MICROSCALE MODELING OF NEAR-ROADWAY AIR QUALITY BY NUMERICAL TECHNIQUES

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The type of microscale modeling considered here is that based on the numerical solution of partial differential equations that govern the conservation of pollutant species throughout specified regions of the atmosphere. The regions considered are small, generally including a roadway and nearby points at distances of tens or hundreds of meters. Thus the use of the term microscale.

Figure 1 shows a schematic diagram of the modeling approach under consideration. The arrows represent processes leading to products shown in boxes. A pollutant species within any selected volume of the atmosphere is conserved by a balance of transport into and out of the volume, production (or depletion) by chemical reactions, and other internal sources or sinks. Mathematically this can be specified by requiring that, for any given species at any time within a volume about a general point x, y, z,

Rate of increase = rate transported in - rate transported out
+ net rate of chemical production
+ net rate of production from internal sources and sinks

By considering the limit as the volume becomes infinitesimally small, this conservation can be expressed in the form of a governing partial differential equation:

$$\frac{\partial x}{\partial t} = -u\frac{\partial x}{\partial x} - v\frac{\partial x}{\partial y} - w\frac{\partial x}{\partial z} + \frac{\partial}{\partial x}\left(K_x\frac{\partial x}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial x}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial x}{\partial z}\right)$$

$$+ R_c + R_s$$

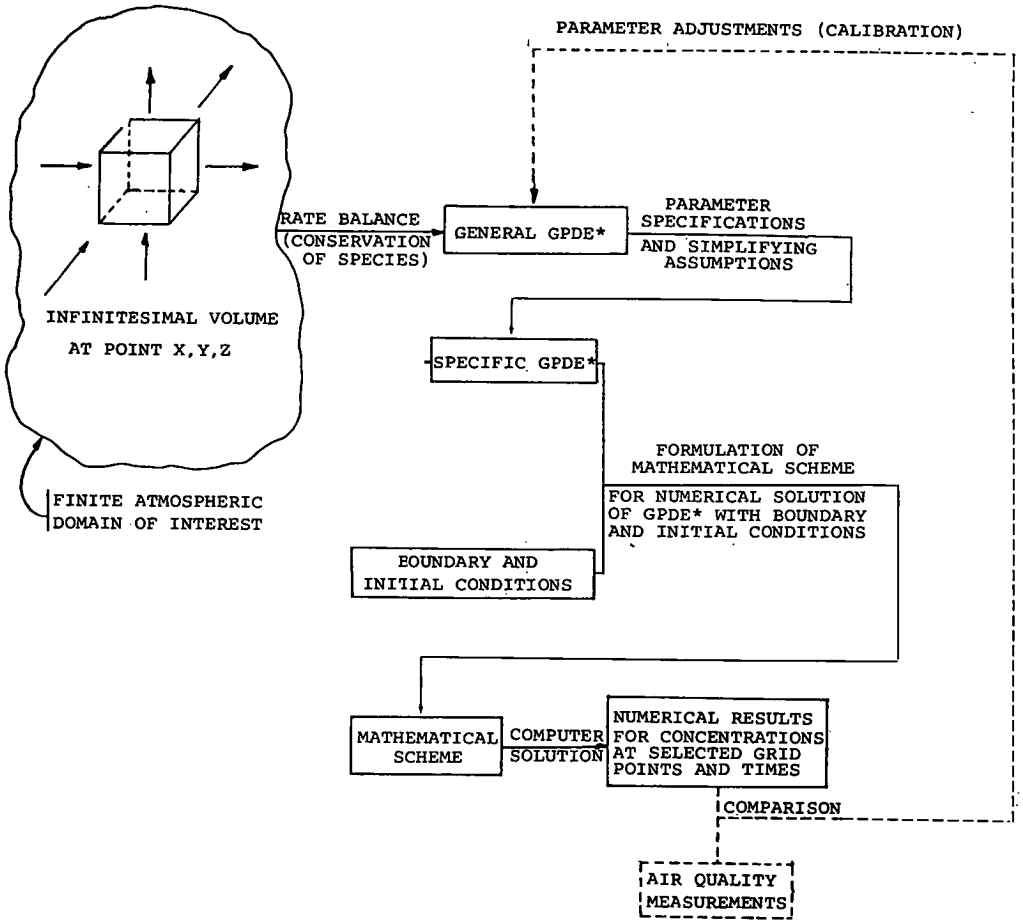
where

x = concentration;
u,v,w = mean wind velocity components in x, y, z directions respectively;
K_x,K_y,K_z = turbulent diffusion coefficients in x, y, z directions respectively;
R_c = net rate of chemical production per unit volume; and
R_s = net rate of production per unit volume from sources and sinks.

