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MODELING POLLUTANT DISPERSION OVER IRREGULAR TERRAIN
WITH SECOND MOMENTS AND CUBIC SPLINES

by

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INTRODUCTION

Under ideal conditions, dispersion can be reasonably predicted with analytical methods, such as Gaussian puff/plume theory (Pasquill, 1974; Shir and Sheih, 1974; Gifford, 1968; and Lamb and Neiburger, 1971). Gaussian puff/plume models still continue to be used with reasonable success even when pushed beyond their intended limits. However, analytical methods are typically inflexible under variable wind conditions, particularly in cases where dispersion occurs over irregular surfaces. An alternative to these constraints appears to be possible at the present time only by the use of sophisticated numerical models. A review of numerical methods for predicting air pollution dispersion is given by Pasquill (1974), Gifford (1975), and Hoffman, et al (1977).

A specific need exists for more detailed study into the effect of surface irregularities on dispersion. The Pasquill-Gifford dispersion curves are valid only for level, uniform terrain — which is ideal in most instances. The roughness can normally be accounted for by using on-site turbulence data, but such data are usually sparse. As a consequence, many models omit the effect of topography. Studies have been undertaken to calculate flow fields and dispersion patterns over complex terrain. (Reynolds, et al, 1973; Yocke, et al, 1977; Lantz, et al, 1977; Anthes and Seaman, 1976; and Egan and Bass, 1976).

The requirement is to establish an accurate and efficient numerical solution algorithm for three-dimensional mesoscale atmospheric transport and diffusion over irregular terrain. Herein, a three-dimensional method-of-moments technique is employed to calculate pollutant advection. The method is based on the calculation of moment distributions of a concentration within a cell (volume), as developed by Egan and Mahoney (1972), and used by Pedersen and Prahm (1974), Fischer (1977), and Pepper and Long (1978). By summing moments over the solution domain, and using a Lagrangian advection scheme, concentration can be transported without generation of numerical dispersion error.

Because the method maintains subgrid scale resolution, problems involving steep gradients can be calculated without significant computational damping.

Three-dimensional diffusion is solved by the method of cubic splines (Price and MacPherson, 1973; Rubin and Graves, 1975; Ahlberg, et al, 1967). The cubic spline method is based on continuous-curvature cubic spline relations used as interpolation functions for first and second derivative terms. After solution of the diffusion terms, the first and second moments are recalculated to ensure continuity with the advection terms. To reduce computer programming complexity, the procedure of fractional steps (Yanenko, 1971) is used to calculate the three-dimensional solutions. A coordinate transformation is employed to transform the terrain-lid variability into regular intervals in the computational domain.

Simple tests are conducted to determine the accuracy of the numerical methods. The effect of topography on a continuous emission is examined under ideal conditions and the results compared with values obtained from an analytical Gaussian plume relation.

PROBLEM STATEMENT

The cell-averaged transport equation requiring solution is (Deardoff, 1973):

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial}{\partial x_j} [\bar{U}_j \bar{C} + \overline{u_j' c'}] + S = 0 \quad (1)$$

where the overbar signifies the mean value, superscript prime denotes deviation from the mean, \bar{U}_j is the wind field ($1 \leq j \leq 3$), \bar{C} is the mean concentration, and S is any source/sink term. The correlation $\overline{u_j' c'}$ is typically expressed in terms of an effective diffusion coefficient

$$\overline{u_j' c'} \approx K_{ij} \frac{\partial \bar{C}}{\partial x_i} \quad (2)$$

where K_{ij} is a (directional) diffusion coefficient. An initial condition corresponding to a concentrated or continuous release is

$$\bar{C}(x_i, t=0) = \bar{C}_0(x_i) \quad (3)$$

For mesoscale analysis, the solution domain is the three-dimensional space bounded by the topography, the mixed height, and a suitable box surrounding the release location. The coordinate transformation used to account for the terrain-lid variability is (Reynolds, et al, 1973)

$$\rho = \frac{x_3 - h(x_i)}{H(x_i, t) - h(x_i)}, \quad i = 1, 2 \quad (4)$$

where h and H are topography and lid parameters, respectively. Horizontal and lateral boundaries are transformed as

