Guide for Applying the EPA Class I Screening Methodology with the CALPUFF Modeling System

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1. Introduction

These instructions are designed to guide a user through the process of preparing input files to run the CALPUFF, CALPOST and POSTUTIL programs to implement the U.S. EPA Screening Methodology for Class I areas (U.S. EPA, 1998). This methodology is referred to as "CALPUFF-lite" because it by-passes the need to generate a full three-dimensional wind field with CALMET. Instead, an ISCST3 single-station meteorological field is used.

Because the methodology designed by the EPA is meant to be a conservative screening technique, a number of assumptions are made that will tend to result in the overprediction of impacts. However, due to the complexity of wind fields in rough terrain and the physical mechanisms incorporated in the CALPUFF model, the screening procedure is not necessarily conservative in every case. However, it will usually predict larger impacts (sometimes much larger) than those obtained with a complete CALPUFF analysis using a three-dimensional wind field generated by CALMET.

This guide does not establish the EPA screening methodology, nor does it address all aspects of such an application. Many details will vary from application to application. Use this guide to learn about features of the CALPUFF modeling system that can be used to implement specific requirements.

Graphical User Interfaces (GUIs) are provided as part of the CALPUFF modeling package for the CALMET, CALPUFF and CALPOST programs. For the screening assessment, CALMET is not required. A postprocessor called POSTUTIL, which is needed for the application of the deposition screening procedure does not currently have a GUI associated with it. Therefore, the POSTUTIL inputs must be prepared by editing the POSTUTIL control file (POSTUTIL.INP) with any text editor. The file must be saved as a DOS ASCII file in order to be compatible with POSTUTIL.

These instructions assume that the CALPUFF modeling system has already been installed, and that the user has executed the initial CALMET/CALPUFF/CALPOST test cases to verify that the system is properly installed. It is highly recommended that users become familiar with the CALPUFF User's Guide (Scire et al., 2000) to understand the major features of the modeling system, and the types of input and output files required to run CALPUFF.

Use of the processor POSTUTIL is also addressed, as it facilitates the manipulation of the dry

and wet deposition flux files produced by CALPUFF prior to using CALPOST to characterize total sulfur and total nitrogen deposition fluxes. This processor is distributed as part of the CALPUFF modeling package, which is available from Earth Tech's CALPUFF web-page (http://www.src.com).

Meteorological data for the EPA screening procedure must be assembled in the form of an extended ISCST3 file. The program normally used for preparing the ISCST3 meteorological file is the PCRAMMET program, available from the EPA's Scram web site (http://www..epa.gov/scram001). However, see the notes below on limitations of the PCRAMMET program to drive CALPUFF. No guidance for this process is included here, just the admonition that meteorological parameters essential to simulating transport, dispersion, chemical transformation, and both wet and dry deposition must be present every hour of the year. These essential parameters include wind speed, wind flow direction, temperature, stability class, mixing height, friction velocity, Monin-Obukhov length, precipitation rate, short-wave solar radiation, and relative humidity.

It should be noted that incompatibilities exist between the U.S. EPA's version of PCRAMMET and CALPUFF. These include:

- PCRAMMET will not produce extended ISCST3 meteorological record variables (e.g., friction velocity, Monin-Obukhov length, relative humidity and solar radiation) when input data are provided in the CD144 format.   PCRAMMET will produce these variables only when SAMSON or HUSWO meteorological data are used. The extended record variable fields are left blank when CD144 data are used.

- PCRAMMET will not report a solar radiation value when an observed value is missing from the SAMSON or HUSWO datasets. Instead the solar radiation field is left blank.

Earth Tech has modified PCRAMMET to produce the ISCST3 extended record variables, when using CD144 surface meteorological data as input. Also, Earth Tech has incorporated an estimate of solar radiation (based on the solar elevation angle and cloud cover) when it is not reported in any of the meteorological input file formats (CD144, SAMSON, or HUSWO). This modified version of PCRAMMET is called "CPRAMMET" short for "CALPUFF-RAMMET". It is available on the Earth Tech web page in the CALPUFF section (http://www.src.com).

2. CALPUFF GUI

The CALPUFF GUI prepares an ASCII control file that is read by the CALPUFF model. The description below describes the steps needed to implement the EPA Class I screening methodology for a typical application.

-- Enter the CALPUFF GUI. (click on the CALPUFF icon, or run PUFMENU.EXE)

-- Change the WORKING DIRECTORY to the location where you wish to do the modeling. On the menu bar, select **File** and then **Change Directory**. Navigate to the directory that you wish to use. The full pathname should be displayed next to 'Set Current Working Directory:'.

