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Current Progress In the AERMIC Model Development Program

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INTRODUCTION

Background

In 1991, the American Meteorological Society (AMS) and the Environmental Protection Agency (EPA) initiated a formal collaboration with the designated goal of introducing recent advances in boundary layer meteorology into regulatory dispersion models. A working group (AMS/EPA Regulatory Model Improvement Committee, AERMIC) of three AMS and four EPA scientists was formed for this collaborative effort. AERMIC members are listed as the authors of this paper.

For many years now, we have known that a comprehensive overhaul of EPA's basic regulatory models is needed (e.g., see Weil[1]). Responding to this need, AERMIC was formed to update EPA models with current state-of-the-art Planetary Boundary Layer (PBL) parameterizations. The early efforts of AERMIC are described by Weil[2]. As we went through the design process and considered the nature of present regulatory models, AERMIC's goal became more comprehensive. In addition to improving how regulatory models characterize the PBL, we decided that other areas such as terrain interactions and surface releases needed immediate attention. This broadened scope is best expressed in AERMIC's present objective which is to develop a complete replacement for EPA's Industrial Source Complex model version 3 (ISC3)[3] by: 1) adopting ISC3's input/output computer architecture; 2) updating, where practical, antiquated ISC3 model algorithms with newly developed or current state-of-the-art modeling techniques; and 3) insuring that all processes presently modeled by ISC3 will continue to be handled by the AERMIC Model (AERMOD). A detailed description of the areas, within the ISC3 model, that are being improved by AERMOD can be found in Perry, et al.[4]

In developing AERMOD, we have strived to follow certain design criteria to yield a model with desirable regulatory attributes. We felt that the model should: 1) be robust in estimating regulatory design concentrations (i.e., provide reasonable estimates under a wide variety of conditions with minimal discontinuities); 2) be easily implemented (user friendly, reasonable input requirements and computer resources), as is the current ISC3 model; 3) be based on state-of-the-art science that captures the essential physical processes while remaining fundamentally simple; and, 4) accommodate modifications with ease as the science evolves.

We chose a phased approach in developing AERMOD. Relative to ISC3, AERMOD currently contains new or improved algorithms for: 1) dispersion in both the convective and stable boundary layers; 2) plume rise and buoyancy; 3) plume penetration into elevated inversions; 4) treatment of elevated, near-surface, and surface level sources; 5) computation of vertical profiles of wind, turbulence, and temperature; and 6) the treatment of receptors on all types of terrain (from the surface up to and above the plume height). Terrain handling is done with a simple approach while still considering the dividing streamline concept in stably-stratified conditions. Where appropriate the plume is modeled as either impacting and or following the terrain. High priority for future efforts include new or improved algorithms dealing with building downwash and both wet and dry deposition.

The complete AERMOD modeling system consists of two pre-processors and the model itself. The AERMIC METeorological preprocessor (AERMET) is a stand-alone program which provides AERMOD with the information it needs to characterize the state of the surface and mixed layer, and the vertical structure of the PBL. The AERMIC MAPping program (AERMAP) is a stand-alone terrain preprocessor which is used to both characterize terrain and generate receptor grids for AERMOD. In addition to the full scale version of AERMOD, we are developing a screening version. When completed, the screening version will operate as an option within the AERMOD code.

Model Development Process

The process we are following in the development of AERMOD includes, in the following sequence: 1) initial model formulation; 2) developmental evaluation; 3) peer review and beta testing; 4) revised model formulation; 5) performance evaluation and sensitivity testing; and 6) submission to EPA's Office of Air Quality Planning and Standards (OAQPS) for consideration as a regulatory model.

Starting with the ISC2[5] code, we built the initial formulation of AERMOD by replacing many of ISC's modules with new or more current formulations. For certain processes (e.g., terrain treatment) AERMOD was coded with more than one formulation to facilitate testing of various ideas during development. The initial formulation of AERMOD is summarized in Perry, et al.[4] Once formulated, we then test the model (i.e. the developmental evaluation) against a variety of field measurements in order to improve and/or replace its algorithms, and provide a basis for selecting formulation options.

We are using five data bases in the developmental evaluation (also referred to as the Phase I Evaluation). Three of the data bases are event-based tracer releases, while the other two each contain up to a full year of continuous SO_2 measurements. The data bases cover both elevated and surface releases, complex and simple terrain, and both rural and urban boundary layers. We present below a summary of the data bases and some results from the developmental evaluation. For a detailed description of the developmental evaluation see Lee, et al.[6] To date, this evaluation has resulted in many revisions to AERMOD, which we discuss below. At the present time, we are nearing completion of the developmental evaluation.

Both peer review and beta testing are included in the model development plan. An internal EPA peer review of the AERMOD model formulation (AERMIC[7]) and evaluation is in progress. This will be followed by an external peer review which will be conducted prior to the performance evaluation. Beta testers have been selected from among federal, state, and private sector users. In addition, a preliminary version of the model and its documentation are available to the public in the Sixth Modeling Conference docket, and through the OAQPS TTN (Office of Air Quality Planning and Standards Technology Transfer Network) electronic bulletin board system.

Based on the results of the developmental evaluation and comments from peer reviewers, beta testers, and the Sixth Modeling Conference, we are constructing a final version of AERMOD. This final version will then be subjected to a comprehensive performance evaluation (also referred to as the Phase II Evaluation), which is designed to assess how well AERMOD's concentration estimates compare against a variety of independent data bases.

The major purpose of the performance evaluation is to assess the adequacy of AERMOD for use in regulatory decision making. As a regulatory model, the operational performance evaluation must be designed to focus on how well the model predicts concentrations at the high end of the concentration distribution. The design details of the performance evaluation appear in AERMIC.[8] At this time, we intend to evaluate AERMOD against at least five independent data bases (three in flat terrain and two in complex terrain), each containing at least one full year of continuous SO_2 measurements. AERMOD's performance will be compared against appropriate EPA Guideline models following the procedures in EPA's "Protocol for Determining the Best Performing Model[9]." Once the performance evaluation is completed, we intend to submit AERMOD to OAQPS for possible inclusion in the Guideline on Air Quality Models[10]. The results of the performance evaluation will be used by OAQPS to decide what proposal should be made regarding the regulatory status of AERMOD. Should AERMOD replace ISC3? If not, what role, if any, should AERMOD play?

In addition, a sensitivity analysis is being designed which will help us determine the degree of precision and accuracy needed for input data; thereby providing a basis for developing guidance for regulatory implementation. In addition, we will use the results from this analysis to examine the stability of AERMOD's estimates to small changes in the input data. As stated in the design criteria above, we are committed to developing a model that produces robust results and minimizes discontinuities.

Basic Model Structure

Design Overview. In this section, we give a very general overview of the most important features of AERMOD. As a replacement for ISC3, AERMOD will be applicable to rural and urban areas, flat and complex terrain, surface and elevated releases, and multiple sources (including, point, area and volume sources). Every effort is being made to avoid model formulation discontinuities wherein large changes in calculated concentrations can result from insignificant changes in input parameters.

AERMOD is a steady-state plume model. In the Stable Boundary Layer (SBL), the concentration distribution is assumed to be Gaussian in both the vertical and horizontal. In the Convective Boundary Layer (CBL), the horizontal distribution is assumed to be Gaussian, but the vertical distribution is described with a bi-Gaussian probability density function (p.d.f.) to accommodate observed[11,12] vertical concentration distributions that are skewed.

Also, in the CBL, AERMOD is designed to treat the phenomenon of "plume bumping," whereby a portion of plume mass, released from a buoyant source, hugs the top of the boundary layer before becoming mixed into the CBL. In addition, AERMOD also tracks any plume mass which penetrates an elevated stable layer allowing it to re-enter the boundary layer when appropriate.