$$\eta_i = \frac{x_i - x_b}{x_o - x_b}, \quad i = 1, 2 \quad (5)$$

where $x_o(i)$ and $x_b(i)$ denote boundaries of x_i . Both η_1 and η_2 normalize the coordinate span of the ground plane. Hence

$$\begin{aligned} \frac{\partial}{\partial t} + \frac{\partial}{\partial t} + \frac{\partial}{\partial \eta_j} \frac{\partial \eta_j}{\partial H} \frac{dH}{dt} \\ \equiv \frac{\partial}{\partial t} + \Gamma_j(H, t) \frac{\partial}{\partial \eta_j} \end{aligned} \quad (6)$$

$$\begin{aligned} \frac{\partial}{\partial j} + \frac{\partial}{\partial \eta_k} \frac{\partial \eta_k}{\partial H} \frac{dH}{dx_j} + \frac{\partial \eta_k}{\partial h} \frac{dh}{dx_j} \\ \equiv [\Gamma_{jk}(H, x_j) + \Gamma_{jk}(h, x_j)] \frac{\partial}{\partial \eta_k} \end{aligned} \quad (7)$$

where Γ_j and Γ_{jk} are specified functions of their arguments and directly related to topography and lid parameters.

For a sloping topography, for example, Equation (7) takes the form

$$\frac{\partial}{\partial x_2} + \frac{\partial}{\partial \eta_2} + \frac{-\eta_3}{H-h} \frac{dH}{dx_2} + \frac{\eta_3-1}{H-h} \frac{dh}{dx_2} \frac{\partial}{\partial \eta_3} \quad (8)$$

Using Equations (6) and (7), Equation (1) becomes

$$\begin{aligned} \frac{\partial \bar{C}}{\partial t} + \Gamma_j(H, t) \frac{\partial \bar{C}}{\partial \eta_j} \\ + [\Gamma_{jk}(H, x_j) + \Gamma_{jk}(h, x_j)] \frac{\partial}{\partial \eta_k} [\bar{U}_j \bar{C} + \bar{u}_j' \bar{C}'] \\ + S = 0 \end{aligned} \quad (9)$$

The boundary conditions are specified as follows

$$x_3 = h(x_i) \quad - K_{ij} \nabla \bar{C} \cdot \hat{n}_h = f_o \quad (10)$$

$$x_3 = H(x_i, t) \quad - K_{ij} \nabla \bar{C} \cdot \hat{n}_H = 0 \quad (11)$$

$$x_i = x_o, x_b \quad - K_{ij} \nabla \bar{C} \cdot \hat{n} = 0, \quad \bar{U}_j \cdot \hat{n} > 0$$

$$(\bar{U}_j \bar{C} - K_{ij} \nabla \bar{C}) \cdot \hat{n} = \bar{U}_j C_o, \quad \bar{U}_j \cdot \hat{n} < 0 \quad (12)$$

where f_o is the mean flux of concentration at the surface (for puffs or plumes $f_o = 0$), \hat{n}_h is the

unit vector normal to the topographic surface while \hat{n}_H is the outward directed unit vector normal to the inversion lid surface; \hat{n} is the outward directed unit vector normal to the horizontal boundaries.

To account for deposition at the surface, the flux at the ground is expressed in terms of a deposition velocity, (Calder, 1968), as

$$p\bar{C} = V_g + K_{ii} \frac{\partial \bar{C}}{\partial x_i} \approx (1-r) K_{ii} \frac{\partial \bar{C}}{\partial x_i}, \quad i = 3 \quad (13)$$

where V_g is the actual settling velocity, p is the deposition velocity, and r is the reflection coefficient. Varying r from 0 to 1 simulates the effect of losses at the surface by deposition (Rao, 1976).

The three-dimensional wind field and diffusion coefficient distribution are required for solution of Equations (9)-(13). The winds are assumed to be known prior to solution of the equation set; the diffusion tensor is obtained from an empirical model — the off-diagonal terms are assumed to be negligible (in global coordinates).

