ADDENDUM

AERMOD: Model Formulation Document

Introduction

This Addendum to the AERMOD Model Formulation Document (MFD) (Cimorelli, *et al.*, 2002) provides a technical description of the implementation of the Plume Volume Molar Ratio Method (PVMRM) for modeling the conversion of NO_x to NO_2 in AERMOD. Hanrahan (1999a) provides a technical description of the PVMRM algorithm. Hanrahan also implemented and evaluated the PVMRM algorithm as a post-processor for the ISCST3 model (Hanrahan, 1999b). The design and implementation of PVMRM in AERMOD is based on the description in Hanrahan (1999a) and the ISCST3 post-processor code. However, the implementation was adapted for the AERMOD dispersion algorithms, as described below.

Definition of Plume Volume for PVMRM

Total vs. Relative Dispersion

The PVMRM determines the conversion rate for NO_x to NO_2 based on a calculation of the NO_x moles emitted into the plume, and the amount of O_3 moles contained within the volume of the plume between the source and receptor. The dispersion algorithms in AERMOD and other steady-state plume models are based on the use of total dispersion coefficients, which are formulated to represent the time-averaged spread of the plume. A more appropriate definition of the volume of the plume for purposes of determining the ozone moles available for conversion of NOx is based on the instantaneous volume of the plume, which is represented by the use of relative dispersion coefficients, (Cole and Summerhays, 1979; Bange, 1991). The implementation of PVMRM in AERMOD is based on the use of relative dispersion coefficients to calculate the plume volume. Weil (1996 and 1998) has defined formulas for relative dispersion that are consistent with the AERMOD treatment of dispersion, and which can be calculated using meteorological parameters available within AERMOD.

Calculation of Relative Dispersion Coefficients

The formula for relative dispersion combines the effects of buoyancy-induced turbulence, which should dominate close to the source, and ambient turbulence, which begins to dominate further downwind. Since the travel time from the source to the receptor is important for defining relative dispersion, the relative dispersion coefficients are calculated based on the radial distance from source to receptor. Weil (1996 and 1998) assumes relative dispersion (σ_r) to be isotropic, so that $\sigma_{rx} = \sigma_{ry} = \sigma_{rz} = \sigma_r$. The relative dispersion (σ_r) due to the combined effects of buoyancy-induced turbulence (σ_{rb}) and ambient turbulence (σ_{ra}) is parameterized as follows:

$$\sigma_r = (\sigma_{rb}^3 + \sigma_{ra}^3)^{1/3} \tag{1}$$

The buoyancy-induced dispersion term, σ_{rb}, is calculated in AERMOD as

$$\sigma_{rb} = \frac{0.4\Delta h}{\sqrt{2}} \tag{2}$$

where Δh is the plume rise. Relative dispersion due to ambient turbulence, σ_{ra}, is parameterized by

$$\sigma_{ra} = \frac{a_1 \varepsilon^{1/2} t^{3/2}}{1 + a_2 t / T_{Lr}} \tag{3}$$

where a_1 is a constant (= 0.57), $a_2 = 0.62\ a_1$, t is the plume travel time (= x/U), and T_{Lr} is a Lagrangian time scale for relative dispersion defined as

$$T_{Lr} = a_{r1} \frac{z_i}{\sigma_w} \tag{4}$$

where $a_{r1} = 0.46$, z_i is the mixing height, and σ_w is the vertical turbulence parameter. The turbulence dissipation rate, ε, is calculated as follows, based on Weil (1996):

$$\varepsilon = \frac{b\sigma_w^2}{T_{Lr}} \tag{5}$$

where b is a constant (= 0.78).

The values of wind speed (U) and σ_w used in Equations 3 through 5 are the effective values, calculated as averages across the layer from the plume centroid height to the receptor height (up to $2.15\sigma_z$), following the procedure used in AERMOD to calculate effective values. Using the effective values of σ_w, AERMOD calculates effective values of the turbulence dissipation rate, ε.

Since the relative dispersion coefficients are source- and meteorology-dependent in AERMOD, the model generates a table of relative dispersion coefficients as a function of distance for the dominant source for each receptor and each hour in order to complete the plume volume calculation.