The above equation was developed with a coordinate system fixed in space (Eulerian formulation). An alternative but equivalent form is sometimes developed with a coordinate system moving with the atmosphere (Lagrangian formulation).

The first 3 terms on the right side of the equation represent net transport in the

Figure 1. Schematic diagram of microscale model.



*GPDE: GOVERNING PARTIAL DIFFERENTIAL EQUATION TO BE SATISFIED AT EACH TIME T AND EACH POINT X, Y, Z WITHIN ATMOSPHERIC DOMAIN OF INTEREST. (NOT A SOLUTION OR EXPLICIT EQUATION FOR POLLUTANT CONCENTRATION)

various directions by the mean wind components; the second 3 terms represent the transport by the turbulent components, i.e., by turbulent diffusion. Molecular diffusion is negligible in comparison and thus does not appear. An equation of this form applies to each pollutant, except that the chemical reaction and source production terms (R_c and R_s) are different. The chemical reaction term complicates the analysis considerably because it involves not only the particular pollutant of interest but all others with which it reacts. Thus, the governing equation is coupled to similar equations for other pollutants, making it necessary to solve simultaneously a set of partial differential equations. However, carbon monoxide for microscale purposes is essentially an inert species, and therefore the chemical reaction term will be neglected. Thus, we need to solve only a single, uncoupled, partial differential equation. The resulting equation is the general governing partial differential equation (GPDE) referred to in Figure 1. The word general should be qualified since the equation has a specific form that treats turbulent transport as a function proportional to the gradient of concentration. The coefficients of proportionality are the turbulent diffusion coefficients K_x, K_y, K_z. This form of the equation is used because it is the classical and most common

formulation and the one used in the models being considered.

It may be helpful to point out that modeling of the type considered here is frequently described in the air pollution literature by the terms K-theory and conservation of mass. The K-theory designation is attributable to the use of the symbol K as the turbulent diffusion coefficient. Conservation of mass refers to the governing partial differential equation and its derivation based on the conservation of a particular species of pollution. This term may be somewhat confusing to those familiar with the literature on fluid dynamics and transport phenomena. In these sciences, conservation of mass generally refers to the equation for conservation of the total mass made up of the sum of the masses of all species. The equation for an individual species, such as that being treated here, is then referred to as the conservation of species equation, or some similar terminology.

The modeling approach shown in Figure 1 proceeds by specifying the spatial and temporal distribution of parameters (such as u, K_x, and R_s) and by making simplifying assumptions, thus reducing the general GPDE to a specific form applicable to a particular problem of interest. The coefficients u, v, w, K_x, K_y, and K_z can be specified on the basis of micrometeorological data, empirical profiles, fluid dynamics, and turbulence theory or by solving partial differential equations for u, v, and w based on conservation of mass, momentum, and energy. The emission rate R_s is of course based on a source inventory involving traffic data with emission factor analysis (25). Simplifying assumptions can involve neglecting terms of the GPDE or using simplified forms of the coefficient terms u, v, w, K_x, K_y, and K_z. Bases for neglecting terms completely include boundary layer theory, steady state, and dimensional homogeneity or uniformity, e.g., neglecting the direction parallel to a long, uniform highway line source. The resulting specific GPDE must then be satisfied at every point in the atmospheric domain of interest. To complete the mathematical formulation of the problem, however, requires that conditions be specified on the boundaries of the atmospheric domain (boundary conditions) and at some initial time throughout the domain (initial conditions). These conditions are given in terms of either the concentration or the concentration gradient or a combination of both. Physically such conditions are related to either the pollutant flux or the pollutant concentration, which in turn can be related to emission rates and background, measured, or other known concentrations. Frequently all sources can be accounted for at the boundaries, thus eliminating the internal source term R_s from the GPDE.

The above boundary and initial conditions together with the specific GPDE constitute the mathematical differential statement of the specific problem of interest. Solution of such problems can be achieved, or attempted, by any of a number of methods including techniques for exact solution leading to analytical expressions (explicit or implicit algebraic-transcendental equations for concentration), techniques for approximate solution leading to analytical expressions, or numerical techniques leading directly to numerical results at an array of grid points and at specific times. Our present consideration is directed toward the last approach, i.e., numerical techniques. The Gaussian equation, on the other hand, is an exact solution to a highly simplified GPDE.