AERMOD incorporates, with a new simple approach, current concepts about flow and dispersion in complex terrain. We have designed this approach to be physically realistic and simple to implement while avoiding the distinction, made by all other regulatory models, among simple, intermediate and complex terrain. As a result, AERMOD removes the regulatory need for defining complex terrain regimes; all terrain is handled in a consistent manner.

One of the major improvements which AERMOD brings is its ability to characterize the PBL through both surface and mixed layer scaling. AERMOD constructs vertical profiles of required meteorological variables based on measurements and extrapolations of those measurements using similarity (scaling) relationships. Vertical profiles of wind speed, wind direction, turbulence temperature, and temperature gradient are estimated using all available meteorological observations. Although we designed AERMOD to operate without the need to collect extensive on-site data, all evaluations to date have included a complete complement of on-site meteorological measurements. Since it has been AERMIC's goal to develop a model which works well using readily available meteorological data (such as National Weather Service data), we will be testing the model's veracity with degraded (reduced from complete on-site) meteorological data sets during the performance evaluation.

Unlike existing regulatory models, AERMOD accounts for the vertical inhomogeneity of the PBL. We accomplish this by "averaging" the parameters of the actual PBL into "effective" parameters of an equivalent homogeneous PBL. With these effective parameters, AERMOD accounts for the inhomogeneity of the PBL, in an averaged sense.

Structure of the Modeling System. As explained above, AERMOD is constructed with one main program (AERMOD) and two pre-processors (AERMET and AERMAP). The major purpose of AERMET is to calculate boundary layer parameters for use by AERMOD. The meteorological INTERFACE, internal to AERMOD, uses these parameters to generate profiles of the needed meteorological variables. In addition, AERMET passes all meteorological observations to AERMOD.

Surface characteristics in the form of albedo, surface roughness and Bowen ratio, plus standard meteorological observations, are input to AERMET. AERMET then calculates the PBL parameters: friction velocity (u_*), Monin-Obukhov length (L), convective velocity scale (w_*), temperature scale (θ_*), CBL height (z_i), SBL height (h), and surface heat flux (H). These parameters are then passed to the INTERFACE where vertical profiles are calculated, from similarity expressions, for wind speed (u), wind direction, lateral and vertical turbulent fluctuations (σ_v, σ_z), potential temperature gradient ($d\theta/dz$), and potential temperature (θ).

The AERMIC terrain pre-processor AERMAP uses gridded terrain data to calculate a representative terrain-influence height (h_c). This height scale h_c is used to calculate the dividing streamline height[13], and is uniquely defined for each receptor location. The gridded data needed by AERMAP is either user supplied or preferably selected by AERMAP from Digital Elevation Mapping (DEM) data. AERMAP is also used to create receptor grids. If DEM data are used, the elevation for each specified receptor can be automatically assigned through AERMAP. AERMAP passes to AERMOD, for each receptor, a location (x,y), a terrain height (z), and a terrain height scale (h_c).

Purpose of Paper

This paper describes the changes that have been made in the formulation of AERMOD since our original formulation (as described in Perry, et al.[4]). When read with Perry, et al.[4], the reader should gain a complete understanding of the current state of development of the AERMIC modeling system: AERMOD (dispersion model), AERMET (meteorological preprocessor), and AERMAP (terrain preprocessor). Since the model's original formulation, AERMIC has been engaged in a developmental evaluation of AERMOD (Lee, et al.[6]). Results from this evaluation have been used to examine the adequacy of the model formulation. In addition, the model has been submitted for public comment, beta testing, and peer review. The major focus of this paper is to describe those changes in formulation that have resulted, to date, from the developmental evaluation and peer review. In addition, we summarize the performance of the current model using the developmental data bases.

MODEL FORMULATION - TECHNICAL DESCRIPTION

In this section, we describe those changes that have occurred since our original discussion of AERMOD in Perry, et al.[4] Except where necessary for clarity, we have not included those portions of the model that have remained unchanged since the initial formulation. Therefore, in order to obtain a complete description of the present model this paper should be read in conjunction with Perry, et al.[4]. It is important to note that at the time of this writing the technical formulation of AERMOD is still subject to revision.

General Structure of AERMOD Including Terrain Handling

The general form of AERMOD's concentration equation has not changed since its inception. AERMOD assumes that the plume dispersion near terrain is characterized by two states. The concentration at a receptor, located at a position (x,y,z), is the weighted sum of two concentration estimates: one for which the plume trajectory is horizontal (i.e., the "horizontal plume state" - representing plume material below the dividing streamline) and the other for which the plume travels over the terrain (i.e., the "terrain responding state" - representing plume material above the dividing streamline). The relative weighting of the two terms depends on: 1) the degree of atmospheric stability; 2) the wind speed; and 3)the plume height relative to terrain. In flat terrain, the concentration equation reduces to the form for a single plume. The general form for the total concentration at any receptor is:

$$C_T(x,y,z) = f \cdot C(x,y,z) + (1-f) \cdot C(x,y,z_{eff}) \tag{1}$$

The two terms in eq. (1) correspond to the contributions from the "horizontal" and "terrain-responding" plume states. The coefficient f is a weighting factor which relates to the fraction of plume material and z_{eff} is an "effective" receptor height which is defined below.

In AERMOD, H_c does not relate to the geometry of a specific hill. As such, it is conceptually different from the traditional context in which it is used. AERMOD uniquely defines H_c for each receptor. The height scale (traditionally the height of the hill being modeled), used for calculating H_c in AERMOD, is based on the general nature of the terrain within the modeling domain and the location of the specific receptor for which it is defined. The terrain height scale (h_c) is described in detail in Perry, et al.[4].

In the initial formulation of AERMOD, we developed two options for defining f and z_{eff} in eq. (1). The two possible formulations for terrain are:

Option 1:

$$f = \Phi$$
$$\text{and} \qquad z_{eff} = 0.5 \cdot Min(h_c, z_t) + (z - z_t) \tag{2}$$

Option 2:

$$f = 0.5\cdot(1 + \phi)$$
$$\text{and} \qquad z_{eff} = (z - z_t) \tag{3}$$

where: h_p is the plume height; z_t is the height of the terrain; and, z is the receptor height.

The CBL's Three Plume Model

To treat the interactions of plume material with the height of the CBL, AERMOD uses a three plume approach: direct, indirect, and penetrated plumes. The "direct source (at the stack) describes the dispersion of plume material that reaches the ground directly via downdrafts. The "indirect" source, located above the CBL, is included to treat the zero-flux condition at $z=z_i$ for material that initially rises to the CBL top in updrafts and is returned to the ground by downdrafts; this material does not have sufficient buoyancy to penetrate the stable air aloft. That is, mass which reaches the height of the CBL, but does not penetrate the stable layer aloft, is permitted to hug the top of the CBL until the amount of entrained air is sufficient to allow the plume to mix downward. The "penetrated" source describes the dispersion of plume material that initially penetrates the elevated stable layer but can re-enter the CBL. We have made slight changes in the mathematical formulation of the three plume mode since Perry, et al.[4] (see AERMIC[7] for a complete description).

