ADDENDUM

USER'S GUIDE FOR THE AMS/EPA REGULATORY MODEL - AERMOD

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USER INSTRUCTIONS FOR THE
REVISED AERMOD MODEL (DATED 04300)

This document provides user instructions for revisions of the AERMOD dispersion model. Two sets of revisions are included in this Addendum. The first set of revisions includes deposition algorithms, first introduced with version 03273 of AERMOD, and the second set of revisions includes the Plume Volume Molar Ratio Method (PVMRM) inccript ver set(. udes deposition algorit4m)8.3(2(iorit4mple docum)8.nclude the AEin (ent prcludean EPAM

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Modeling Options

The dispersion options are controlled by the MODELOPT keyword on the CO pathway. The syntax, type, and order of the MODELOPT keyword are summarized below:

Syntax:	`CO MODELOPT DFAULT CONC/DEPOS/DDEP and/or WDEP AREADPLT FLAT NOSTD NOCHKD NOWARN SCREEN TOXICS SCIM PVMRM or OLM`
Type:	Mandatory, Non-repeatable
Order:	Must precede POLLUTID, HALFLIFE and DCAYCOEF

where:

CONC - Specifies that concentration values will be calculated;

DEPOS - Specifies that total deposition flux values (both dry and wet) will be calculated;

DDEP - Specifies that dry deposition flux values will be calculated;

WDEP - Specifies that wet deposition flux values will be calculated;

AREADPLT - Specifies that an optimized method for plume depletion due to dry removal mechanisms will be included in calculations for area sources;

PVMRM - Specifies that the non-default Plume Volume Molar Ratio Method (PVMRM) for NO_2 conversion will be used; and

OLM - Specifies that the non-default Ozone Limiting Method (OLM) for NO_2 conversion will be used.

The other keywords on the MODELOPT card are described in the AERMOD user's guide (EPA, 2002a).

The user may select any or all of the output types (CONC, DEPOS, DDEP and/or WDEP) to be generated in a single model run. The order of these secondary keywords on the MODELOPT card has no effect on the order of results in the output files - the outputs will always be listed in the order of CONC, DEPOS, DDEP, and WDEP. The model will also assume CONCentration calculations if neither the CONC, DEPOS, DDEP nor WDEP keywords are specified.

The dry and/or wet removal (depletion) mechanisms (the DRYDPLT and WETDPLT options in earlier versions of AERMOD) will automatically be included in the calculated concentrations or deposition flux values if the dry and/or wet deposition processes are considered. Note that dry and wet removal effects on calculated concentration values can be included even if deposition flux values are not being calculated. However, the additional data requirements for dry and wet deposition, described below, must be met in order for dry and wet removal to be included in the calculations.

The PVMRM and OLM options for modeling NO_2 conversion are non-default options, and only one of these options can be specified for a given model run. Both options require that the pollutant ID be specified as NO2 on the CO POLLUTID card (see Section 3.2.5 of the AERMOD User's Guide).

Modeling Increment Credits with PVMRM and OLM

Due to the ozone-limiting effects of the PVMRM and OLM options, the predicted concentrations of NO_2 are not linearly proportional to the emission rate. Therefore, the approach of modeling increment credits through the use of a negative emission rate for credit sources cannot be used with the PVMRM and OLM options as currently implemented. The user should check with the appropriate reviewing authority for further guidance on modeling increment credits for NO_2.