The use of numerical techniques involves the formulation of some mathematical scheme for the calculation of numerical results that will satisfy the specific GPDE with its associated boundary and initial conditions. The mathematical scheme is then computerized for calculation of the results. In most cases the numerical technique used is the finite difference approach. Most cases, however, differ from one another by application of different variations of the finite difference approach. Although these variations do not change the basic objective of satisfying the GPDE with associated conditions, they can have an effect on the accuracy of doing so and, probably more significant, they can have considerable impact on computation efficiency and therefore on computer requirements.

This discussion covers all ingredients essential to description of our modeling approach. Figure 1, however, also shows how the approach can be improved, and usually is, by comparison with air quality data and calibration through adjustment of the coefficient parameters.

EXISTING NUMERICAL MODELS: STATE OF THE ART

Following is a brief description of existing capabilities and some specific models (1, 2, 3, 4, 5, 6, 7, 8, 9, 10) based on numerical techniques. The list of models is not all inclusive, but is representative of the various degrees and avenues of development. Figure 1 shows the primary elements that distinguish models: atmospheric domain, boundary conditions, parameter specifications and simplifying assumptions, and mathematical scheme. Although these factors determine the capabilities of models, a definitive evaluation should also consider the degree and success of model validations. Unfortunately, validations have not been performed for all models, and those that have been performed are not adequate for evaluation of the relative merits of models. Along these lines it would be helpful if all modelers evaluated a common set of validation criteria, such as correlation coefficients and standard error of estimate.

Atmospheric domain and boundary conditions essentially determine the problem that is solved; parameters and assumptions determine the limitations and rigor with which it is solved, and the mathematical scheme determines the computational efficiency. The problems most commonly solved by existing models involve elevated, at-grade, and depressed roadways. In addition, however, there are models of complexity sufficient to deal with 3-dimensional multiroadway systems in the presence of complex building and topographical features.

Specifications for wind and turbulence parameters include analytical profiles such as power and logarithmic laws, separated flow regions with backflow and vortex motions in the vicinity of obstructions, and, in the most sophisticated cases, flows determined by solution of the partial differential equations governing conservation of mass and momentum. Although each existing model has been applied with only selected wind and turbulence profiles, all the models have the mathematical capability, and are generally programmed on the computer, to accept any prescribed profiles. However, one qualification that is usually built into the program, or should be, is the constraint that winds must be such as to conserve total mass at all points of the atmospheric domain; i.e., they must satisfy the partial differential equation for conservation of mass (total mass). In this way the models prevent impossible flow fields that artificially create or destroy atmospheric mass, including mass of the particular species of interest. With the flexibility of accepting arbitrary wind and turbulence input, models may be readily upgraded as more accurate information, data, or analysis becomes available for each input.

Regarding the simplifying assumptions, most models assume 2-dimensional steady-state behavior, although some include 3-dimensional and transient effects. The 2-dimensional assumption is applicable to long roadways with uniform topography and emissions along their length. Except near the ends of such roadway sections, variations parallel to the road are negligible.

Details of the mathematical scheme employed are quite complex and diverse and are thus difficult to evaluate except on the basis of their effect on the relative computational efficiency of the various models. The efficiencies in terms of computer requirements such as running time and storage have been surveyed and reported by Darling (11) for numerous models including both numerical and Gaussian types. An updated version including additional models would be valuable and should be available in the near future.

Egan and Lavery (1) treat elevated, at-grade, and depressed roadways and also include applications to at-grade and elevated roadways upwind of an obstacle. The model is 2-dimensional steady-state with perpendicular or near-perpendicular winds. Validations have been performed for vertical power law wind and turbulence profiles with eddy recirculation regions in the vicinity of obstacles.

The General Research Corporation (GRC) model (2) incorporates several unique features. The mathematics is composed of a hybrid of finite differences in the vertical, the Gaussian distribution in the cross-wind direction, and a Lagrangian formulation for the windward transport. As a result the model is capable of handling 3-dimensional time-dependent problems of arbitrary wind direction with greatly reduced computer requirements. The model also takes advantage of advanced aerodynamics to simulate wake velocity and turbulence distributions both behind vehicles and downwind of elevated roadways (open underneath). Unfortunately the model has not been validated.