In order to specify the wind field throughout the three-dimensional region, a subjective analysis and interpolation scheme is used to calculate a first-guess wind field based on available data, i.e., wind speeds and directions obtained from instrumented towers and NWS data. The mean velocity field is assumed parallel to the ground. A mass consistent wind field model is then used to calculate corrections to the interpolated wind vectors at each node point such that continuity is satisfied, i.e.,

$$\frac{\partial U_j}{\partial x_j} = 0 \quad (14)$$

Based on the techniques of Dickerson (1975) and Sherman (1977), a Sasaki variational statement is minimized to determine the mass-consistent correction to the initial velocity field. The Poisson equation of Lagrangian multipliers obtained from the Euler-Lagrange equations are solved by a three-dimensional strongly implicit procedure (Pepper and Harris, 1978). Only a few iterations are normally required for each time step. The velocity components are readjusted with the converged values of the Lagrangian multipliers. Direct solutions can also be obtained with cyclic reduction/fast Fourier transform techniques; this is presently being undertaken.

An O'Brien (1970) K-theory model is used in conjunction with similarity theory to determine the diffusion coefficient distribution (Yu, 1977, and Liu and Durran, 1977). Surface similarity theory is used to calculate K_{33} from the Monin-Obukhov universal relations with measured wind velocities and temperatures from an instrumented TV tower within the transition layer region ($x_3 \sim 60$ m). The O'Brien cubic profile is then used to calculate the vertical diffusivity above the transition layer region to the top of the mixing layer. This procedure was also used by Pepper and Kern (1978) to model atmospheric dispersion with linear finite element (chapeau functions) and cubic spline methods.

THE NUMERICAL MODEL

Equation (9) can be expanded and written in global coordinates as

$$\begin{aligned} \frac{\partial(\bar{Z}C)}{\partial t} + \frac{\partial}{\partial \xi} \left(\frac{U\bar{Z}C}{X} \right) + \frac{\partial}{\partial \eta} \left(\frac{V\bar{Z}C}{Y} \right) + \frac{\partial}{\partial \rho} (WC) = \\ \frac{1}{X^2} \frac{\partial}{\partial \xi} \left(K_x \bar{Z} \frac{\partial C}{\partial \xi} \right) + \frac{1}{Y^2} \frac{\partial}{\partial \eta} \left(K_y \bar{Z} \frac{\partial C}{\partial \eta} \right) + \frac{\partial}{\partial \rho} \left(\frac{K_z}{Z} \frac{\partial C}{\partial \rho} \right) + S\bar{Z} \end{aligned} \quad (15)$$

where the general tensor notation has been transformed to $x_1(\eta_1) \equiv \xi(x)$, $x_2(\eta_2) \equiv \eta(y)$, $x_3 = \rho(z)$, $X = x_a(1) - x_b(1)$, $Y = x_a(2) - x_b(2)$ and $\bar{Z} = H(x_i, t) - h(x_i)$, $i = 1, 2$.

The vertical velocity, W , is given as

$$W = w - U \left(\frac{\partial h}{\partial \xi} + \rho \frac{\partial \bar{Z}}{\partial \xi} \right) - V \left(\frac{\partial h}{\partial \eta} + \rho \frac{\partial \bar{Z}}{\partial \eta} \right) - \rho \frac{\partial \bar{Z}}{\partial t} \quad (16)$$

Equation (15) has been reduced by neglecting terms containing $\partial h / \partial \xi$, $\partial h / \partial \eta$, $\partial \bar{Z} / \partial \xi$, and $\partial \bar{Z} / \partial \eta$, as done by Reynolds, et al (1973). Equation (15) is split into two equations such that

$$\frac{\partial(\bar{Z}C)}{\partial t} + \frac{\partial}{\partial \xi} \left(\frac{U\bar{Z}C}{X} \right) + \frac{\partial}{\partial \eta} \left(\frac{V\bar{Z}C}{Y} \right) + \frac{\partial}{\partial \rho} (WC) - S\bar{Z} = 0 \quad (17a)$$

$$\begin{aligned} \frac{\partial(\bar{Z}C)}{\partial t} = \frac{1}{X^2} \frac{\partial}{\partial \xi} \left[K_x \bar{Z} \frac{\partial C}{\partial \xi} \right] + \frac{1}{Y^2} \frac{\partial}{\partial \eta} \left[K_y \bar{Z} \frac{\partial C}{\partial \eta} \right] \\ + \frac{\partial}{\partial \rho} \left[\frac{K_z}{Z} \frac{\partial C}{\partial \rho} \right] \end{aligned} \quad (17b)$$

Successive solutions to Equation (17) give the final solution at one time step.