-- Begin with a NEW control file. On the menu bar, select **File** and then **New**. This establishes many of the model default values, and avoids the problem of accepting information from an existing control file that may not be appropriate to this modeling task. If there is an existing control file that you know is appropriate, you may start with that file instead by selecting **File** and then **Open**. Remember to rename the file now so that the existing file will not be inadvertently over-written. Do this with the **File**, **Save As** feature.

-- Enter SEQUENTIAL INPUT mode. On the menu bar, select **Input** and then **Sequential**. This is recommended even when you start with an existing control file because it gives you the opportunity to review all of the information contained in the file. In this mode, you are guided through all of the main screens in a rational sequence.

-- Screen 1: Run Information. Enter 3 lines of text that sufficiently identify this CALPUFF application. Turn OFF the option to **Check selections against Regulatory Guidance** because this application does not use a CALMET meteorological data file and will not pass the regulatory guidance checks. Use the option to **Run all periods** contained in the meteorological data file, and supply the starting **Year** for the simulation (YYYY format) and the **Time Zone** associated with the meteorological data. Do not use the **Model Restart** option. **(NEXT)**.

-- Screen 2: Grid Settings. The top panel contains information that establishes the meteorological modeling domain. This application uses meteorological data from a single ISC-type file, so there is no spatial variation in meteorological or geophysical properties. Therefore, the minimum grid cell configuration (**NX**=2, **NY**=2, **NZ**=1) is used. A single layer is used in the vertical because the wind speed measured at anemometer height will be scaled to 'stack-top', as in ISC. Select **Edit Cell Face Heights** and place **cell face 2** at a height above ground of 3000m to 5000m (this height should exceed the maximum expected mixing height). Although few cells are needed in the horizontal, they must be large enough to cover an area swept out by a radius equal to the maximum distance from the source to the farthest boundary of a Class 1 area, plus a buffer zone of about 50km. This buffer zone allows CALPUFF to track puffs that may return to

a Class I area in a recirculating wind pattern. If the farthest Class I boundary is 60km from the source, for example, then the cell size (**Grid Spacing**) would be 110km. With the source at the center of the cluster of the 4 cells that define this grid, the modeling domain covers an area that is 220km by 220km, and the **Grid Origin** is 110km south and 110km west of the source location (the grid origin is the southwest corner of the grid). The source location determines the **UTM Zone**. Now, the bottom panel can be filled in. The computational domain is the same as the meteorological domain, so the grid cells in both the **X-Direction** and the **Y-Direction** are 1,2. **(Next)**.

-- Screen 3: Modeled Species. Assessments require chemical property data for chemical transformations and deposition. Use the **Load Library** option on this screen to install default values for commonly modeled species (file SPECIES.LIB). Now select the species for the run. Visibility assessments use the MESOPUFF II chemical transformation scheme which includes **SO2**, **SO4**, **NOX**, **HNO3**, and **NO3**. Highlight and add these species names (in this order) by creating an entry in the species list using **ADD**, and then dragging the name from the library table to the vacant line in the species list. Other species may then be included in the run if emitted (e.g., PM10). If chemical transformation is not required for an application, then the species emitted can be provided in any order. An alternate method for selecting the species for the MESOPUFF II chemical transformation scheme is to use the "quick-start" option. Select the **5-Species MESOPUFF II** entry in the pull-down box beneath the species list, and then click **Quick-Start**. This will load the species into the list in the correct order. (**Next**).

-- Screen 4: Chemical Transformation. Class I impact assessments typically require the chemical transformation option, so select the **MESOPUFF II Scheme**. Do NOT read ozone concentrations from an external file. Instead, provide constant **background concentrations** of ozone (**O3**) and ammonia (**NH3**) expressed in ppb. These values should be specified monthly for your modeling region by selecting **Monthly O3** and **Monthly NH3**, and filling in the concentration for each month. Retain the default **nightime conversion rates** (SO2 loss rate=0.2%/hr, NOX loss rate=2%/hr, and HNO3 formation rate=2%/hr). (**Next**).

-- Screen 5: Deposition. All of the species in the run appear in the table on this screen, but no deposition has been selected. Using the pull-down options under **Dry Deposited**, change None to either **Gas Phase** (SO2, NOX, and HNO3) or **Particle Phase** (SO4 and NO3). Under **Wet Deposited**, click on the check-box for each species to turn on wet deposition. All of the species-dependent deposition parameters are loaded from the species library when these selections are made. Note that the scavenging coefficients for NOX are zero, so NOX will not be removed or deposited by precipitation. Few, if any, changes should be made to any of the **Advanced Variables**. The most likely change will be in the selection of the **Vegetation State** if the modeling domain has stressed (due to drought) or inactive vegetation. (**Next**).