Elevated roadways are of 2 basic types: those that are filled underneath and those that are open underneath. The aerodynamics of the 2 cases, and therefore the resulting concentration fields, are considerably different. Thus, a model derived and calibrated for one type should not be expected to give good results for the other. Similarly, caution should be exercised in the application of models for depressed roads, since the depressions modeled can be quite different, ranging from shallow to deep, with vertical or sloping walls and with other irregularities such as cantilevered overhands.

Kirsch and Mason (3) describe a model known as EXPLOR. It allows arbitrary wind direction and has been validated for elevated, at-grade, and depressed roadways. Effects of irregular terrain are accounted for by constructing a wind field that satisfies the equation for conservation of total mass. A related model is called NEXUS (4). This is essentially a 3-dimensional version of EXPLOR. Recently EXPLOR and NEXUS have been upgraded, primarily by incorporation of a subprogram called W-FIT, which determines an improved wind distribution by solving the governing partial differential equations for conservation of momentum of an inviscid fluid. In addition, the models have been expanded to allow more than 1 roadway, currently as many as 8, with arbitrary vertical and horizontal spacing. The new NEXUS is particularly suited for treatment of 3-dimensional stacked roadway configurations as found in typical interchanges. The upgraded versions of NEXUS and EXPLOR are called MROAD 2 and MROAD 3 respectively. Draft copies of user manuals for the new programs have been provided, under contract, to the Oregon Department of Transportation (5).

Eschenroeder (6) describes an adaptation of a larger scale 2-dimensional photochemical model to microscale at-grade roadway applications. For such applications, however, that model has apparently been supplanted by the more powerful GRC model (2). Ragland and Pierce (7) consider only at-grade roadways but incorporate highly realistic wind and turbulence profiles while also considering 3-dimensional effects. One of the most advanced models is described by Hotchkiss and Harlow (8). This model treats systems of streets and cross streets with complex 3-dimensional obstacles. The flow field is determined by solution of the 3-dimensional conservation of momentum equations including viscous effects (Navier-Stokes equations) as described by Hirt and Cook (12). Validations show good agreement with field data. Danard (9) treats at-grade and depressed roadways by assuming 2-dimensional behavior. A limitation of the application described is the assumption of calm winds within the depression. Kondo (10) deals with only depressed or street canyon roadways and considers specifically a vortex wind field between the buildings.

Perhaps a few words should be said about the assumption of vortex flow in a depression. Such flows have been observed in the field by a number of investigators (13, 14). Further the expected consequence of such motion is to cause higher pollution levels on the upwind side of the depression, and this too has been observed. At one time there was a reluctance by some to accept the notion of such a flow pattern. Today, however, the opposite seems to be true; the acceptance or assumption of such flow patterns is excessive. They do not always exist, even for wind perpendicular to the street. Although fluid dynamics theory has long been aware of such vortices in similar flows, e.g., flow past fins in annuli (15, p. 197), their formation is understood to be dependent on both Reynolds number and aspect ratio, i.e., the depression height to width ratio. Accordingly, it is expected that at least for very deep depressions vortices are not always formed, especially near the bottom of the depression. In addition, mobile laboratory measurements by the New York City Department of Air Resources in deep city street canyons have indicated a preference for channeled flow instead, i.e., flow parallel to the canyon. More definitive evidence of this effect has been observed in a monitoring program recently conducted for New York City by Environmental Systems Laboratory, Inc., and will be reported on in the future.

FUTURE MODELING NEEDS: ADVANCEMENT OF THE ART

In trying to construct a list of areas that are in most urgent need of further work and that will also bear the greatest fruit, I found that all items relate in one way or another

to one primary overriding need, namely the improvement of input parameter specifications, i.e., wind and turbulence. The mathematics and computer capabilities are already sufficiently powerful to handle most problems of interest. In complex 3-dimensional cases with highly irregular terrain and man-made obstacles, computer demands may still be impractical for many engineering analyses. However, the development of improved math schemes and computer programs to reduce computer requirements is an area of active research and steady progress.