The method of second moments (Egan and Mahoney, 1972) is used to solve Equation (17). The method calculates the zeroth, first, and second moments of the concentration within a mesh and then advects and diffuses the concentration by maintaining conservation of the moments. The moments correspond to the mean concentration, center of mass, and scaled distribution variance (moment of inertia), respectively, and are given by the relations

$$C_i^{n+1} = \sum C^n(\xi_i) \quad (18)$$

$$F_i^{n+1} = \frac{\sum C^n(\xi_i) F_i^n}{C_i^{n+1}} \quad (19)$$

$$\begin{aligned} (R_i^{n+1})^2 = \frac{\sum C^n(\xi_i) R_i^{n2}}{C_i^{n+1}} \\ + 12 \left[\frac{\sum C^n(\xi_i) F_i^{n2}}{C_i^{n+1}} - \left(\frac{\sum C^n(\xi_i) F_i^n}{C_i^{n+1}} \right)^2 \right] \end{aligned} \quad (20)$$

where ξ_i denotes the relative displacement of material within the i th cell and varies from -0.5 to +0.5 (corresponding to the left and right hand extreme boundaries of a cell); F_i is the first moment, and R_i is the second moment. For a simple rectangular mesh, the integrals are evaluated by summation for each grid element in terms of the concentration distributions of the

portions remaining and newly transported in for each successive time step. Figure 1 shows scaling parameters used to advect a distribution in one, two, or three dimension. For illustration, the transport of a single cell of concentration (peak value = 100) is shown in Figure 2 for two-dimensional advection. Note the single cell is advected without numerical dispersion or computational damping errors. Similar tests on hyperbolic equations including finite difference and finite element techniques are discussed by Long and Pepper (1976) and Baker, et al (1978).

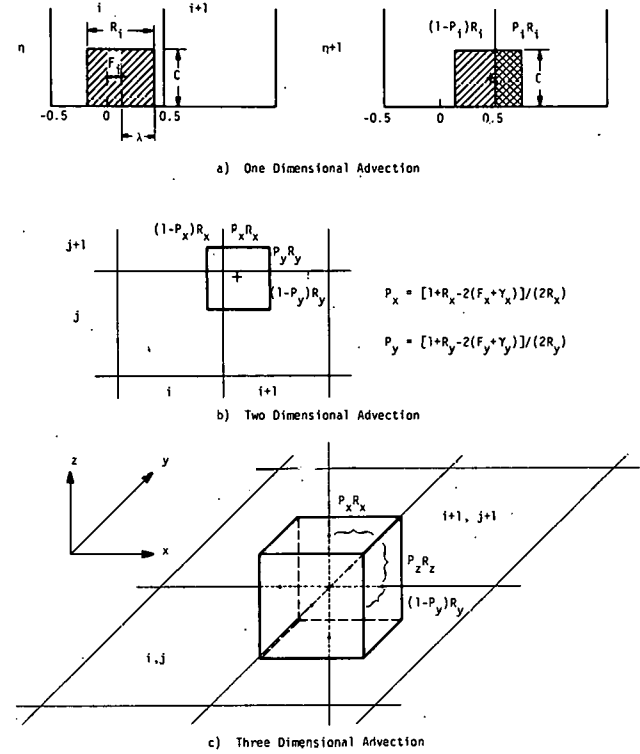


FIGURE 1. Scaling Parameters Used in the Advection of a Cell of Concentration

Equation (17b) is recast as an algebraic equation system using cubic spline interpolation to establish derivatives. For example, the equation

$$\frac{\partial C}{\partial t} - \frac{\partial^2 C}{\partial x^2} = 0 \quad (21)$$

is solved by letting $F = \frac{\partial^2 C}{\partial x^2}$ such that

$$\frac{\partial C}{\partial t} - F = 0 \quad (22)$$

F values are solved by the relation

$$\begin{aligned} \frac{\Delta x_i}{6} F_{i-1} + \frac{\Delta x_i + \Delta x_{i+1}}{3} F_i + \\ \frac{\Delta x_{i+1}}{6} F_{i+1} = \frac{(C_{i+1} - C_i)}{\Delta x_{i+1}} - \frac{(C_i - C_{i-1})}{\Delta x_i} \end{aligned} \quad (23)$$