-- Screen 6: Meteorological/Landuse. In the **Meteorological Data Format** box, select **ISC ASCII File**. Place the cursor in the **File Name** box, and either type the name of the meteorological data file, or use the **Browse** feature to locate the file.   All defaults listed in the

Edit Advanced Variables should be retained. In the panel labeled **Single-Station Met Data Inputs**, enter data consistent with the meteorological data file that was prepared for the application. Note that the **Elevation Above Sea Level** is used to set the surface elevation of the modeling domain. Use the elevation of the area near the source location for this input. The panel below this configures the wind speed power law extrapolation function used to estimate the wind speed at stack-top, and identifies the minimum valid wind speed for non-calm conditions. The default values seen in this panel should be retained. (**Next**).

-- **Screen 7: Plume Rise.** Configure the plume rise options so that only **Stacktip Downwash** is modeled. (**Next**).

-- **Screen 8: Dispersion.** Retain all default settings on this screen, and on the **Edit Advanced Variables** screen. (**Next**).

-- **Screen 9: Terrain Effects.** Retain all default settings on this screen, so that any terrain effects will be simulated using the **Partial plume path adjustment** method. (**Next**).

-- **Screen 10: Point Sources.** Enter the location and characteristics of all point sources for this run. Coordinates should be consistent with those used earlier to define the grid system for the simulation, placing the sources near the center of the modeling domain. The vertical **Momentum Flux Factor** should remain at the default setting of 1.0 unless the release is capped, in which case the factor should be set to 0.0. Select **Edit Emission Rates** to provide the emissions of each species from each source. Species that are not emitted (but are formed by chemical transformation) should have a zero emission rate. No initial sigmas are typically used for point sources, but may be provided if appropriate for a source (use the **Initial Sigmas** checkbox, then select **Edit Initial Sigmas**). If any source is subject to building downwash, the wind-direction-specific building dimensions must be entered. Identify such sources using the **Building Downwash** checkboxes, and then either select **Load BPIP ...** or **Edit Building Dimensions**. The former prompts you for the name of the "BPIP.OUT" file generated by the BPIP program, and loads the effective building dimensions directly. The latter allows you to enter or edit the dimensions by hand. No sources should be provided in an external file. (**Next**).

-- **Screens 11, 12, 13: Area Sources, Volume Sources, and Buoyant Line Sources.** Follow similar procedures to provide information for sources other than point sources. (**Next**).

-- **Screen 14: Boundary Sources.** Do not include any boundary sources. (**Next**).

-- **Screen 15: Gridded Receptors.** Do not use gridded receptors. (**Next**).

-- **Screen 16: Discrete Receptors.** All receptors are generated using the receptor ring feature in this screen. These rings should be centered on the source, which should be located at the center of the modeling grid, and each should be given a radius such that the set of rings covers the distance from the nearest boundary of the Class 1 area to the farthest boundary. Multiple Class I

areas located at different distances may require multiple sets of rings. Receptors along each ring should be spaced at 1-degree intervals (360 receptors/ring). A single elevation should be used for each ring, representing the average elevation at this distance within the Class 1 area. If the terrain elevations in the Class 1 area vary substantially, then the ring may be entered twice: once with the minimum elevation and once with the maximum elevation. To create a set of receptors, select **Add Ring Receptors ...** to bring up the **Ring Receptors** screen. This screen requests the coordinates of the **Center of Ring**, the **Angular Separation Along Ring**, and it allows the receptors generated to be placed into the discrete receptor table either before or after any existing receptors in the table. The **Radius** and **Ground Elevation** columns of the table provide the remaining information needed to create the receptor entries. Initially, ground elevations and height above ground are zero. Enter the appropriate elevation for each ring, but leave the receptor height above ground at zero because all receptors must remain on the ground. Select **OK** to return to the **Discrete Receptor** screen. Repeat this process to add new groups of rings. Note that receptor information in this table may be exported to disk (**Save As**) and imported later (**Load**) for use in other CALPUFF applications. (**Next**).

