,              0.0   *
*END*
```