Treatment of Volume and Area Sources

If the dominant source is a volume source, then the initial lateral and vertical dimensions of the volume source are included in the calculation of the relative dispersion coefficients for purposes of calculating the plume volume, as follows:

$$\sigma_r = \left(\sigma_{rb}^3 + \sigma_{ra}^3 + \sigma_0^3\right)^{1/3} \tag{6}$$

where σ_0 is the initial dispersion coefficient of the volume source calculated as $\sqrt{\sigma_{y0}\ \sigma_{z0}}$ based on the initial lateral (σ_{y0}) and vertical (σ_{z0}) dimensions input by the user. If a volume source is included among the major contributing sources it is treated the same as a point source in defining the combined plume volume.

For application of PVMRM to area sources, the plume volume is extended laterally if necessary to include the projected width of the area source or sources that are included among the major contributing sources. The emissions from an area source are included in the calculation of the NO_x moles emitted into the plume if the centroid of the area source is within the box defined by the alongwind and crosswind extent of major contributing sources. In addition, if an area source is the dominant source, then the relative dispersion coefficients are calculated based on the radial distance from the centroid of the area source to the receptor.

Defining Extent of Plume

Since relative dispersion coefficients are used to define the plume volume, the number of standard deviations from the plume centerline, n_z, used in the calculation of plume volume was increased from the value used by Hanrahan (1999) for ISCST3. The ISCST3 postprocessor version used a value of 1.282 for n_z, corresponding to 80 percent of the area under the normal curve. The plume volume calculations for AERMOD are based on a value of $n_z = 4.0$, which corresponds to about 99.99 percent of the area under the normal curve. The minimum value of the dispersion coefficient was also reduced from the 15m minimum used with ISCST3 to a minimum of 5m for AERMOD in order to maintain approximately the same minimum plume volume in AERMOD as used for ISCST3. A minimum value of 4.8m in AERMOD would provide the same minimum plume volume as used by ISCST3 with $n_z = 1.282$ and a minimum dispersion coefficient of 15m.

Adaptation for AERMOD Terrain Algorithm

The vertical dimension of the plume volume is based on the relative dispersion coefficient for the dominant source and the range in plume heights for the major contributing sources. Since the effective plume heights differ for the terrain following and terrain responding components, the vertical dimension was modified to calculate the range of plume heights separately for both the terrain following and terrain responding components, and then use a weighted value for the vertical dimension based on the terrain (plume state) weighting factor, f, defined in Section 5.1 of the MFD.

Treatment of Penetrated Plumes

For unstable conditions with partial or full plume penetration above the mixing height, z_i, separate relative dispersion coefficients are calculated for the penetrated portion of the dominant plume. For cases with partial penetration for the dominant plume, AERMOD calculates two plume volumes, one based on relative dispersion coefficients for the direct source and another based on the relative dispersion coefficients for the penetrated source. Since AERMOD uses the same dispersion coefficients for the direct and indirect sources, separate values of relative dispersion coefficients for the indirect source are not needed. The effective plume volume used in the application of PVMRM is based on a weighted average of the direct and penetrated plume volumes using the plume penetration factor (PPF) for the dominant source. The model stores the plume centroid heights for both the direct and penetrated plumes for all sources at each receptor, and these are used to incorporate the effect of the major contributing sources on the volumes for the direct and penetrated plumes.

Minimum Ozone Concentration for Stable Conditions

Hanrahan (1999a) applied a minimum ozone concentration of 40 ppb for stable conditions for implementation with ISCST3, due to the fact that surface measurements may be artificially low during nighttime stable conditions due to the formation of a stable vertical temperature gradient. Since the AERMOD model does not use Pasquill-Gifford (P-G) stability categories, this minimum ozone concentration was modified to use Monin-Obukhov length as the stability parameter. The AERMOD model first keeps track of the maximum ozone concentration over the previous 24 hours. If the Monin-Obukhov length is positive (i.e. stable), with a value of less than 50 meters (very stable), then the maximum ozone concentration over the previous 24 hours is used as the minimum value, with an upper limit of 40 ppb. If the Monin-Obukhov length is positive and the value is over 500 meters (nearly neutral), then no minimum ozone concentration is applied for that hour. If the Monin-Obukhov length is between 50 meter and 500 meters, then the minimum ozone concentration is determined by linear interpolation, i.e., the minimum value is calculated as MIN(40ppb, O3MAX) * (500 – L)/450, where O3MAX is the maximum ozone concentration over the previous 24 hours, and L is the Monin-Obukhov length in meters.

References

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