-- Screen 17: Output. Configure the outputs for the run so that all concentrations and deposition fluxes that are needed for the application are written to binary files on disk. The postprocessing step will require these files. Limited output (for informational purposes only) should be written to the list file, since no averaging is available for this output, and the format of the list file will result in a very large file if all of the hourly results are written to it. Typically, no model output is written to the list file. In the top panel of the screen, use the check-boxes under **Create Binary Disk File** to select the required **Concentration**/**Dry Flux**/**Wet Flux**/**RH(visibility)** files, and provide a **Binary File Name** for each. Entries for the **Print Interval for the List File** will be ignored unless output to the list file is selected. The file for hourly relative humidity (**RH**) data should be created if visibility calculations will be done in CALPOST using any method other than **Method 6**. Select the output options for the run by clicking on the **List Output** and **Binary Output** tabs of the species table. No boxes should be checked for the list file output, while all boxes appropriate for the application should be checked for the binary file output. Note that only those species that are explicitly written to binary concentration and deposition flux files will be available for postprocessing. Complete the output configuration by selecting **Progress Messages to Screen** and **Use Data Compression in Binary Files**, and provide the name for the list file. (**Done**).

The information for the CALPUFF control file is now complete. Use **File**, **Save As** to save this control file to disk, choosing an appropriate name for it.

A utility can be used prior to running CALPUFF that screens the meteorological file for values that are out of range. It does not change any data, but it does report problems to a list file. Select **Utilities, Check Met File** to enter this utility. Identify the **Met Data File** name to be tested, and assign a name for the **List File** produced by this utility. Select the **Met File Type** and check the **Extended Records** box so that data needed for deposition and chemical transformation are

included. **Run** the utility, and then review the list file that is created for warning messages.

Now, run CALPUFF. Use **Run**, **Run CALPUFF** to bring up the screen that shows the name of the executable that will be run, and the name of the control file that you have created. Select the **Test Run** option to instruct the model to process all of the information in the control file and then halt before starting the simulation. Pressing **OK** loads the final screen that lists the input and output files for your run. If these are correct, launch CALPUFF by pressing **Run**. A DOS window will open and the CALPUFF model will execute. After this window closes, review the contents of the list file created by CALPUFF to make sure that no errors or warnings were produced. Then, repeat the run-sequence, this time selecting the **Regular Run** button, which will produce the full simulation. After CALPUFF stops, always review the list file to be sure that the application used the intended files and parameter settings, and that no errors arose during the simulation.

When modeling 5 years of meteorological data, use the control file for the first year as a starting-point to create the remaining 4 control files. Open the first in the CALPUFF GUI, save it to a different filename, and then edit the newly-named control file in the GUI to indicate the different input and output files and the year simulated (remember to update the title lines to clearly identify the simulation).

3. POSTUTIL

After completing the 5 CALPUFF runs, one for each year modeled, you will have 5 sets of binary files. Each set includes one file for the modeled concentrations (we shall simply refer to this file as 'conc.dat'), one file for the modeled dry deposition fluxes ('dflx.dat'), and one file for the modeled wet deposition fluxes ('wflx.dat'), calculated at every receptor, for each hour of the year. Using these files, the post-processing tasks include characterizing peak concentrations of several species (e.g., SO_2, NO_x and PM10) for several averaging times, characterizing peak annual deposition rates of total sulfur and total nitrogen, and characterizing the change in visibility associated with modeled sulfates, nitrates, and any emitted particulates.

Prior to applying CALPOST to obtain these types of outputs, POSTUTIL should be used to consolidate the deposition fluxes. In particular, POSTUTIL can sum the wet and dry deposition fluxes into the total deposition flux of each species, and it can convert sulfate and nitrate fluxes to the total sulfur and total nitrogen fluxes. It should be configured to read the 'dflx.dat' and 'wflx.dat' files, and produce a new binary file 'tflx.dat' with total sulfur and total nitrogen added. CALPOST can then be used to process the total fluxes in 'tflx.dat'.

POSTUTIL is driven by a control file that is configured using any standard text editor (e.g., NOTEPAD). It uses the general CALPUFF control file structures explained in the CALPUFF

users guide, containing several input groups with module inputs set within a pair of special delimiter characters (!). All documentation associated with these inputs is written outside of these delimiters.

A sample control file that illustrates a POSTUTIL application for the screening assessment is provided in Table 1. The top of the control file contains three lines that are reserved for identifying the application. These lines are written to the output file, and become part of the documentation in subsequent processing.

Input Group: 0

Input Group 0 identifies the input and output files for the application. The output consists of a list file that documents how this application of POSTUTIL is configured, and a data file that is identical in form to the binary data files created by CALPUFF. As stated above, the data file is given the generic name 'tflx.dat' in Table 1 (!UTLDAT = TFLX.DAT!) to indicate that wet and dry fluxes are summed, and that total sulfur and total nitrogen are added the list of species in the file. The list file is given the default name (!UTLLST = POSTUTIL.LST!). More specific names should be used in typical applications.