where $\Delta x_i = x_i - x_{i-1}$ and $\Delta x_{i+1} = x_{i+1} - x_i$

A slightly different expression is obtained for first derivative values but the recursion relation still retains its tri-diagonal nature as in Equation (23). Equation (17b) can either be solved by time-splitting the equation into three one-dimensional relations, or solved with a tri-tri-diagonal algorithm (von Rosenberg, 1969) in an alternating direction sequence. The method of cubic splines was chosen in lieu of other methods (e.g., chapeau functions) because of its ability to easily accommodate variable grid spacing with minimal computational dispersion errors (Pepper and Kern, 1978) and ease in handling boundary conditions.*

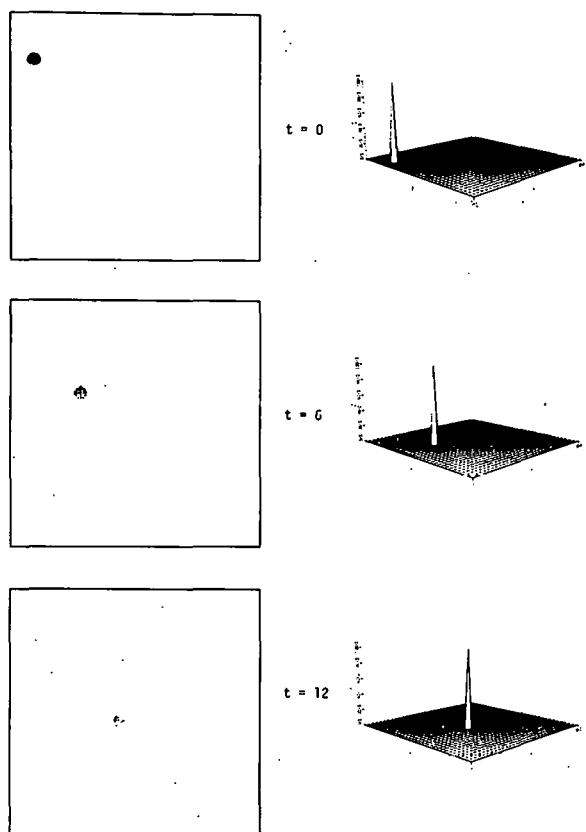


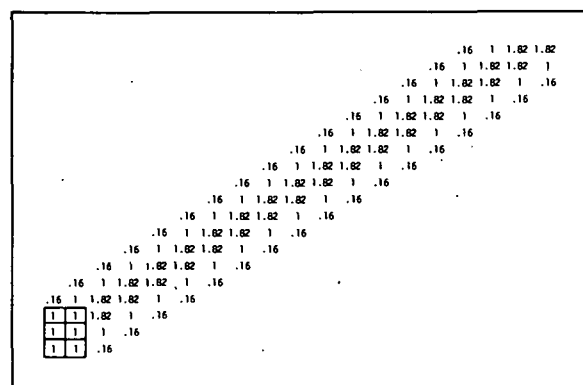
FIGURE 2. Advection of a Cell of Concentration ($C=100$) in Two Dimensions; $U=(1,-1,0)$, $\Delta X=\Delta Y=1$; $\Delta t=0.5$

NUMERICAL RESULTS

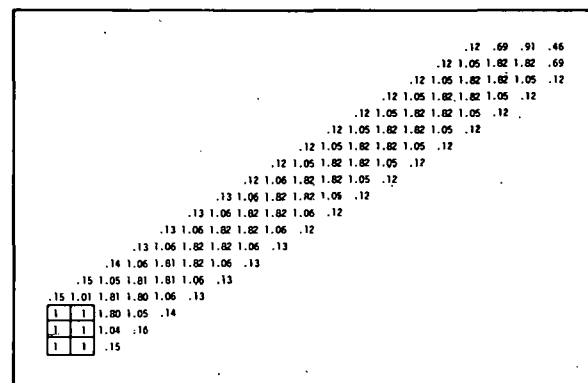
The computational domain normally consists of 10,890 cells; 33 cells in the longitudinal direction (ξ), 33 cells in the lateral direction (η), and 10 levels in the vertical direction (ρ). Mesh spacing can either be arbitrarily set (such as a telescoping grid network) or equally spaced with $\Delta \xi = \Delta \eta$. The vertical spacing is established between ground level values for topography and the height of the lid. User input values for the remaining levels, i.e., levels corresponding to instrumented tower locations, are automatically transformed to non-dimensional values such that $0 < \rho < 1$ throughout the computational domain.