Definition of Seasons for Gas Dry Deposition

The new deposition algorithms include land use characteristics and some gas deposition resistance terms based on five seasonal categories, defined in Table 2 of the ANL report as:

Seasonal Category 1: Midsummer with lush vegetation
Seasonal Category 2: Autumn with unharvested cropland
Seasonal Category 3: Late autumn after frost and harvest, or winter with no snow
Seasonal Category 4: Winter with snow on ground
Seasonal Category 5: Transitional spring with partial green coverage or short annuals

The user correlates these seasonal definitions to calendar months through the GDSEASON keyword on the CO pathway. The syntax and type of the GDSEASON keyword are:

Syntax:	`CO GDSEASON Jan Feb Mar ... Dec`
Type:	`Optional, Non-repeatable`

where a numeric value from 1 to 5 is entered for each of the twelve calendar months to associate it with the seasonal definitions given above. This keyword is optional for the model, but mandatory when applying the new gas deposition algorithms. Some of the seasonal categories defined above may not apply for certain regions, such as Category 4 for southern latitudes.

Definition of Land Use Categories for Gas Dry Deposition

The new deposition algorithms include some gas deposition resistance terms based on five seasonal categories, defined above, and on nine land use categories as follows (from Table 1 of the ANL report):

Land Use Category	Description
1	Urban land, no vegetation
2	Agricultural land
3	Rangeland
4	Forest
5	Suburban areas, grassy
6	Suburban areas, forested
7	Bodies of water
8	Barren land, mostly desert
9	Non-forested wetlands

The user defines the land use categories by wind direction through the GDLANUSE keyword on the CO pathway. The syntax and type of the GDLANUSE keyword are:

Syntax:	`CO GDLANUSE Sec1 Sec2 Sec3 ... Sec36`
Type:	`Optional, Non-repeatable`

where a numeric value from 1 to 9 is entered for each of the 36 wind direction sectors (every 10 degrees) to associate it with the land use definitions given above. This keyword is optional for the model, but mandatory when applying the new gas deposition algorithms. The first value, Sec1, corresponds with the land use category for winds blowing toward 10 degrees, plus or minus 5 degrees. The downwind sectors are defined in clockwise order, with Sec36 corresponding to winds blowing toward 360 degrees (North). The user can specify "repeat values" by entering a field such as "36*3" as a parameter for the GDLANUSE keyword. The model will interpret this as "36 separate entries, each with a value of 3." Since the model must identify this as a single parameter field, there must not be any spaces between the repeat-value and the value to be repeated.

Option for Overriding Default Parameters for Gas Dry Deposition

An optional keyword is available on the Control (CO) pathway to allow the user to override the default values of the reactivity factor (f_o), and the fraction (F) of maximum green leaf area index (LAI) for seasonal categories 2 and 5, for use with the gas dry deposition algorithms.

The syntax and type of the GASDEPDF keyword are summarized below:

Syntax:	`CO GASDEPDF  React  F_Seas2  F_Seas5  (Refpoll)`
Type:	`Optional, Non-repeatable`

where the parameter React is the value for pollutant reactivity factor (f_o), and F_Seas2 and F_Seas5 are the fractions of maximum green LAI for seasonal categories 2 and 5, respectively. The parameter Refpoll is the optional name of the pollutant. If the GASDEPDF keyword is omitted, then the default value of 0 is used for React, and default values of 0.5 and 0.25 are used for F_Seas2 and F_Seas5, respectively. A reactivity factor value of 1 should be input for ozone (O_3), titanium tetrachloride ($TiCl_4$), and divalent mercury (Hg^{2+}), and a value of 0.1 should be input for nitrogen dioxide (NO_2). A value of F=1.0 is used for seasonal categories 1, 3, and 4.

Specifying Ozone Concentrations for PVMRM and OLM Options

The background ozone concentrations can be input as a single value through the OZONEVAL keyword on the CO pathway, or may be input as hourly values through a separate data file specified through the OZONEFIL keyword on the CO pathway. The user must specify either the OZONEVAL or OZONEFIL keywords, or both, in order to use the PVMRM or OLM options. If both keywords are entered, then the value entered on the OZONEVAL keyword will be used to substitute for hours with missing ozone data in the ozone data file.