Input files include a CALMET meteorological data file and one or more CALPUFF binary files. The CALMET file is not needed for this application because no nitrate partitioning will be calculated (MNITRATE=0). Two CALPUFF binary files are needed for this application: one for the dry deposition flux, and one for the wet deposition flux. Therefore !NFILES = 2! and two filenames are provided in Subgroup 0b:

! MODDAT =WFLX.DAT   !   !END!
! MODDAT =DFLX.DAT   !   !END!

Note the location of the input terminator !END!. This terminator signals the end of a group or a subgroup in the control file, and it also signals the end of an assignment for variables such as MODDAT that appear multiple times.

Input Group: 1

Input Group 1 identifies the period to process, and sets parameters that configure POSTUTIL. Note that there is no "run all periods" option, so that the period must be explicitly stated. Typically, full years of 8760 hours (8784 hours for leap years) are processed in the screening assessments.

Three "nspec" variables are set:
NSPECINP identifies the number of species that are stored as the input data files are read.
NSPECOUT identifies the number of species that are written to the output data file.
NSPECCMP identifies the number of new species that are computed from those that are stored.

For example, you may wish to store 7 of 12 species from the input files, and you may wish to compute 3 new species from these 7, and write the 3 new species plus 5 of the stored species to the output data file for analysis with CALPOST. In the screening assessment sample, the 5 MESOPUFF II chemical transformation species are stored (! NSPECINP = 5 !), because all 5 are needed to compute the 2 new species (! NSPECCMP = 2 !), the total sulfur and the total nitrogen fluxes. The original 5 plus the 2 new species are written to the output data file (! NSPECOUT = 7 !) so that the sum of the wet and dry fluxes are available for further analysis.

Table 1
Sample POSTUTIL Control File (POSTUTIL.INP)
Input Group 0

```
Example application for total nitrogen & sulfur deposition
Nitrogen deposition due to NOX(as NO2), HNO3, NH4NO3, and (NH4)2SO4
Sulfur deposition due to SO2, (NH4)2SO4
---------------- Run title (3 lines) ------------------------------------------

                  POSTUTIL MODEL CONTROL FILE
                  ---------------------------


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INPUT GROUP: 0 -- Input and Output File Names
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Subgroup (0a)
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Output Files
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 File            Default File Name
 ----            -----------------
 List File       POSTUTIL.LST        ! UTLLST =POSTUTIL.LST   !
 Data File       MODEL.DAT           ! UTLDAT =TFLX.DAT    !


Input Files
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 Meteorological data file for the HNO3/NO3 partition option.
 Used only if MNITRATE > 0.
 The met data file is the 'CALMET.DAT' format file used in the CALPUFF
 simulation.  If multiple CALMET files had been used in sequence, then
 POSTUTIL must be applied multiple times, once for each CALMET file.

 File            Default File Name
 ----            -----------------
 Met Data        MET.DAT             ! UTLMET =CALMET.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 = 2   !

 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!

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 NOTE: file/path names can be up to 70 characters in length
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Subgroup (0b)
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Input File      Default File Name
----------      -----------------
    1           CALPUFF.DAT         ! MODDAT =WFLX.DAT     ! !END!
    2           (none)              ! MODDAT =DFLX.DAT     ! !END!
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INPUT GROUP: 1 -- General run control parameters
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     Starting date:   Year  (ISYR) --   No default   ! ISYR  =  1990 !
                      Month (ISMO) --   No default   ! ISMO  = 1   !
                      Day   (ISDY) --   No default   ! ISDY  = 1   !
                      Hour  (ISHR) --   No default   ! ISHR  = 1   !

     Number of periods to process
                              (NPER) -- No default   ! NPER  = 8760 !

     Number of species to process from CALPUFF runs
                         (NSPECINP) -- No default    ! NSPECINP = 5 !

     Number of species to write to output file
                         (NSPECOUT) -- No default    ! NSPECOUT = 7 !

     Number of species to compute from those modeled
     (must be no greater than NSPECOUT)
                         (NSPECCMP) -- No default    ! NSPECCMP = 2 !

 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  =  0  !
        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 !

 Option to recompute the HNO3/NO3 concentration partition prior to
 performing other actions.  This option will NOT alter any deposition
 fluxes contained in the CALPUFF file(s).  Two partition selections
 are provided.  The first (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 a previous application
 of POSTUTIL) to compute the partition for individual source groups.

 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

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

     Ammonia concentrations may be available as a modeled species in
     the CALPUFF files.  When NH3 is listed as a processed species in
     Subgroup (2a) (as one of the NSPECINP ASPECI entries), the
     modeled values will be used in the chemical equilibrium calculation.
     If NH3 is not on this list, the default background value listed
     below will be used.
     Default ammonia concentration (ppb) used for HNO3/NO3 partition:
     (BCKNH3) in ppb                 Default: 10.      ! BCKNH3 = 1. !
!END!
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11

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INPUT GROUP: 2 -- Species Processing Information
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Subgroup (2a)
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   The following NSPECINP species will be processed:

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

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Subgroup (2b)
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   The following NSPECOUT species will be written:

! ASPECO =          SO2 !          !END!
! ASPECO =          SO4 !          !END!
! ASPECO =          NOX !          !END!
! ASPECO =         HNO3 !          !END!
! ASPECO =          NO3 !          !END!
! ASPECO =            N !          !END!
! ASPECO =            S !          !END!

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Subgroup (2c)
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   Supply this Subgroup only if NSPECCMP > 0.
   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):

! CSPECCMP =          N !
!     SO2  =      0.0        !
!     SO4  =      0.291667 !
!     NOX  =      0.304348 !
!    HNO3  =      0.222222 !
!     NO3  =      0.451613 !
!END!

! CSPECCMP =          S !
!     SO2  =      0.500000 !
!     SO4  =      0.333333 !
!     NOX  =      0.0 !
!    HNO3  =      0.0 !
!     NO3  =      0.0 !
!END!

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Subgroup (2d)
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   Supply this Subgroup only if NSCALED > 0.
   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 =WFLX.DAT     @
@     SO2  =      1.0,                0.0   @
@     SO4  =      1.0,                0.0   @
@END@
```