* In instances where advection is the dominant means of transport, second order central difference techniques are adequate in representing the diffusion terms.

To assess model accuracy, the advection of a continuous area source was analyzed using a six cell source, each with a unit release advected in a two-dimensional constant wind field. Figure 3 compares numerical predictions to the analytical solution (Pedersen and Prahm, 1974). The results are nearly identical, with computed peak centerline values as well as the width of the plume accurately maintained. All remaining values in the computational domain are zero, in contrast to predictions using standard finite difference procedures (which tend to produce wider plume width and associated loss of centerline concentration). The numerical values are identical to those of Pedersen and Prahm (1974) obtained using a two-dimensional method of moments technique. In both cases, a width correction procedure has been used to eliminate small lateral dispersion at the plume edge.



Analytical Solution (Pedersen & Prahm, 1974)



Numerical Solution

FIGURE 3. Advection of an Area Source ($Q=1/\text{cell}$) $U=(1,1,0)$; $\Delta X=\Delta Y$; $\Delta t=0.5$

A test of two-dimensional advection-diffusion in the x - y plane is shown in Figure 4 for a continuous area source emission consisting of four cells each containing 250 units. Analytical results (assuming Fickian diffusion) were obtained by Christensen and Prahm (1976). Lateral diffusion (K_y) was set equal to $0.10 \text{ m}^2/\text{s}$ with $K_x = K_z = 0$. Advection occurred only in the longitudinal direction (ξ) with $U = 1 \text{ m/s}$, $V = W = 0 \text{ m/s}$. This test case was also analyzed by Christensen and Prahm (1976) with a pseudospectral method. Peak centerline values are predicted by the numerical model within 3 percent (average) of the analytical values. The lateral spread of concentration is nearly identical, deviating by only a few percent within each cell.

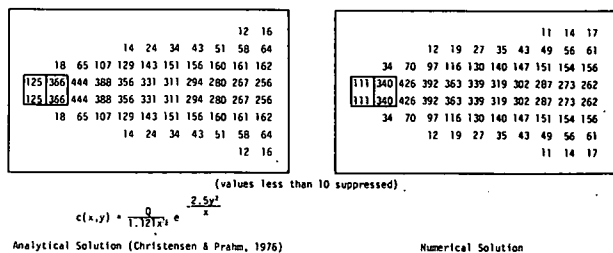


FIGURE 4. Advection-Diffusion from Four Sources ($Q=250/\text{cell}$); $U=(1,0,0)$; $K_y=0.1$; $\Delta x=\Delta y=1$ $\Delta t=0.5$

Dispersion of a continuous source over a hill is shown in Figure 5. The effect of source location and downwind dispersion pattern about bluff bodies has been analyzed by Hunt and Mulhearn (1973) and Brighton (1978). If the source is below the peak of the hill and the velocity light, part of the concentration will bifurcate around the hill (Figure 5a,b). When the source is at peak height or above, the ground level concentration is perturbed such that the maximum value occurs at peak height. As the wind velocity increases, entrainment of the concentration begins to occur in the wake of the hill (providing recirculation occurs). In these two tests, $K_y = 100 \text{ m}^2/\text{s}$ with neutral stability. Emphasis has not been placed on the appropriate turbulence diffusion coefficients (or methodology) but on the ability of the transformed moment/cubic spline code to portray physically realistic dispersion patterns. Other tests were conducted but are not shown because of space limitations. In order to visualize the spread of concentration about the hill, particles* are used to represent discrete amounts of concentration. The scatter of particles downwind of the hill is due to the perturbation of the wind field about the hill.