The syntax of the OZONEVAL keyword is as follows:

```
CO OZONEVAL  O3Value  (O3Units)
```

where the O3Value parameter is the background ozone concentration in the units specified by the O3Units parameter (PPM, PPB, or UG/M3). If the optional O3Units parameter is missing, then the model will assume units of micrograms/cubic-meter (UG/M3) for the background ozone values. If units of PPM or PPB are used, then the model will convert the concentrations to micrograms/cubic-meter based on the reference ambient temperature and the base elevation specified on the ME PROFBASE card. The OZONEVAL keyword word is optional and non-repeatable.

The syntax of the OZONEFIL keyword is as follows:

```
CO OZONEFIL  O3FileName  (O3Units)  (Format)
```

where the O3FileName parameter is the filename for the hourly ozone concentration file, the optional O3Units parameter specifies the units of the ozone data (PPM, PPB, or UG/M3, with UG/M3 as the default), and the optional Format parameter specifies the Fortran FORMAT to read the ozone data. If the optional Format parameter is missing, then the model will read the ozone data using a Fortran free format, i.e., assuming that commas or spaces separate the data fields. The contents of the ozone data file must include the year (2-digits), month, day, hour and ozone value in that order (unless specified differently through the Format parameter). The date sequence in the ozone data file must match the date sequence in the hourly meteorological data files. As with the OZONEVAL keyword, if units of PPM or PPB are used, then the model will convert the concentrations to micrograms/cubic-meter based on the reference ambient temperature and the base elevation specified on the ME PROFBASE card.

Values of ozone concentrations in the ozone data file that are less than zero or greater than or equal to 900.0 will be regarded as missing. If a background ozone value has been specified using the OZONEVAL keyword, then that value will be used to substitute for missing ozone data from the ozone file. If no OZONEVAL keyword is used, then the model will assume full conversion for hours with missing ozone data.

Specifying the Equilibrium NO2/NOx Ratio

The PVMRM option for modeling conversion of NO to NO_2 incorporates a default NO_2/NO_x equilibrium ratio of 0.90. A NO_2/NO_x equilibrium ratio other than 0.90 can be specified through the optional NO2EQUIL keyword on the CO pathway. The syntax of the NO2EQUIL keyword is as follows:

```
CO NO2EQUIL NO2Equil
```

where the NO2Equil parameter is the NO_2/NO_x equilibrium ratio and must be between 0.10 and 1.0, inclusive.

Open Pit Source Option

The open pit source option is invoked by specifying a source type of OPENPIT on the source location (SO LOCATION) card. The OPENPIT source algorithm can be used to model particulate emissions from open pits, such as surface coal mines and rock quarries. A technical description of the OPENPIT source algorithm is provided in the ISC3 Model User’s Guide - Volume II (EPA, 1995b). The OPENPIT algorithm uses an effective area for modeling pit emissions, based on meteorological conditions, and then utilizes the numerical integration area source algorithm to model the impact of emissions from the effective area sources. A complete technical description of the OPENPIT source algorithm is provided in the ISC3 Model User’s Guide - Volume II (EPA, 1995b).

The AERMOD model accept rectangular pits with an optional rotation angle specified relative to a north-south orientation. The rotation angle is specified relative to the vertex used to define the source location on the SO LOCATION card (e.g., the southwest corner). The syntax, type and order for the SRCPARAM card for OPENPIT sources are summarized below:

Syntax:	`SO SRCPARAM  Srcid Opemis Relhgt Xinit Yinit Pitvol (Angle)`
Type:	`Optional, Repeatable`
Order:	`Must follow the LOCATION card for each source input`

where the Srcid parameter is the same source ID that was entered on the LOCATION card for a particular source, and the other parameters are as follows:

Opemis - open pit emission rate in g/(s-m2),

Relhgt - average release height above the base of the pit in meters,

Xinit - length of X side of the open pit (in the east-west direction if Angle is 0 degrees) in meters,

Yinit - length of Y side of the open pit (in the north-south direction if Angle is 0 degrees) in meters,

Pitvol - volume of open pit in cubic meters, and

Angle - orientation angle for the rectangular open pit in degrees from North, measured positive in the clockwise direction (optional).