Dispersion

The standard deviations for both the lateral and vertical concentration distributions (σ_y and σ_z respectively) result from the combined effects of: ambient dispersion (σ_a); dispersion induced by plume buoyancy (σ_b); and, enhancements from building effects (σ_d). Combining these effects, we produce the following general expression for σ_y or σ_z

$$\sigma_{y,z} = \sqrt{\sigma^2_{ya,za} + \sigma^2_{yb,zb} + \sigma^2_{yd,zd}} \tag{4}$$

Ambient dispersion ($\sigma_{ya,za}$) is known to vary significantly with height; having its strongest variation near the earth's surface. Unlike present regulatory models, we designed AERMOD to account for this height variation. In our original formulation, both σ_{ya} and σ_{za} were taken directly from Taylor's statistical theory of dispersion[14]. In the following sections eqs. (5), (8), (11), and (12) each represent the complete expression, used in our original formulation, to calculate σ_{ya} and σ_{za} for the CBL and SBL respectively.

Changes to these expressions have been made based on our analysis of the Prairie Grass data. We now have separate expressions for dispersion from surface and elevated sources. In the following sections we will describe our present formulation for σ_{ya} and σ_{za}, first for the CBL and then for the SBL.

Ambient Lateral Dispersion (σ_{ya}) in the CBL. In AERMOD, the ambient portion of the lateral dispersion is composed of an elevated and surface portion. The elevated part (σ_{ye}) follows directly from Taylor[14] as:

$$\sigma_{ye} = \frac{\sigma_v x/U}{\left(1 + \frac{0.5x}{UT_{Ly}}\right)^{1/2}} \tag{5}$$

where σ_v is the lateral turbulent fluctuation; x is the downwind distance; U is the wind speed; and, T_{Ly} is the lateral Lagrangian time scale.

The surface portion, σ_{ys}, which we developed empirically from the Prairie Grass data is written as:

$$\sigma_{ys} = \frac{\sigma_v x/U}{\left(1 + 78\frac{\sigma_v x}{U z_i}\right)^{0.3}} \tag{6}$$

In order to insure a smooth transition between eqs. (5) and (6), we perform an interpolation. At any given height within the PBL, the ambient portion of the lateral dispersion is determined by means of the following formula:

$$\sigma_{ya} = f_\sigma \sigma_{ys} + (1 - f_\sigma)\sigma_{ye} \tag{7}$$

At the present time we are formulating the expression for the interpolation factor, f_σ.

Ambient Vertical Dispersion (σ_{za}) in the CBL. The ambient portion of the vertical dispersion is also composed of an elevated and surface portion. The elevated part (σ_{ze}) is given by the following:

$$\sigma_{ze} = \alpha_b \left(b_j \frac{\sigma_w x}{U} \right) \tag{8}$$

where: σ_w is the vertical turbulent fluctuation; and,

$$\alpha_b = 0.6 + 0.4\left(\frac{H_e}{0.1\, z_i}\right) \qquad for \quad H_e \le 0.1 z_i$$

$$\alpha_b = 1.0 \qquad for \quad H_e > 0.1 z_i$$

The coefficient α_b was developed to insure a smooth transition between the SBL and CBL. That is, we designed α_b such that in the neutral limit ($L \to \infty$), the SBL and CBL expressions for σ_z are equal. The form of σ_{ze} is again from Taylor with the assumption that $T_{Lz} = \infty$ during convective conditions. The b_j in eq. (8) results directly from the assumed bi-Gaussian p.d.f. for the vertical CBL.

The expression used for σ_{zs} (the surface portion) is taken from Venkatram[15].

$$\sigma_{zs} = b_c[1 - 10\cdot(H_e/z_i)]^{\alpha}(u_*/U)^2\cdot\frac{x^2}{|L|} \qquad for \quad \frac{H_e}{z_i} \le 0.1$$
$$and, \qquad \sigma_{zs} = 0.0 \qquad for \quad \frac{H_e}{z_i} > 0.1 \tag{9}$$

We determined the values of the coefficient b_c and the exponent α empirically from the Prairie Grass data. In the present version of the model, they are 0.5, and 1.0, respectively.

The total ambient portion of the vertical dispersion can now be written as:

$$\sigma_{za}^2 = \alpha_b^2\left[b_j\frac{\sigma_{w^*}x}{U}\right]^2 + \sigma_{zs}^2 \tag{10}$$

Ambient Lateral Dispersion (σ_{ya}) in the SBL. As with the CBL, the ambient portion of the lateral dispersion in the SBL is composed of an elevated and surface portion. The elevated part (σ_{ye}) is given by the following[16]:

$$\sigma_{ye} = MAX\left[0.05; \frac{\sigma_v}{U}\right]x \tag{11}$$

The surface portion, σ_{ys}, is given by the same empirical expression presented above for the CBL (i.e., eq. (6)) with z_i (the height of the CBL) replaced by h (the SBL height). As with the CBL, the interpolation formula, eq. (7), is used to insure a smooth transition between the surface and elevated components of σ_{ya}.

Ambient Vertical Dispersion (σ_{za}) in the SBL. The ambient portion of the vertical dispersion is also composed of an elevated and surface portion. The elevated part (σ_{ze}) is given by the following:

$$\sigma_{ze} = \frac{\sigma_w x/U}{\left(1 + \frac{0.5x}{UT_{Lz}}\right)^{1/2}} \qquad (12)$$

where,

$$T_{Lz} = \frac{kz}{1.3\,\phi_h(z/L)\,\sigma_w}; \qquad and \qquad \phi_h(z/L) = 0.74 + 4.7(z/L) \qquad (13)$$

The surface portion of the ambient vertical dispersion σ_{zs} is taken from Venkatram[15].

$$\sigma_{zs} = \sqrt{\frac{2}{\pi}}\,\frac{u_* x}{U}\left(1 + 0.7\,\frac{x}{L}\right)^{-1/3} \qquad (14)$$

As with the CBL, interpolation in the form of eq. (7) is used to weight the surface and elevated portions of the ambient vertical dispersion (i.e., eqs. (12) and (14)).

Reflection From The Top of the SBL.
The original formulation of AERMOD included reflections from the top of the SBL. The reflecting surface was set equal to h or the plume height, whichever was larger. Results from the Lovett evaluation showed that performance improved if these reflections were eliminated. Therefore, we do not include reflection from the top of the SBL in the present version of AERMOD.

Urban Dispersion
In our original formulation of AERMOD we did not explicitly account for the difference between the urban and rural boundary layers. However, in order for us to achieve acceptable comparisons with the Indianapolis data it was necessary to consider these effects. By adding an additional anthropogenic contribution (50 watts/m^2)[17] to the surface energy balance, AERMOD interpreted the PBL as convective, and selected algorithms accordingly.

Inhomogeneity in the Boundary Layer
AERMOD, unlike existing regulatory models, is designed to treat the effects on dispersion from vertical variations in wind and turbulence. This treatment is primarily needed to properly handle surface releases and to provide a mechanism by which the penetrated source can re-enter the CBL. The algorithms in AERMOD function under the assumption that the atmospheric boundary layer is vertically homogeneous (single values of the meteorological parameters represent the layer). Therefore, we designed a method to "convert" the inhomogeneous values (as measured or estimated) into equivalent (representative)

homogeneous values. AERMOD uses equivalent values for wind speed, σ_w, and σ_v as needed throughout the computations. We refer to these equivalent values as effective parameters (α_{eff}).

In our original approach to inhomogeneity (see Perry, et al.[4]), we basically interpolated (with downwind distance) between two observations of plume behavior: 1) near the source, plume dispersion is dominated by meteorological variables near the release point; 2) when the plume later disperses through the depth of the mixed layer, it is reasonable to assume that plume behavior is governed by meteorological variables averaged through the layer. The interpolation had an exponential form which was controlled by travel time and T_{Lz}.

This original approach has subsequently been revised since we were unable to adequately describe what was observed in the Prairie Grass experiment. The revised approach, used in the present version of the model, is described below.