The great power of numerical models is their ability to account for the complexities of wind and turbulence distributions in the real world; unfortunately, this is also the major source of difficulty, for it requires determination of those distributions. Especially difficult is the determination of the turbulent diffusion coefficients. This has been, and still is, the central problem of turbulence theory. The use of improperly specified wind and turbulence can cause gross errors and is an injustice to the modeling technique. Although it is agreed that wind and turbulence distributions are not easily determined, it is also believed that they are not so mysterious as often alleged and that difficulties are in large part due to a failure to take advantage of existing knowledge. The sciences of fluid dynamics and micrometeorology are not new and have developed a large body of data and methods of analysis for flow around obstacles and over irregular boundaries. This information is readily available in fluid dynamics and micrometeorology texts. Also available in the literature are considerations specifically pertaining to atmospheric flows around obstacles (16, 17, 18). (Scales involved in roadway microscale modeling are at the lower end of, and in some cases smaller than, the scales of classical micrometeorology.) Existing knowledge can be of critical value in numerical modeling, and therefore its exploitation should be a first priority objective. This will be helpful not only in the specification of wind and turbulence but also in the design of more meaningful and effective field measurement programs. This leads to the second need: more field data.

Measurement programs in the past tended to emphasize output, i.e., air quality, while input parameters other than traffic were in general inadequately measured, at least from the point of view of numerical models. Therefore, future measurement programs intended for the development and validation of numerical models should give greater consideration to the wind and turbulence input and should do so in a rational, organized, and optimized way based on the existing knowledge. Such an approach should influence not only the measurement of wind and turbulence but also the placement of pollutant monitors. For purposes of data acquisition as well as improved understanding of the governing phenomena, small-scale physical experiments, as in wind tunnels, should also be more actively pursued. Examples of wind tunnel investigations for atmospheric problems have been published (19, 20, 21, 22). In fact, Hoydysh and Sabetta (22) deal directly with use of wind tunnel results to calibrate numerical models. Although wind tunnel data have been challenged with regard to quantitative validity on the microscale, they can at least reveal qualitative effects and contribute to experiment design for full-scale measurement programs.

Finally, there is an urgent need, and to date a general failure, to be careful. Once models have been developed for particular situations, their limitations should be realized and respected. Subtle changes in terrain or meteorology can have drastic impact on air quality whereas other seemingly major differences in these input factors might have only minor effects on the air. A roadway near an obstacle may cause high pollution near the obstacle while another road only 1 or 2 road-widths farther from the obstacle might have practically no impact at the obstacle. In the first case, the road is contained within a recirculating vortex region formed by the obstacle; in the second case, the road is outside the region. As discussed above, elevated roads with fill are significantly different from those without. Similarly, a depressed road with vertical walls may cause a large eddy to be formed whereas in another depressed roadway, because it is deeper or shallower or has sloped walls, the eddy is not formed. Application of a model developed for vortex flow would give good results in the first case and poor results in the second, not to mention a bad name for numerical models.

Unfortunately many users select a model simply on the basis of general category; e.g., if the user has an elevated roadway, then any model developed for an elevated

roadway is assumed applicable. Fault is not only with the user alone but also with the model developer who does not adequately determine and define applicability of the model. To correct this situation as well as to launch a more organized attack on microscale problems, we should investigate and carefully specify the applicability of particular models in terms of quantified ranges of characteristic parameters. These might include geometric parameters such as aspect ratios, roughness heights, and basic shapes and flow parameters such as wind vectors, Reynolds numbers, and Froude numbers. They should cover both the microscale of interest and the larger background scale.

Advancement of the art of numerical modeling is most urgently in need of, and can most effectively be achieved by, improved specification of wind and turbulence fields. To this end it is recommended that the sciences of fluid and atmospheric flows be more thoroughly exploited, that additional data be acquired including field measurements as well as small-scale physical experiments, and that the applicability of models be determined and defined on a more comprehensive and organized basis, with users carefully selecting models accordingly.

NUMERICAL VERSUS GAUSSIAN MODELS

The vast majority of existing microscale models are either Gaussian or numerical (finite difference). Gaussian models are considerably more expedient and less demanding of the computer, but numerical models are more powerful, more realistic, and, therefore, if properly developed and applied, more accurate.

These advantages of numerical models are claimed on the basis that Gaussian equations and numerical models are both solutions of governing partial differential equations (GPDE) for conservation of species, but that the GPDE solved by the Gaussian equation is much less realistic than the GPDE solved numerically. In particular, the Gaussian equation is a solution to the conservation of species GPDE in which the wind and turbulence profiles are both assumed to be uniform in space or more generally where they have the same profiles. Unfortunately, this is unrealistic in the atmosphere except at higher elevations beyond the disturbing influence of obstacles and the boundary layer effects of the ground. On the other hand, numerical techniques, as already discussed, are capable of handling arbitrary wind and turbulence of almost unlimited complexity. Of course, as also pointed out above, use of improper wind and turbulence in numerical models can cause results that are wrong, in fact, possibly much worse than Gaussian results. Thus, it seems fair to say that numerical models at least have the potential to produce more accurate results and handle more complex situations than Gaussian models.