The same emission rate is used for both concentration and deposition calculations in the AERMOD model. It should also be noted that the emission rate for the open pit source is an emission rate per unit area, which is different from the point and volume source emission rates, which are total emissions for the source. The Relhgt parameter cannot exceed the effective depth of the pit, which is calculated by the model based on the length, width and volume of the pit. A Relhgt of 0.0 indicates emissions that are released from the base of the pit.

If the optional Angle parameter is input, and the value does not equal 0.0, then the model will rotate the open pit clockwise around the vertex defined on the SO LOCATION card for this source. The relationship between the Xinit, Yinit, and Angle parameters and the source location, (Xs,Ys), for a rotated pit is the same as for rectangular area sources. The Xinit dimension is measured from the side of the area that is counterclockwise along the perimeter from the vertex defined by (Xs,Ys), while the Yinit dimension is measured from the side of the open pit that is clockwise along the perimeter from (Xs,Ys). Unlike the area source inputs, the Yinit parameter is not optional for open pit sources. The Angle parameter is measured as the orientation relative to North of the side that is clockwise from (Xs,Ys), i.e. the side with length Yinit. The Angle parameter may be positive (for clockwise rotation) or negative (for counterclockwise rotation), and a warning message is generated if the absolute value of Angle is greater than 180 degrees. The selection of the vertex to use for the source location is not critical, as long as the relationship described above for the Xinit, Yinit, and Angle parameters is maintained.

The aspect ratio (i.e., length/width) of open pit sources should be less than 10 to 1. However, since the pit algorithm generates an effective area for modeling emissions from the pit, and the size, shape and location of the effective area is a function of wind direction, an open pit cannot be subdivided into a series of smaller sources. Aspect ratios of greater than 10 to 1 will be flagged by a warning message in the output file, and processing will continue. Since open pit sources cannot be subdivided, the user should characterize irregularly-shaped pit areas by a rectangular shape of equal area. Receptors should not be located within the boundaries of the pit; concentration and/or deposition at such receptors will be set to zero. Such receptors will be identified during model setup and will be flagged in the summary of inputs.

An example of a valid SRCPARAM input card for an open pit source is given below:

```
SO SRCPARAM  NORTHPIT  1.15E-4  0.0  150.0  500.0  3.75E+6  30.0
```

where the source ID is NORTHPIT, the emission rate is 1.15E-4 g/(s-m2), the release height is 0.0 m, the X-dimension is 150.0 m, the Y-dimension is 500.0 m, the pit volume is 3.75E+6 cubic meters (corresponding to an effective pit depth of about 50 meters) and the orientation angle is 30.0 degrees clockwise from North.

Since the OPENPIT algorithm is applicable for particulate emissions, the particle categories for an open pit source must be defined using the PARTDIAM, MASSFRAX, and PARTDENS keywords on the SO pathway.

Specifying Source Parameters for Gas Deposition

The input of source parameters for dry and wet deposition of gaseous pollutants is controlled by the GASDEPOS keyword on the SO pathway. The gas dry deposition variables may be input for a single source, or may be applied to a range of sources.

The syntax, type, and order for the GASDEPOS keyword are summarized below:

Syntax:	SO GASDEPOS Srcid (or Srcrng) Da Dw rcl Henry
Type:	Optional, Repeatable
Order:	Must follow the LOCATION card for each source input

where the Srcid or Srcrng identify the source or sources for which the inputs apply, the parameter Da is the diffusivity in air for the pollutant being modeled (cm^2/s), Dw is the diffusivity in water for the pollutant being modeled (cm^2/s), rcl is the cuticular resistance to uptake by lipids for individual leaves, and Henry is the Henry's Law constant (Pa m^3/mol). Values of the physical parameters for several common pollutants may be found in the appendices to the ANL report (Wesely, et. al, 2002).