In our current formulation, the effective parameters are determined by averaging their values over that portion of the layer between $h_p(x)$ (plume height) and z_r (the height of the receptor above ground) that contains plume material. The layer through which α_{eff} is calculated is controlled by $\sigma_z(x_r)$ (where x_r is the distance from source to receptor) and is bounded by $h_p(x)$ and z_r.

Since $\sigma_z(x_r)$ depends on the effective values of σ_z, u, and T_{Lz} the plume size is estimated through a series of iterations. We use $\sigma_w(h_p(x))$, $u(h_p(x))$ and $T_{Lz}(h_p(x))$ as initial values in the calculation of $\sigma_z(x_r)$. We then use $\sigma_z(x_r)$ to determine the layer over which $\sigma_w(x_r)_{eff}$, $u(x_r)_{eff}$ and $T_{Lz}(x_r)_{eff}$ are calculated. This process is continued for a number of iterations. The number of iterations depends on convergence and computational considerations. At the end of the iterative process, we calculate $\sigma_w(x_r)_{eff}$, $u(x_r)_{eff}$ and $T_{Lz}(x_r)_{eff}$ over the final layer.

We then calculate α_{eff} from the following expression:

$$\alpha_{eff} = \frac{1}{(h_t - h_b)} \int_{h_b}^{h_t} \alpha(z)\, dz \tag{15}$$

where:

$$h_b = \begin{cases} h_p(x), & \text{if } h_p(x) < z_r \\ MAX\{[h_p(x) - 2.15\,\sigma_z(x_r)], z_r\}, & \text{if } h_p(x) > z_r \end{cases}$$
$$h_t = \begin{cases} h_p(x), & \text{if } h_p(x) > z_r \\ MIN\{[h(x_r) + 2.15\,\sigma_z(x_r)], z_r\}, & \text{if } h_p(x) < z_r \end{cases} \tag{16}$$

PBL Height. Since our original formulation we have made two changes to AERMOD which are designed to prevent temporal discontinuities in the growth of the PBL. First, at the time of transition from a stable to a convective boundary layer (i.e., at sunrise), we prevent the PBL from artificially collapsing by requiring z_i to be greater than or equal to the value of h during the last hour of the previous nocturnal period. Secondly, we avoid sudden (and unrealistic) drops in h for those hours that experience a large decrease in wind speed by controlling its time evolution as follows[7]:

$$\frac{dh}{dt} = \frac{h_d - h}{\tau}, \qquad where \quad \tau = \beta h / u_* \tag{17}$$

This technique performs a temporal smoothing on the original SBL height (h_d) as calculated by Nieuwstadt[18].

Turbulence Parameterizations. Based primarily on peer review comments, we have revised the manner in which turbulence is parameterized. In our original formulation for the SBL, $\sigma_v(h)$ and $\sigma_w(h)$, the turbulence at the top of the SBL, were based on their values at the surface. Since the surface is generally decoupled from higher layers, we have adopted a formulation based on parameterized turbulent intensity. This revised approach is presented below.

Turbulence in the SBL. For L > 0, we develop the vertical profile of σ^2_v by linearly interpolating between the value of σ^2_v at the surface (σ^2_{vo}) and its value at the top of the SBL ($\sigma^2_v(h)$). As in the original formulation the expression for σ^2_{vo} is given as follows[19].

$$\sigma^2_{vo} = 3.6 \cdot u^2_* \tag{18}$$

The expression we use for $\sigma_v(h)$ has changed based on peer review comments[20], which noted that turbulence above the mechanically mixed SBL is decoupled from surface effects. We are now using the following expression for $\sigma_v(h)$:

$$\sigma_v(h) = U(h)\, i_y \tag{19}$$

where i_y is the horizontal component of the turbulent intensity. Based on Briggs[21], i_y is set equal to 0.04 (its parameterized value for Pasquill Gifford Turner (PGT) "F" stability). For σ_v above h, we simply persist its value at h. That is:

$$\sigma_v(h) = 0.04\, U(h), \quad for\ z > h \tag{20}$$

The vertical profile of σ_w in stable conditions takes on the following new form[20]:

$$\sigma_w(z) = MAX\left\{\sigma_{wo} \exp\left[-\frac{0.8z}{h}\right];\ 0.05;\ U(h)\, i_z\right\} \qquad for\ all\ z \tag{21}$$

where the expression we use for σ_{wo} (i.e., $\sigma_{wo}^2=1.7u_*^2$) is unchanged; and, i_z (the vertical component of the turbulent intensity) we set equal to 0.016 after Briggs[21] (its parameterized value for PGT "F" stability).

The exponential from allows some turbulence above h due to occasional nocturnal downbursts, but effectively gives lower vertical turbulence that approaches zero as the height increases above h. The minimum value of 0.05 m/s is based upon a variety of measurement programs. The minimum formulation involving the vertical component of the turbulence intensity is consistent with the decoupling of turbulence in the vertical that is also used in eq. (19).

Turbulence in the CBL. For L<0 and $z<z_i$, our original σ_v formulation has remained unchanged. That is, from the surface to z_i we assume a constant profile for σ_v which, in the absence of measurements we calculate from:

$$\sigma_v^2 = 3.6 \cdot u_*^2 + 0.35 \cdot w_*^2 \tag{22}$$

If observations of σ_v are available, then AERMOD persists the value at the lowest level down to the surface and at the highest level up to z_i. Between z_i and $1.2z_i$, we allow σ_v^2 to decrease linearly. We originally set the value of σ_v equal to $0.5\ \sigma_v(z_i)$ at $z=1.2z_i$; however, based on peer review comments, we now estimate $\sigma_v(1.2z_i)$ from

$$\sigma_v(1.2z_i) = U(z_i)\, i_y \tag{23}$$

Again, based on Briggs[21], i_y is set equal to 0.04. Above $1.2z_i$, we simply persist the value that σ_v attains at $1.2z_i$.

In the absence of measurements, we calculate the profile of σ_w from, Hanna and Paine[19]:

$$\sigma_w^2 = \left(1.7 - \frac{z}{z_i}\right) \cdot u_*^2 + 1.6 \cdot \left(\frac{z}{z_i}\right)^{2/3} \cdot w_*^2\ , \quad for\ \frac{z}{z_i} \le 0.1 \tag{24}$$

and,

$$\sigma_w^2 = \left(1.7 - \frac{z}{z_i}\right) \cdot u_*^2 + 0.35 \cdot w_*^2\ , \quad for\ 0.1 \le \frac{z}{z_i} \le 1.0 \tag{25}$$

Eq. (24), which represents a change from our original formulation, was revised to insure continuity between the surface layer and mixed layer formulations (i.e., eqs. (24) and (25) respectively); whereas, eq. (25) has remained unchanged. As with σ_v, σ_w is linearly interpolated between z_i and $1.2z_i$. In our original formulation $\sigma_v(1.2z_i)=.01\sigma_v(z_i)$, whereas in the present version $\sigma_v(1.2z_i)=U(z_i)i_z$, where i_z is set equal to 0.016, its value for PG class "F" after Briggs[22].

Temperature Gradient. In unstable conditions ($L < 0$), the potential temperature gradient $(d\theta/dz)$ is assumed to be zero for all heights within the convective mixed layer. In our original formulation we set $d\theta/dz$ equal to 0.005°K/m for $z > Z_i$. However, based on typical lapse rates found at the top of the "mixed layer" and above the "interfacial layer," we presently assume that $d\theta/dz=0.01$°K/m for $z_i<z<1.2z_i$ and $d\theta/dz=0.005$°K/m for $z\geq1.2z_i$.

In the SBL, AERMOD estimates vertical profiles of $d\theta/dz$ using an expression developed by Businger[22] for $z\leq10m$ and the profiling equation of Stull[23] for $z>10m$. In addition we assume a minimum value for $d\theta/dz$ of 0.002°K/m for all $z>10m$, Paine[24].