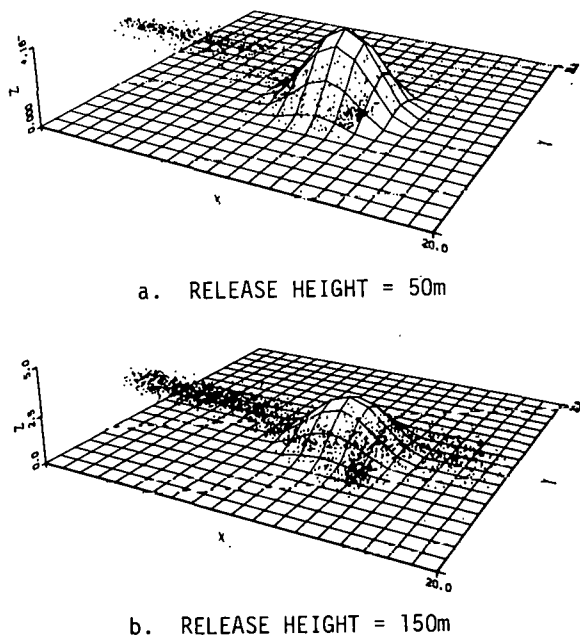


FIGURE 5. Dispersion Over a Hill; $Q=1\text{g/s}$; $K_z=f(z)$; $K_y=100 \text{ m}^2/\text{s}$

*Particles within each cell based on the total mass within each cell volume.

The effect of a series of surface irregularities on a continuous elevated emission is shown in Figures 6-7. Figure 6 shows the distribution of the ground plane, along with concentration isopleths and mass consistent wind field in the x - z plane of the computational domain. The continuous release occurs at a height of 200 m at the left-center cell denoted with a dot (Figure 6a). A 200 m peak surface elevation occurs 11 km downwind from the source. The height of the lid is kept constant at 650 m; grid intervals are $\Delta x = \Delta y = 1000 \text{ m}$ and $\Delta z = 100 \text{ m}$ (equally incremented). The source rate is equal to 1 gm/s and the atmospheric stability condition assumed neutral. The transport coefficients are $K_y = 33 \text{ m}^2/\text{sec}$ and K_z obtained from Pasquill stability curves at 1000 m distances (Slade, 1968). The initial velocity field is given as $\vec{U} = [5(z/0.2)^{0.14}, 0, 0] \text{ m/s}$. In Figure 6b, the length of an individual vector denotes the magnitude of the wind speed; the vertical scale is increased to enhance visualization of the small vertical velocities. The wind field is held constant after readjustment. Essentially steady-state concentration isopleths are shown in Figure 6c. For reference, Figure 6d illustrates centerline topography; maximum ground level concentration occurs at the peak elevation.

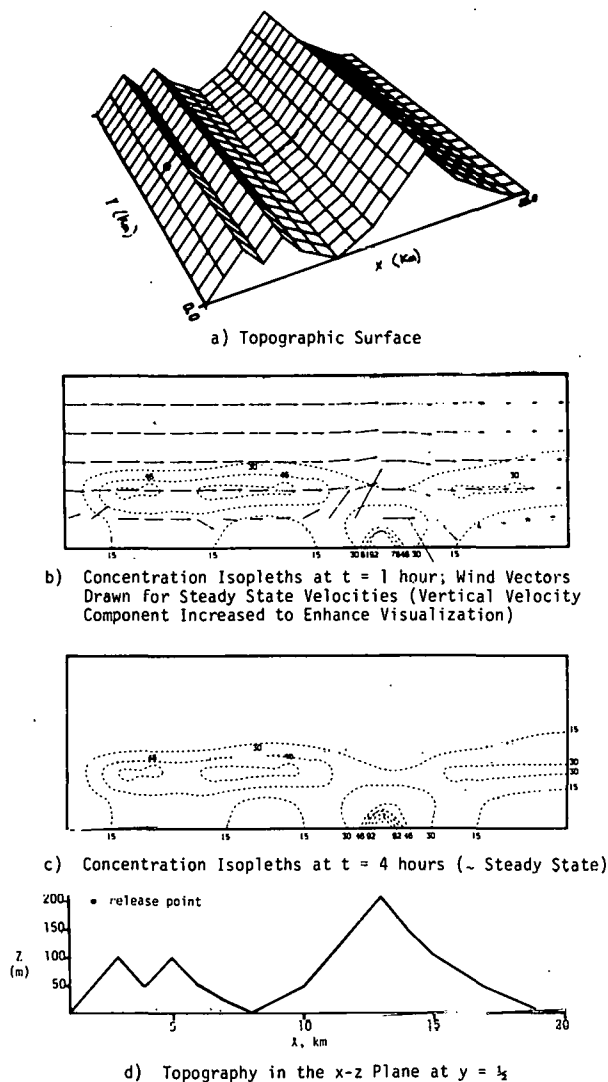


FIGURE 6. Concentration Isopleths in the x - z Plane at $n=1/2$ (Dotted Lines Denote C/Q Values in m^{-3})