Specifying Source Parameters for Particle Deposition

The AERMOD model includes two methods for handling dry deposition of particulate emissions. Method 1 is used when a significant fraction (greater than about 10 percent) of the total particulate mass has a diameter of 10 μm or larger. The particle size distribution must be known reasonably well in order to use Method 1. Method 2 is used when the particle size distribution is not well known and when a small fraction (less than 10 percent of the mass) is in particles with a diameter of 10 μm or larger. The deposition velocity for Method 2 is given as the weighted average of the deposition velocity for particles in the fine mode (i.e., less than 2.5 μm in diameter) and the deposition velocity for the coarse mode (i.e., greater than 2.5 μm but less than 10 μm in diameter).

Specifying Particle Inputs for Method 1:

The input of source variables for particle deposition using Method 1 are controlled by three keywords on the SO pathway, PARTDIAM, MASSFRAX, and PARTDENS. The particle variables may be input for a single source, or may be applied to a range of sources.

The syntax, type and order for these three keywords are summarized below:

Syntax:	`SO PARTDIAM  Srcid (or Srcrng) Pdiam(i),i=1,Npd`
	`SO MASSFRAX  Srcid (or Srcrng) Phi(i),i=1,Npd`
	`SO PARTDENS  Srcid (or Srcrng) Pdens(i),i=1,Npd`

Type:	`Optional, Repeatable`
Order:	`Must follow the LOCATION card for each source input`

where the Srcid or Srcrng identify the source or sources for which the inputs apply, and where the Pdiam array consists of the particle diameter (microns) for each of the particle size categories (up to a maximum of 20 set by the NPDMAX PARAMETER in the computer code), the Phi array is the corresponding mass fractions (between 0 and 1) for each of the categories, and the Pdens array is the corresponding particle density (g/cm^3) for each of the categories.

The number of categories for a particular source is Npd. The user does not explicitly tell the model the number of categories being input, but if continuation cards are used all inputs of a keyword for a particular source or source range must be contiguous, and the number of categories must agree for each of the three keywords input for a particular source. As many continuation cards as needed may be used to define the inputs for a particular keyword. The model checks the inputs to ensure that the mass fractions sum to 1.0 (within 2 percent) for each source input, and that the mass fractions are within the proper range (between 0 and 1).

Specifying Particle Inputs for Method 2:

The Method 2 particle information is input through the METHOD_2 keyword on the SO pathway. The syntax, type, and order for the METHOD_2 keyword are summarized below:

Syntax:	`SO METHOD_2  Srcid (or Srcrng)  FineMassFraction   Dmm`
Type:	`Optional, Repeatable`
Order:	`Must follow the LOCATION card for each source input`

where the Srcid or Srcrng identify the source or sources for which the inputs apply, the parameter FineMassFraction is the fraction of particle mass emitted in the fine mode, less than 2.5 microns, and Dmm is the representative mass mean particle diameter in microns. Estimated values of fine particle fractions and mass mean diameters for various pollutants are provided in Appendix B of the ANL report (Wesely, et al, 2002).

<u>Specifying Emission and Output Units</u>

Since the AERMOD model allows for both concentration and deposition to be output in the same model run, the EMISUNIT keyword cannot be used to specify emission unit factors if more than one output type is being generated. The AERMOD model therefore allows for concentration and deposition units to be specified separately through the CONCUNIT and DEPOUNIT keywords, respectively. The syntax and type of the CONCUNIT keyword are summarized below:

Syntax:	`SO CONCUNIT  Emifac  Emilbl  Conlbl`
Type:	`Optional, Non-repeatable`

where the parameter Emifac is the emission rate unit factor, Emilbl is the label for the emission units (up to 40 characters), and Conlbl is the output unit label (up to 40 characters) for concentration calculations. The syntax and type of the DEPOUNIT keyword are summarized below:

Syntax:	`SO DEPOUNIT  Emifac  Emilbl  Deplbl`
Type:	`Optional, Non-repeatable`

where the parameter Emifac is the emission rate unit factor, Emilbl is the label for the emission units (up to 40 characters), and Deplbl is the output unit label (up to 40 characters) for deposition calculations.