Although unreported in Perry, et al.[4], AERMOD develops the vertical profile of potential temperature from its estimate of the temperature gradient.

Summary. In the past two years, since AERMOD was initially formulated, we have made significant revisions to certain areas of the model based primarily on the developmental evaluation. Although the fundamental structure of the model has not changed, revisions, which were discussed above, have been made in the areas of: 1) dispersion; 2) turbulence and temperature profiling; 3) treatment of the urban boundary layer; 4) SBL reflections; 5) growth of the PBL height and, 6) vertical inhomogeneity. Furthermore, prior to the start of the performance evaluation, we intend to: 1) develop a generalized treatment for the urban boundary layer, and 2) make all final algorithm selections in areas where options now exist.

RESULTS OF THE DEVELOPMENTAL EVALUATION

AERMOD contains many algorithms that are new to routine regulatory modeling and although in most cases these algorithms are based on existing published work, their comparison against field data within the AERMOD framework must be tested. Since AERMOD is intended to handle pollutants from a wide variety of source types in a variety of modeling situations, it is important to challenge the model as much as possible in the development process. Where performance is poor, improved approaches have been included and tested. While some of the improvements to AERMOD noted previously are the result of peer review comments or simply further consideration by the AERMIC committee, most improvements are the result of unacceptable model performance during the developmental evaluation phase of the project. The results shown here are those provided by the most recent version of AERMOD which includes the revisions described in this paper.

The Data Bases

Five data bases were selected for the developmental evaluation.

1.The Prairie Grass data base (Barad[25]) involves a near-surface, non-buoyant SO_2 release, in a rural area, with flat terrain. Surface sampling arrays were positioned in arcs from 50m to 800m downwind of the source. Both convective and stable conditions are included.

2. The Kincaid SF_6 data base (Liu, et al.[26]) involves an elevated, buoyant release in a rural area with flat terrain. Approximately 200 SF_6 monitors were placed in arcs from about 500m to 50km downwind of

the single 187m stack.

3. The Indianapolis SF_6 data base (Murray, et al.[27]) involves an elevated, buoyant release in an urban area with flat terrain. Data were obtained from 177 SF_6 monitors in arcs from 250m to 12km downwind of an 84m stack.

4. The Lovett Power Plant SO_2 data base (Paumier et al.[28]) involves an elevated, buoyant release in a rural area with complex terrain. This one-year data set involves a 145m stack and 12 SO_2 monitoring sites on terrain features rising 250 to 330m above the stack base. The monitors are generally 2 to 3km downwind of the stack.

5. The Kincaid SO_2 data base (Liu, et al.[26]) involves an elevated, buoyant release in a rural area with flat terrain. There were 30 SO_2 monitoring stations from about 2km to 20km downwind of the 187m stack. This data base contains a total of 248 days of valid meteorological observations.

Evaluation Results

As pointed out by Lee et al.[6] the purpose of the developmental evaluation is primarily diagnostic, that is to identify and correct deficiencies of the model during development. Highlights of the evaluation with the above mentioned data bases are presented here using one of the more general tools of our analysis, quantile-quantile (Q-Q) plots of modeled and measured concentrations (all concentrations have been normalized by emission rates). Q-Q plots are simple pairings of predicted concentrations, ranked highest to lowest, with observed concentration, ranked in the same manner. If the ranked distributions are identical, then all points lie on the x = y line. Q-Q plots are an effective method for comparing the distributions of two data sets. They are very useful for assessing the performance of regulatory models since they provide an easy comparison between the high end of the model concentration distribution and the high end of the observations. To assist us in judging AERMOD's relative performance, we have included comparisons with ISC3 in the Q-Q plots. The fractional bias, FB, is also used to evaluate AERMOD. FB provides a quantitative measure with which to compare the models and is defined as:

$$FB_{MEAN} = 2\,(\overline{C_p} - \overline{C_o})\,/\,(\overline{C_p} + \overline{C_o}) \qquad (26)$$

where C_p is the predicted concentration and C_o is the observed concentration with the overbar indicating (for our analysis) the mean of the top 25% of the data values in each set. Note that with this formula, negative FB indicates underprediction and positive FB indicates overprediction. For example, FB = 0.67 is a factor of two overprediction while FB = 1.0 is a factor of three and FB = 1.33 is a factor of five; similarly, -0.67 is an underprediction by a factor of two.

At the time of this writing, we have completed our initial analysis with the three tracer studies (Prairie Grass, Kincaid SF_6, and Indianapolis) and the two full year data bases (Lovett and Kincaid SO_2). Analyses with these data bases will continue until we are satisfied with the performance of the model. At that time we will finalize the model and conduct the performance evaluation. The three tracer-study comparisons have been reported in some detail by Lee, et al.[6] Only a brief overview (focusing on the results of regulatory interest) will be presented here. In addition, since we have now completed our initial analysis of the two full year data bases, we have included a discussion of the results of these preliminary comparisons. All of the tracer comparisons have been stratified by stability (stable or convective) and data base; the full-year comparisons include those for one-hour, three-hour, and twenty-four-hour averages.

Prairie Grass. As reported in Lee, et al.[6] for convective conditions at Prairie Grass, the Q–Q plot of Figure 1 shows that the distribution of AERMOD predictions compare well against the distribution of observations, with the highest observations being underpredicted by a small amount. Almost the entire distribution is within a factor of two for this unpaired comparison. The fractional bias (FB) based on the mean of the top 25% of the distribution is -0.301 (underprediction within a factor of about 1.35). In contrast to AERMOD, ISC3 shows a tendency to overpredict by about a factor of two at the high end of the distribution (Figure 1). The FB for ISC3 is 0.610.

For stable conditions at Prairie Grass, both ISC3 and AERMOD perform well as indicated by the Q-Q plot of Figure 2. Both models provide an upper end distribution which follows that of the observations; however, ISC3 has a slight overprediction tendency (FB = 0.321) while AERMOD is slightly underpredicting (FB = -0.158). In general we have concluded that the present version of AERMOD, which includes previously discussed changes, adequately simulates the observations in this rural, flat terrain, surface release data base. The areas of the model that were improved as a result of our comparison with the Prairie Grass data included: the treatment of vertical inhomogeneity; and, a specific approach for surface dispersion which included development of an empirical relationship for σ_y.

Kincaid, SF_6. Comparison between AERMOD's and ISC3's performance, during convective conditions, is shown in Figure 3 for the Kincaid data. This tracer data base is characterized by a buoyant, elevated gaseous release. The model estimates are compared against surface level peak concentrations. The Q-Q plot of Figure 3 shows a good match between the distribution of AERMOD estimates and the observations (at least over the upper portion) with a poorer comparison over the less interesting and less important lower end the distribution. The dropoff of the distribution at lower concentrations may be related to the relative uncertainty in the observations for low concentrations. The FB for AERMOD during convective conditions is -0.028 (essentially unbiased on average over the top 25%). ISC3 shows similar performance to AERMOD at the upper end of the distribution as seen in Figure 3 (FB of top 25% = -0.188). However, ISC3 does not match the overall distribution quite as well as AERMOD. Based on the good comparisons we obtained with the Kincaid SF_6 data, we have made no notable changes to our original CBL formulations.

Traditionally, worst case surface-level impacts from elevated buoyant releases in flat terrain have been found during convective conditions, where the plume is brought quickly to the ground. Therefore, the Kincaid study focused primarily on daytime conditions. However, there is a limited number of stable cases in the data base against which we examined the performance of both AERMOD and ISC3. For these cases both models performed poorly. We attempted to determine the cause of this poor performance but we have yet to find an adequate explanation. Since the stable data at Kincaid represented only a very small portion of the distribution of expected stable conditions at this site, we concluded that it would not be productive to continue the analysis. As a result, we have not used these comparisons to reformulate the model.