The remaining control parameters in this group should be set as indicated in Table 1. Deposition fluxes of each species are summed (wet+dry), no fluxes are scaled, and no nitrate partitioning is done in the screening assessment.

Input Group: 2

The NSPECINP species that are stored are named in Subgroup 2a. Species names must match those used in the CALPUFF runs, but may be entered in any order. Each is read into the data dictionary name ASPECI. In the sample control file, the 5 MESOPUFF II species names are entered.

Similarly, the NSPECOUT species are named in Subgroup 2b. These names include the 5 MESOPUFF II species, plus the two new species for total sulfur (S) and total nitrogen (N). Each is read into the data dictionary name ASPECO.

Subgroup 2c provides the information required to compute the new species. New species concentrations or deposition fluxes are constructed using a weighted sum of the concentrations or deposition fluxes of all of the stored species. The weight for each species is entered here. Only SO2 and SO4 contribute sulfur mass. Nitrogen mass is contributed by SO4 (CALPUFF tracks ammonium sulfate as SO4), NOX (as NO2), HNO3, and NO3 (CALPUFF tracks ammonium nitrate as NO3). The atomic weights for the constituent elements are sulfur = 32, oxygen = 16, nitrogen = 14, and hydrogen = 1. The molecular formula for ammonium sulfate is $(NH_4)_2SO_4$ and ammonium nitrate is $(NH_4)NO_3$. Therefore:

      1 g of SO2   contributes 0.500000 g of S
      1 g of SO4   contributes 0.333333 g of S

      1 g of SO4   contributes 0.291667 g of N
      1 g of NOX   contributes 0.304348 g of N
      1 g of HNO3 contributes 0.222222 g of N
      1 g of NO3   contributes 0.452623 g of N

As illustrated in the sample in Table 1, identify the new species by name using the data dictionary name CSPECCMP, and then assign the weight for each species by name.

Subgroup 2d is not used in the screening assessment.

Running POSTUTIL

POSTUTIL assumes that the control file prepared for it is called POSTUTIL.INP, and that this file is located in the current directory (or folder). Create the control file for each year of your simulation, with an appropriate name. Then process each year in turn by copying the control file into POSTUTIL.INP, and running POSTUTIL either from a DOS window or within Windows.

4. CALPOST GUI

CALPOST is applied several times to produce the summaries needed for a screening assessment. This process is illustrated here by showing the steps needed to characterize peak SO2 concentrations for 3-hr, 24-hr, and annual averages for one year; peak annual deposition of total nitrogen for one year; and the percent change in daily and annual extinction due to sulfates and nitrates for one year.

4.1 Peak SO2 Concentrations

-- **Enter the CALPOST GUI.** (click on the CALPOST icon, or run POSTMENU.EXE)

-- **Change the WORKING DIRECTORY to the location where you wish to do the processing.** On the menu bar, select **File** and then **Change Directory**. Navigate to the directory that you wish to use. The full pathname should be displayed next to 'Set Current Working Directory:'.