Specifying In-stack NO_2 Ratios

The PVMRM and OLM options for modeling NO_2 conversion assume a default in-stack NO_2/NO_x ratio of 0.10 (or 10 percent). The user can specify in-stack NO_2/NO_x ratios through the optional NO2RATIO keyword on the SO pathway. The syntax of the NO2RATIO keyword is as follows:

```
SO NO2RATIO  SrcID or SrcRange   NO2Ratio
```

where the Srcid or Srcrng identify the source or processed within the model for the OLM model, and the SRCGROUP card simply controls how source impacts are grouped in the model outputs.

If the user identifies one or more groups of sources to apply OLM on a combined plume basis using the OLMGROUP card, the model will still need to calculate the concentration for individual plumes within the OLM group in order to sum the results for the sources listed on the SRCGROUP card(s). The individual source concentrations are calculated by applying the ratio of the combined concentration for the OLM group with and without OLM to each source within the OLM group.

Deposition Velocity and Resistance Outputs

In order to facilitate review and testing of the deposition algorithms in the AERMOD model, the model outputs the main resistance terms and deposition velocities for gaseous and particle sources. The gas deposition data are written to a file called GDEP.DAT, which includes the values of R_a, R_b, R_c, and V_{dg} for each source and for each hour modeled. A header record is included to identify the columns. The particle deposition data are written to a file called PDEP.DAT, which includes the values of R_a, R_p, V_g, and V_d for each source and for each hour modeled. The particle outputs are labeled as being based on either Method 1 or Method 2. For Method 1, results are output for each particle size category. The filename and file units for these data files are hardcoded in the model, and the files are overwritten each time the model is executed.

Meteorological Data for New Deposition Algorithms

The AERMET meteorological processor (dated 04300) has been modified to output additional meteorological parameters needed for the deposition algorithms in AERMOD. The additional variables include the precipitation code, precipitation rate, relative humidity, surface pressure, and cloud cover. These additional variables are automatically included after the standard variables for each hour, and do not require any additional user input. The precipitation data needed for wet deposition calculations in AERMOD can be obtained from the SAMSON, HUSWO or ISHD (TD-3505) formats currently supported by AERMET (EPA, 2002b). The meteorological data file for the new deposition algorithms is read as a free format file, i.e., each field on a record is separated from adjacent fields by a comma or by one or more spaces. The input meteorological data file consists of a header record that includes the surface station ID (e.g., WBAN number), surface station year, upper air (mixing height) station ID, upper air station year, and AERMET version date (see Section D.1 of the AERMOD model user's guide (EPA, 2002a)). Each subsequent record contains the following variables in the order listed:

Variable Description	Format
Year	Integer
Month	Integer
Day of Month	Integer
Julian Day (Day of Year)	Integer
Hour of Day	Integer
Heat Flux (W/m^2)	Real
Surface Friction Velocity, u* (m/s)	Real
Convective Velocity Scale, w* (m/s)	Real
Lapse Rate Above Mixing Height (m)	Real
Convective Mixing Height (m)	Real
Mechanical Mixing Height (m)	Real
Monin-Obukhov Length, L (m)	Real
Surface Roughness Length, z_o (m)	Real
Bowen Ratio	Real
Albedo	Real
Reference Wind Speed (m/s)	Real
Reference Wind Direction (degrees)	Real
Reference Height for Wind (m)	Real
Ambient Temperature (K)	Real
Reference Height for Temperature (m)	Real
Precipitation Code (0-45)	Integer
Precipitation Rate (mm/hr)	Real
Relative Humidity (%)	Real
Surface Pressure (mb)	Real
Cloud Cover (tenths)	Integer

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