Indianapolis. Comparison between AERMOD's and ISC3's performance for data at Indianapolis is shown in Figure 4 for convective conditions and Figure 5 for stable conditions The Q-Q plot for convective conditions shows a remarkable match between model and measurements. The FB of 0.045 confirms this. The reader should note that we found similar favorable comparisons in convective conditions, using the original formulation. ISC3 also performed very well at Indianapolis. For convective conditions, the FB was found to be 0.076.

The model also performed quite well during stable conditions after we reformulated AERMOD to account for the anthropogenic effects that an urban boundary has on the surface energy balance. The Indianapolis area is urban in nature. In stable conditions, where these effects can dominate, AERMOD estimates concentrations well within a factor of two (Figure 5) of the observations (FB = -0.145). ISC3 (also within a factor of two with a FB = 0.476) shows a slight tendency for overprediction. ISC3 accounts for urban effects by replacing the rural PGT dispersion curves with the Briggs urban curves.

Analysis of model performance using the data during nighttime "stable" conditions at Indianapolis is one of the most obvious areas where the developmental evaluation process worked well for AERMIC. At Indianapolis the original model performed poorly against the surface concentrations during stable conditions because of its incorrect characterization of the urban boundary layer. Our initial formulation allowed the boundary layer in Indianapolis to develop a strong stable stratification when, in fact, the urban nature of the area rarely would allow this condition to arise. Consequently, plume material was often not being appropriately mixed in the vertical. As indicated by the current results, the modification (addition of anthropogenic heat) was necessary.

Lovett (Full-Year) SO_2. We have completed our initial analysis of AERMOD's performance against the full-year SO_2 data base collected at the Lovett Power Plant. This plant is located in the complex topography of the Hudson River Valley in New York State. Complex terrain effects are handled by this model in a manner that is totally novel to regulatory models. The two-state model as described above and in Perry, et al.[4] has been coded with two options. The initial performance of each of these options has been examined with this data base. Preliminary comparisons (for one-, three-, and twenty four-hour averages) of AERMOD against ISC3 and the Lovett observations are shown in Figures 6, 7, and 8.

For the one-, and three-hour averages, both options of AERMOD are performing well (within a factor of two) in reproducing the distribution of the observations at Lovett. Option 1 has a tendency to underestimate, while Option 2, showing a similar absolute bias, has a tendency towards overprediction. ISC3, for the shorter averaging times, overpredicts the observations by a factor of three to four.

We have found very little bias in the comparisons of the observed and predicted 24-hour averages, with AERMOD's Option 2. However, predictions using AERMOD's terrain Option 1, were found to underestimate observations, in general, by a factor of two. Furthermore, ISC3 overpredicts the observed concentrations, for this averaging period, by a factor of two to three.

Although these comparisons are encouraging, we are performing an analysis of the models sensitivity to a wide variety of source-receptor-terrain relationships in order to build additional confidence in these methods. If similar good performance is found for both terrain options, we will examine each option in the Phase II performance evaluation.

Kincaid, SO_2. As with Lovett, the Kincaid SO_2 data provides an extensive temporal record which allows us to evaluate predictions of the longer term averages. Our initial analysis of the one-, three-, and twenty four-hour average concentrations have been completed and the results are presented in Figures 9, 10, and 11. For the one-, and three-hour comparisons AERMOD reproduces the observed distribution very well. For the same averaging times, ISC3 is showing a tendency towards underprediction although still generally within a factor of two.

For the twenty four-hour averages, both models provide noticeable underpredictions. With the exception of the highest few points, which are close to the one-to-one line, AERMOD's predictions fall around a factor of two below the observations. Whereas, ISC3's predictions fall generally around a factor of four below the observations.

Summary In summary, AERMOD has gone through considerable modification as a result of the developmental evaluation process and will likely continue to do so over the remaining few months of this phase of the project. For the surface release data (Prairie Grass) AERMOD shows a slight underprediction tendency in both convective and stable conditions while ISC3 has a small overprediction tendency. With the rural elevated release tracer data (Kincaid SF_6) AERMOD exhibits insignificant bias in convective conditions while performing poorly against the few available stable cases. ISC3 performs similarly to AERMOD with this tracer data base. With the urban data, both models perform well with only small biases for all conditions.

For the full year data bases, AERMOD compared well with the observations, particularly for the shorter averaging times.

DISCLAIMER

This paper has been reviewed in accordance with the U. S. Environmental Protection Agency's peer and administrative review policies and approved for presentation and publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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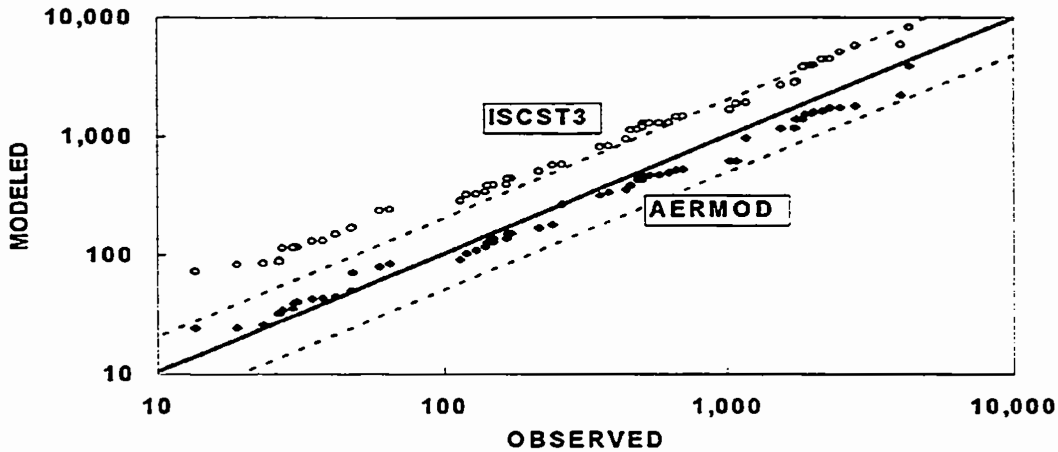

Figure 1. Quantile-quantile plot of predicted versus observed arc-maximum concentrations for AERMOD and ISC3 based on Prairie Grass convective data.

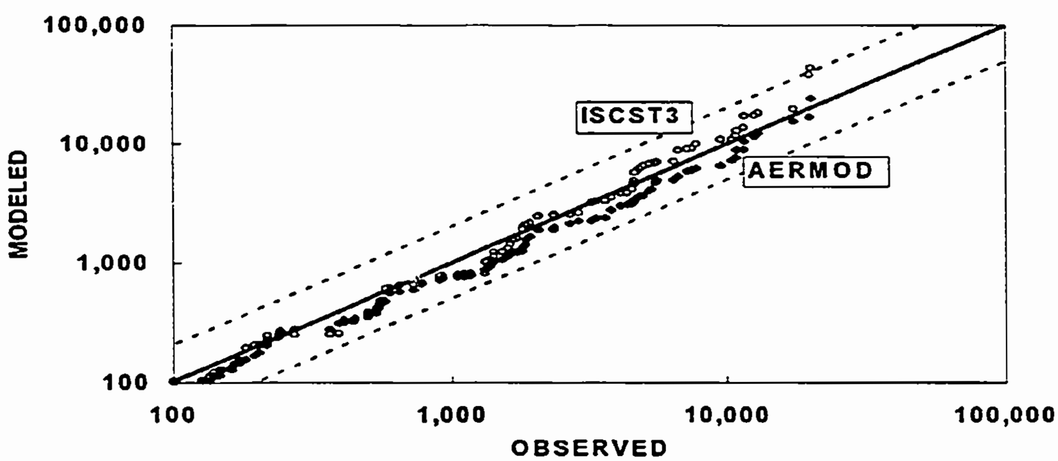

Figure 2. Quantile-quantile plot of predicted versus observed arc-maximum concentrations for AERMOD and ISC3 based on Prairie Grass stable data.