As an aside, all models based on physics, as opposed to those based on statistical, empirical, or other grounds, must conserve mass of the species, that is, in the broader sense including sources, sinks, and chemistry. Thus the label "conservation of mass" applies equally to Gaussian models and to numerical models that solve the GPDE for conservation of species. Unfortunately, this label has been adopted for particular types of models only, such as the numerical, with an implied and frequently assumed exclusion of all other models. This is misleading and unfair to other modelers that are also conserving mass. Therefore, it might be wise to completely avoid the term conservation of mass.

The Gaussian model is generally simpler, more expedient, and less burdensome to the computer. The Gaussian equation is a simple functional relation between receptor and source. Total concentration at a single receptor can therefore be evaluated directly by addition of results from separate Gaussian equations, one for each source. Also the effects of variations in meteorology or sources or both are readily evaluated on either a single or a multiple receptor basis. On the other hand, numerical models require mathematical schemes involving complex algorithms, iterations, matrix inversions, and other procedures that are much more difficult to implement than the simple Gaussian relation. Such procedures can also incur problems with convergence and mathematical instability that can be quite difficult to overcome. Further, the mathematical

schemes involve an interdependence of receptor points that precludes computation at a single receptor and requires in each case the computation of numerical results for an entire array of grid point receptors.

Considering the advantages and disadvantages of both Gaussian and numerical models, I believe that both should play, as they have in the past, an important role in microscale air quality modeling. However, in light of some of the weaknesses, it might be worthwhile to spend somewhat more of our efforts on other types of models. Existing techniques and models incorporate some of the advantages of both Gaussian and numerical models without all of the disadvantages. For example, by approximate techniques such as iterative, asymptotic, and weighted residual methods, it is possible to develop functional relations (algebraic-transcendental equations) that are approximate solutions (i.e., close to exact solutions) to complex GPDEs. Such solutions obtained for GPDEs, which are more realistic and general than the GPDE for which the Gaussian is a solution, would provide models having both the convenience of Gaussian models, i.e., the functional form, and some of the greater realism of the numerical models. Further, exact solutions are already available for more realistic GPDEs. For example, Cresswell and Sutton (23, 24) derive exact solution for the GPDE for an at-grade road and arbitrary vertical power law profiles of wind and turbulent diffusivity. The profiles not only are more representative of atmospheric boundary layers but also lead to the Gaussian solution as a special case. To illustrate, the solution is

$$x = cQ\sigma^{-\frac{n+1}{n}} \exp\left(-\frac{\eta^{\nu}}{\nu}\right)$$

where the wind and turbulent diffusivity are assumed to be

$$u = \beta z^{1/n} \qquad K = \partial z^{1/m}$$

respectively, with n and m being arbitrary constants. In the solution, c is a constant, σ is a function of downwind distance, both given as part of the solution, and

$$\eta = \frac{z}{\sigma}$$

$$\nu = \frac{m - n + 2mn}{mn}$$

For $\nu = 2$, the Gaussian solution is obtained, and further this requires m = n, that is, the same profile for both wind and turbulent diffusivity. However, based on the law of conservation of momentum in boundary layers, m cannot equal n except in the special case of n = 2. Unfortunately, this value of n is not only restrictive but practically nonoccurring, especially over flat terrain. Thus, the Gaussian solution is based on either an unrealistic profile or a violation of the law of conservation of momentum. Considering a value of n = 7, which is more typical of the turbulent boundary layers over flat terrain, it follows from conservation of momentum that m = 7/6 and therefore that $\nu = 9/7$, i.e., the turbulent diffusivity is nearly linear and the conservation is closer to exponential than Gaussian. The above is an example of models with more rigorous physics than Gaussian models, yet greater simplicity than numerical models. They should not be ignored.

SUMMARY

Numerical techniques provide a powerful tool for the assessment of transportation-related air quality impacts. They are potentially capable of accounting for meteorology and topography of almost unlimited complexity. This paper presents a description of their basic nature, a discussion of existing capabilities including some particular models, suggested ways for improvement of models, and consideration of the relative merits of numerical versus Gaussian models.

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