For steady-state (non-varying winds and flat surfaces) concentration isopleths generally become smoothly distributed throughout the vertical plane. At this specific release height, the topography causes the vertical distribution to be perturbed at locations corresponding to surface peaks. A decrease in lid height also causes an increase in ground level maximum at peak height since the effective mixing region over the peak is decreased (Anthes and Seaman, 1976).

The effect of this topography is more evident in Figure 7 where ground level centerline C/Q values are plotted as a function of longitudinal distance. The computed solutions in both cases agree reasonably well with the Gaussian plume analytical solution adjusted for topography by Kao (1977).

Validation tests of actual releases of ^{85}Kr from the Savannah River Plant (SRP) for which experimental data are available are presently being undertaken. Data which has been accumulated over a two-year period consists of wind speeds and directions (from the seven tower network within SRP and the 330 m WJBF-TV tower), ground level concentrations at 13 receptor sites, source terms (combined) from the two release areas, vertical temperatures (TV-tower), and acoustic sounder records (inversion height determination). Detailed comparison will be presented at a later date, (Pendergast, 1977, 1978).

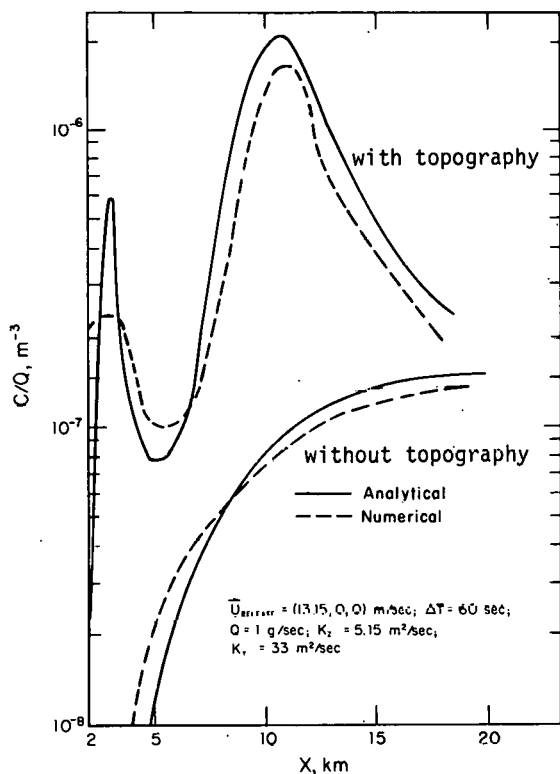


FIGURE 7. Ground Level Centerline C/Q Values With and Without Topography

CONCLUSION

A three-dimensional method of moments numerical solution algorithm has been used to predict pollutant advection within the environment. The algorithm employs a quasi-Lagrangian scheme to minimize numerical dispersion error, with the moment distribution providing sub-grid scale resolution. Cubic spline interpolation functions are used to calculate spatial derivatives appearing in the diffusion terms. Both techniques are computationally efficient and relatively easy to use. The technique of fractional steps is used to reduce programming complexity. Topography and variable lid height are incorporated into the model by transforming the governing equations. Either assumed wind field values or measured wind data are made mass-consistent by performing a Sasaki variational analysis over the entire mesh.

Model results agree with analytical solutions for simple releases over flat surfaces under ideal conditions. Similarly, the three-dimensional numerical results agree with steady state analytical results for ground level values over a horizontal variable terrain. However, the principle advantage of the three-dimensional model is its ability to calculate concentration values for variable wind conditions over complex terrain, with a minimum of numerical error.

The embedding of moment distributions within finite element basis functions is currently being investigated. Further generalization of the computer code is also being undertaken for use in water transport and engineering reactor problems.

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