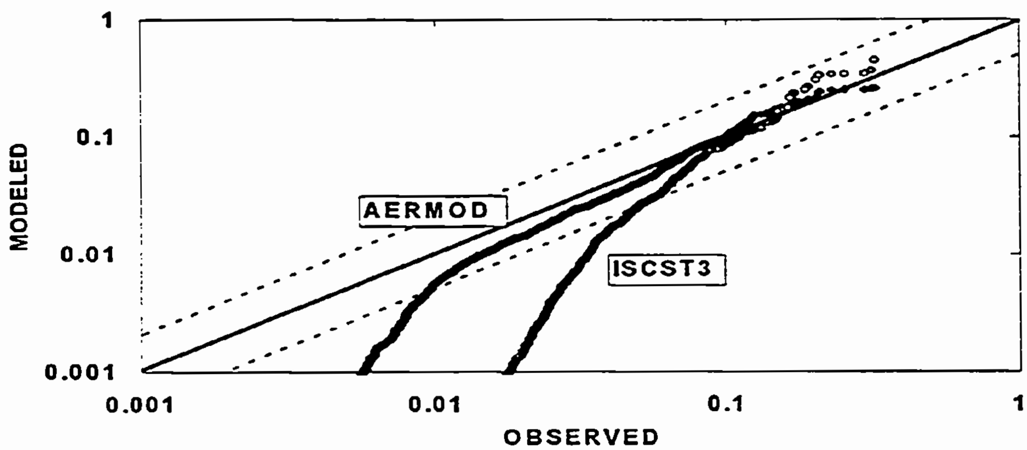

Figure 3. Quantile-quantile plot of predicted versus observed arc-maximum concentrations for AERMOD and ISC3 based on Kincaid SF_6 convective data.

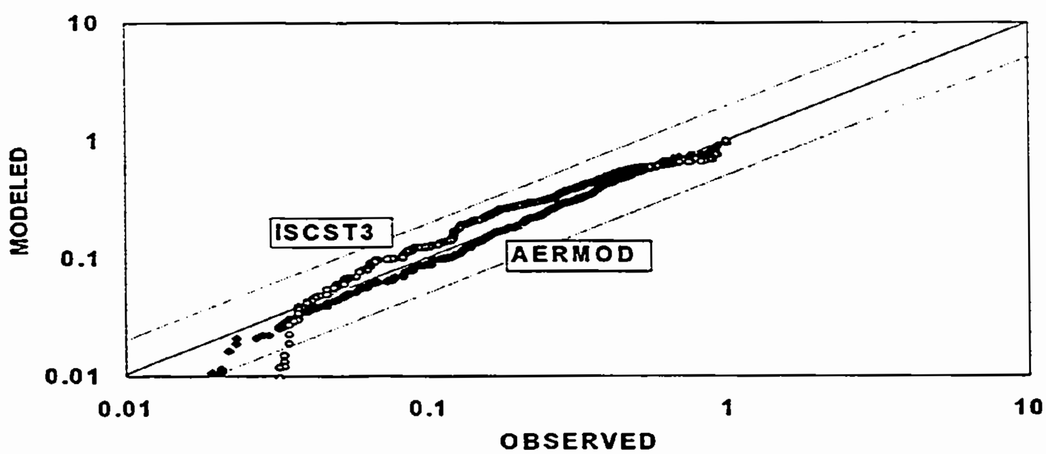

Figure 4. Quantile-quantile plot of predicted versus observed arc-maximum concentrations for AERMOD and ISC3 based on Indianapolis convective data.

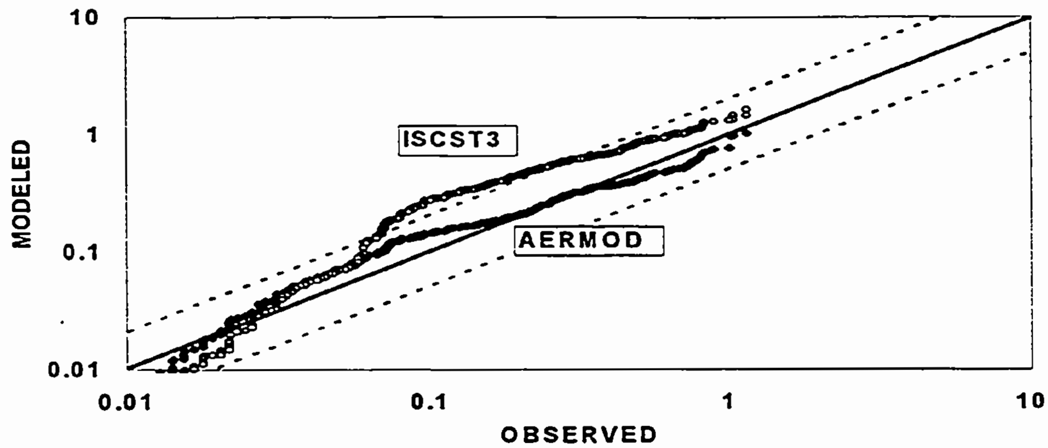

Figure 5. Quantile-quantile plot of predicted versus observed arc-maximum concentrations for AERMOD and ISC3 based on Indianapolis stable data.

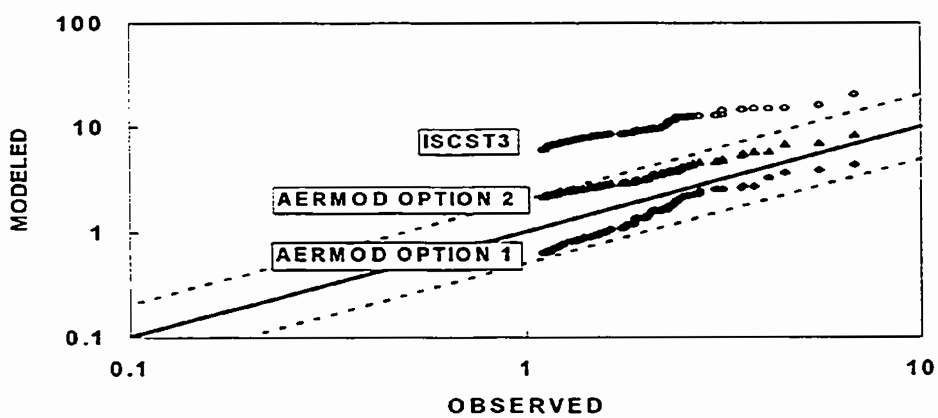

Figure 6. Quantile-quantile plot of predicted versus observed maximum one-hour concentrations for AERMOD and ISC3 based on the Lovett data base. Options 1 and 2 refer to the two complex terrain modeling approaches presently in AERMOD.