-- **Begin with a NEW control file.** On the menu bar, select **File** and then **New**. This establishes many of the model default values, and avoids the problem of accepting information from an existing control file that may not be appropriate to this modeling task. If there is an existing control file that you know is appropriate, you may start with that file instead by selecting **File** and then **Open**. Remember to rename the file now so that the existing file will not be inadvertently over-written. Do this with the **File**, **Save As** feature.

-- **Enter SEQUENTIAL INPUT mode.** On the menu bar, select **Input** and then **Sequential**. This is recommended even when you start with an existing control file because it gives you the opportunity to review all of the information contained in the file. In this mode, you are guided through all of the main screens in a rational sequence.

-- **Screen 1: Process Options.** Enter 3 lines of text that sufficiently identify this CALPOST application. Because CALPOST is typically run several times on the same CALPUFF output file, be specific as to the nature of the CALPOST application. Use the option to run all periods contained in the CALPUFF output file, and supply the starting year for the simulation (YYYY format). In the **Receptors** panel, request only **Discrete** receptors using the checkboxes. Then use the **Select Discrete Subset** button to move into the **Discrete Receptors to Process** screen and mark the check-box to **Include All Discrete Receptors**. In addition, mark the **Report by Ring** check-box to obtain a summary of the results by ring. (**Next**).

-- **Screen 2: Processed Data.** In the **Input Data Type** panel, identify the data that you wish to process. In this application we want to obtain results for SO2 concentrations, so select **Concentration** from the pull-down **Process** menu, type **SO2** into the **Species** box, and provide the **Input Data File Name** for the CALPUFF output file that contains the concentrations. (**Next**).

-- Screen 3: Output Options. Many of the features provided on this screen can be used to obtain detailed information about the CALPUFF results, but only the minimum is discussed here. In the **Output** panel, select the **Averaging Time**(s) of 3-hr, 24-hr, and run-length using the check-boxes, and select the reporting **Units**. Select only the **Ranked Values Table** check-box, and enter a single **Rank** of 1 to obtain the highest concentrations for each averaging time. Make sure that the other output options for top-50 tabulations and exceedance counts are inactive. Complete the entries for this screen by providing the **List File Name** in the **File Names** panel. (**Done**).

The information for the CALPOST control file is complete, and CALPOST may be run. The results of the analyses are reported to the CALPOST list file.

4.2 Peak Total Nitrogen Deposition Flux

-- Enter the CALPOST GUI. (click on the CALPOST icon, or run POSTMENU.EXE)

-- Change the WORKING DIRECTORY to the location where you wish to do the processing. On the menu bar, select **File** and then **Change Directory**. Navigate to the directory that you wish to use. The full pathname should be displayed next to 'Set Current Working Directory:'.

-- Begin with a NEW control file. On the menu bar, select **File** and then **New**. This establishes many of the model default values, and avoids the problem of accepting information from an existing control file that may not be appropriate to this modeling task. If there is an existing control file that you know is appropriate, you may start with that file instead by selecting **File** and then **Open**. Remember to rename the file now so that the existing file will not be inadvertently over-written. Do this with the **File**, **Save As** feature.

-- Enter SEQUENTIAL INPUT mode. On the menu bar, select **Input** and then **Sequential**. This is recommended even when you start with an existing control file because it gives you the opportunity to review all of the information contained in the file. In this mode, you are guided through all of the main screens in a rational sequence.

-- Screen 1: Process Options. Enter 3 lines of text that sufficiently identify this CALPOST application. Because CALPOST is typically run several times on the same CALPUFF output file, be specific as to the nature of the CALPOST application. Use the option to run all periods contained in the CALPUFF output file, and supply the starting year for the simulation (YYYY format). In the **Receptors** panel, request only **Discrete** receptors using the checkboxes. Then use the **Select Discrete Subset** button to move into the **Discrete Receptors to Process** screen and mark the check-box to **Include All Discrete Receptors**. In addition, mark the **Report by Ring** check-box to obtain a summary of the results by ring. (**Next**).

-- Screen 2: Processed Data. In the **Input Data Type** panel, identify the data that you wish to

process. For this example, select **Total Flux** from the pull-down **Process** menu, type **N** into the **Species** box for total nitrogen, and provide the **Input Data File Name** for the CALPUFF output file that contains the total (wet+dry) deposition fluxes. This is the file produced by POSTUTIL. (**Next**).