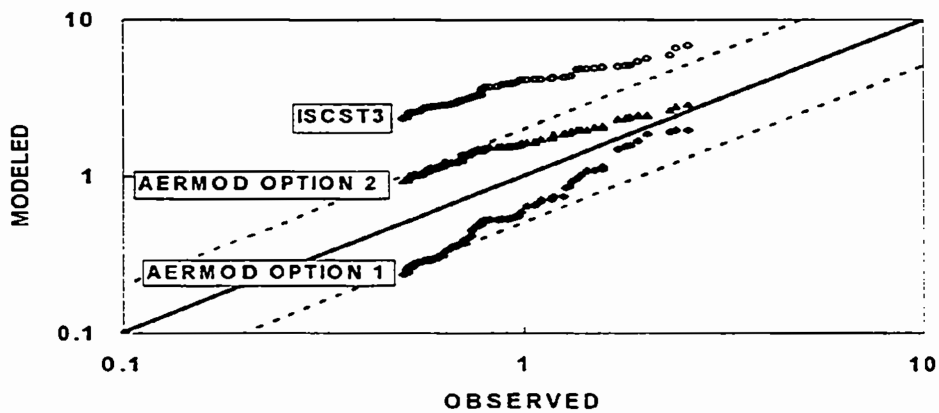

Figure 7. Quantile-quantile plot of predicted versus observed maximum three-hour concentrations for AERMOD and ISC3 based on the Lovett data base. Options 1 and 2 refer to the two complex terrain modeling approaches presently in AERMOD.

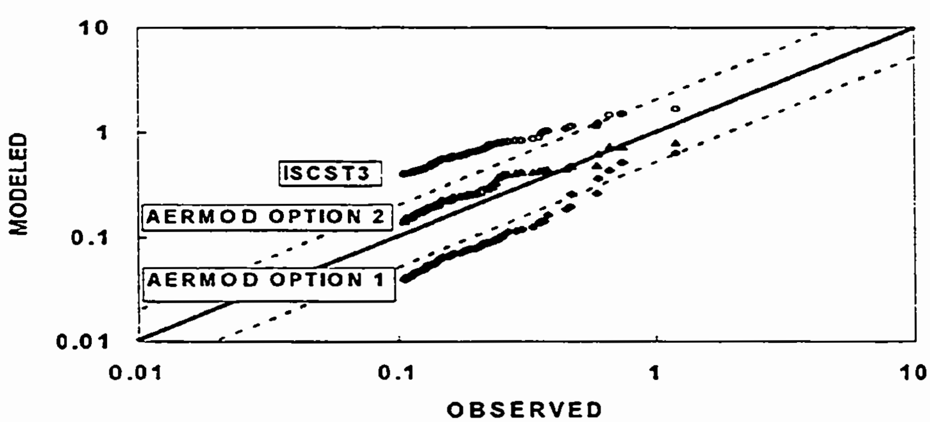

Figure 8. Quantile-quantile plot of predicted versus observed maximum twenty-four hour concentrations for AERMOD and ISC3 based on the Lovett data base. Options 1 and 2 refer to the two complex terrain modeling approaches presently in AERMOD.

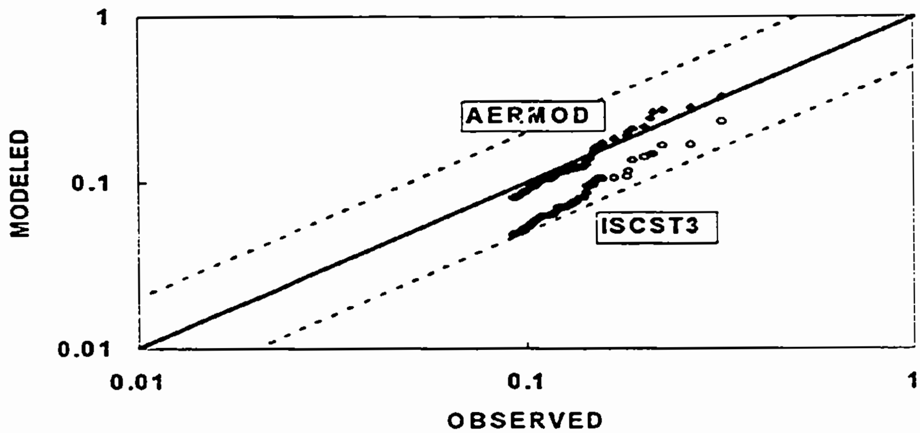

Figure 9. Quantile-quantile plot of predicted versus observed maximum one-hour concentrations for AERMOD and ISC3 based on the Kincaid SO_2 data base.

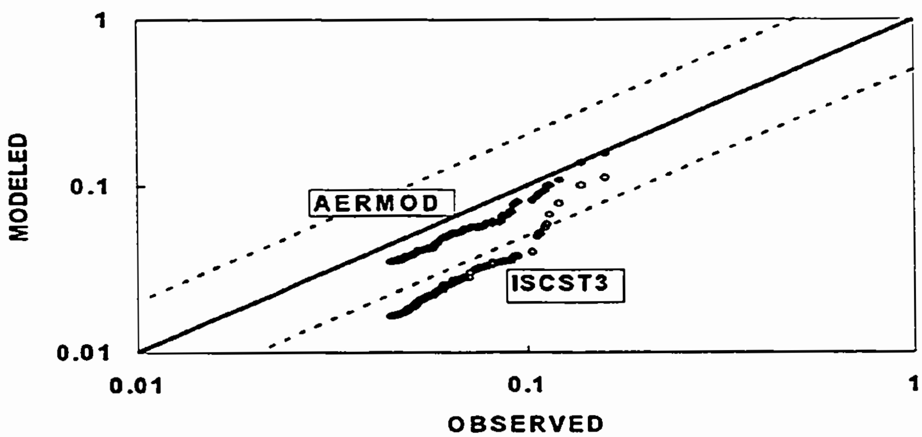

Figure 10. Quantile-quantile plot of predicted versus observed maximum three-hour concentrations for AERMOD and ISC3 based on the Kincaid SO_2 data base.

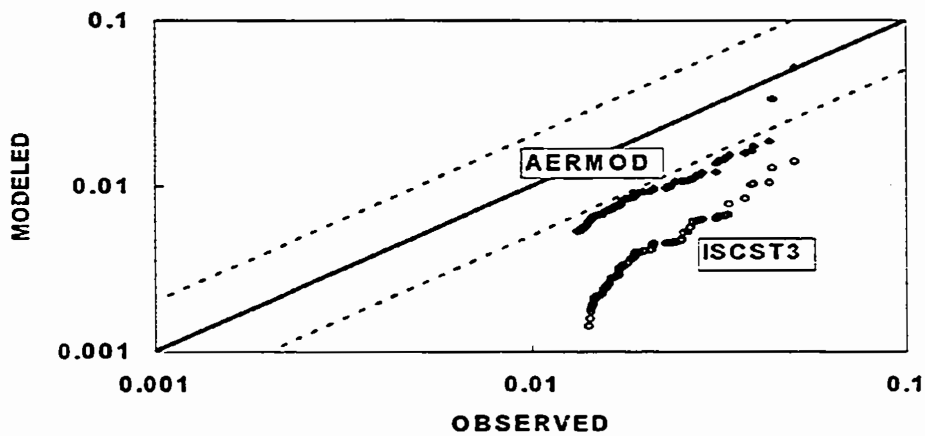

Figure 11. Quantile-quantile plot of predicted versus observed maximum twenty-four hour concentrations for AERMOD and ISC3 based on the Kincaid SO_2 data base.

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6. ABSTRACT

The American Meteorological Society and the Environmental Protection Agency formed a combined working group to develop mproved algorithms for regulatory air dispersion models. This workgroup has developed the AERMOD model which is a steady tate, plume model intended to be applied in those regulatory situations currently modeled with the Industrial Source Complex Model (ISC3). This model development project is moving into its final phases and the purpose of this paper is to examine the echnical basis for the most recent AERMOD algorithms. In addition, there is a discussion of the performance of the model in elation to measurements at five research field studies over a wide variety of meteorological conditions and source configurations.

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