-- **Screen 3: Output Options.** Many of the features provided on this screen can be used to obtain detailed information about the CALPUFF results, but only the minimum is discussed here. In the **Output** panel, select a single **Averaging Time** using the run-length check-box, and select the reporting **Units**. Select the **Ranked Values Table** check-box, and enter a single **Rank** of 1 to report the annual deposition flux at each receptor ring. Make sure that the other output options for top-50 tabulations and exceedance counts are inactive. Complete the entries for this screen by providing the **List File Name** in the **File Names** panel. (**Done**).

The information for the CALPOST control file is complete, and CALPOST may be run. The results of the analyses are reported to the CALPOST list file.

4.3 Daily and Annual Change in Extinction

-- **Enter the CALPOST GUI.** (click on the CALPOST icon, or run POSTMENU.EXE)

-- **Change the WORKING DIRECTORY to the location where you wish to do the processing.** On the menu bar, select **File** and then **Change Directory**. Navigate to the directory that you wish to use. The full pathname should be displayed next to 'Set Current Working Directory:'.

-- **Begin with a NEW control file.** On the menu bar, select **File** and then **New**. This establishes many of the model default values, and avoids the problem of accepting information from an existing control file that may not be appropriate to this modeling task. If there is an existing control file that you know is appropriate, you may start with that file instead by selecting **File** and then **Open**. Remember to rename the file now so that the existing file will not be inadvertently over-written. Do this with the **File**, **Save As** feature.

-- **Enter SEQUENTIAL INPUT mode.** On the menu bar, select **Input** and then **Sequential**. This is recommended even when you start with an existing control file because it gives you the opportunity to review all of the information contained in the file. In this mode, you are guided through all of the main screens in a rational sequence.

-- **Screen 1: Process Options.** Enter 3 lines of text that sufficiently identify this CALPOST application. Because CALPOST is typically run several times on the same CALPUFF output file, be specific as to the nature of the CALPOST application. Use the option to run all periods contained in the CALPUFF output file, and supply the starting year for the simulation (YYYY format). In the **Receptors** panel, request only **Discrete** receptors using the checkboxes. Then use the **Select Discrete Subset** button to move into the **Discrete Receptors to Process** screen

and mark the check-box to **Include All Discrete Receptors**. In addition, mark the **Report by Ring** check-box to obtain a summary of the results by ring. (**Next**).

-- Screen 2: Processed Data. In the **Input Data Type** panel, identify the data that you wish to process. For visibility assessments, select **Visibility** from the pull-down **Process** menu, and the species **VISIB** will automatically appear in the **Species** box. Provide the **Input Data File Name** for the CALPUFF output file that contains the concentrations, since the visibility calculations will be based on CALPUFF concentrations for several species. Identify the **Modeled Species** that will be used to compute light extinction coefficients. These should be **Sulfates**, **Nitrates**, and in some cases **Fine Particles** if such emissions were modeled. Species names for the sulfates and nitrates are fixed in CALPUFF (e.g. via the chemical transformation option), but the **Species Name for Particulates Used in the Input Data File** is not fixed and must be specified here. Select either **Method 2** or **Method 6** in the **Method for Background Light Extinction** menu, depending on instructions from the reviewing agency. Method 2 uses the relative humidity values from the CALPUFF "visibility" file to compute the relative humidity factor f(RH) for each hour. Method 6 uses a single f(RH) factor for the year, specific to the class I area in the simulation. Note that the f(RH) simulates the effect of humidity on the scattering properties of hygroscopic particles such as sulfate and nitrate. For Method 2, set the **Max. Relative Humidity** to 95%, and provide the **Relative Humidity File** name (created by the CALPUFF run). For Method 6, select the **Monthly RH** (relative humidity) **Factors** button, and input the factor each month. Next, supply the **Monthly Background Concentrations**, and the **Extinction Due to Rayleigh Scattering**. These are prescribed for each Class I area, and must be specific to your application. Note that a single set of values is typically provided for an entire year rather than by month. Enter the annual value for each month. All of the other parameters associated with visibility processing should remain set at the default values. (**Next**).

-- Screen 3: Output Options. Many of the features provided on this screen can be used to obtain detailed information about the CALPUFF results, but only the minimum is discussed here. For visibility processing, only the **List File Name** in the **File Names** panel needs to be supplied. Daily visibility results are automatically written to the list file. All other output options should be turned off. (**Done**).

The information for the CALPOST control file is complete, and CALPOST may be run. The results of the analyses are reported to the CALPOST list file. Daily and annual visibility impacts are characterized by either a % change in extinction, or as a change in deciview. Guidance should be provided by the reviewing authority as to which measures are preferred.

5. REFERENCES

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