A PUFF-ON-CELL MODEL FOR COMPUTING POLLUTANT TRANSPORT AND DIFFUSION

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Introduction

Most finite-difference methods of modeling dispersion have been shown to introduce numerical pseudodiffusion, which can be much larger than the true diffusion in the fluid flow and can even generate negative values in the predicted pollutant concentrations.[1] Two attempts to minimize the effect of pseudodiffusion are particularly notable. In the first, Sklarew[2] develops the particle-in-cell (PIC) method. In this method pollutant concentration is represented by the number of particles of an assigned unit pollutant strength. The particles are tracked in a Lagrangian frame, and their displacements during each time step are found by multiplying the time increment by the sum of the mean wind and diffusive velocities. The diffusive velocity is computed from the turbulent eddy diffusivity, the pollutant concentration, and the concentration gradient. The concentration in each grid volume is then calculated by dividing the total pollutant, represented by the particles present in the grid volume, by the grid volume.

Egan and Mahoney[3] developed a different type of numerical scheme. At each time step, after computing the Lagrangian transport, they calculate the first and the second moments of the pollutant concentration distribution in each of the grid volumes. The moments are then used to construct a weighting function for distributing the pollutant from the Lagrangian grid volume to its surrounding Eulerian grids, such that the first and second moments remain the same after the distribution.

The present paper replaces Sklarew's numerous particles in a grid volume, and parameterizes subgrid-scale concentration with a Gaussian puff, and thus avoids the computation of the moments, as in the model of Egan and Mahoney[3] by parameterizing subgrid-scale concentration with a Guassian puff.

Description of the Model

For simplicity in demonstrating the scheme, a one-dimensional diffusion equation will be used, i.e.,

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) , \tag{1}$$

where C is concentration, t is time, x is the spatial coordinate, u is the mean wind velocity, and D is eddy diffusivity. For an incompressible flow, the above equation can be written as

$$\frac{\partial C}{\partial t} + \frac{\partial (u + \xi) C}{\partial x} = 0 , \tag{2}$$

with

$$\xi = - \frac{D}{C} \frac{\partial C}{\partial x} . \tag{3}$$

Equation 2 implies that the pollutant elements in the flow can be considered to be traveling in a Lagrangian frame with an effective velocity of $u + \xi$, as suggested by Sklarew.[2] Consequently, if a volume of pollutant originally corresponding to an Eulerian grid volume is followed in a Lagrangian frame, the total mass is conserved and the problems of numerical instability and negative concentration are easily avoided. Figure 1(a) shows the change experienced by the pollutant in a grid volume in a conventional model. The pollutant concentration is uniform in the shaded grid volume. For each time step, the grid volume is advected for the distance of $u\Delta t$, and the boundary of the grid volume is expanded by the diffusive velocities ξ^+ and ξ^- on the right and the left sides of the volume, respectively. In terms of a finite-difference scheme, the diffusive velocities can be written as

$$\xi_i^+ = \frac{D_i + D_{i+1}}{(C_i + C_{i+1}) \Delta x} (C_i - C_{i+1}) \tag{4}$$

$$\xi_i^- = \frac{D_i + D_{i-1}}{(C_i + C_{i-1}) \Delta x} (C_i - C_{i-1}) . \tag{5}$$

Egan and Mahoney[3] compute the first and second moments of the Lagrangian grid volume and then distribute the pollutant in the Lagrangian grid volume back to the Eulerian grid volumes in such a manner that these moments are

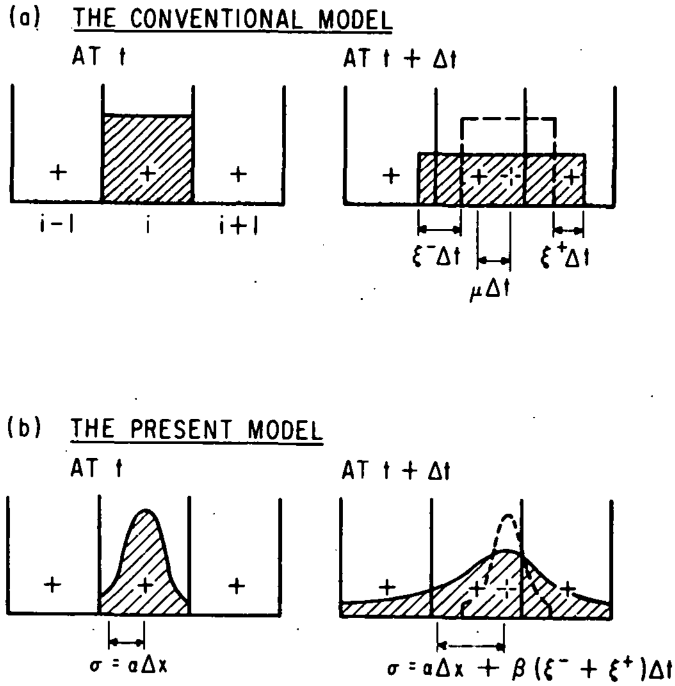

FIG. 1.--Graphical representations of the transport processes of (a) conventional and (b) the present models. Dashed lines are advection without diffusion, shaded areas are total concentrations, and σ is a standard deviation of Guassian distribution. (ANL neg. 149-76-176)

preserved. In addition to a uniform concentration distribution over the grid volume, other distribution functions capable of approximating their criteria could also be used. An obvious candidate is a Gaussian distribution function, which has the advantage that, if one uses it as a weighting function to distribute the pollutant in the Lagrangian puff to its surrounding, the moments will automatically be preserved.. Also, the Gaussian distribution approaches an asymptotic distribution function of the pollutant in the Lagrangian volume if the time increment in the numerical integration becomes very large and if there is no pollutant surrounding the Lagrangian volume. The proposed scheme of the present model is illustrated in Figure 1(b). The distribution functions of the pollutant concentration for an Eulerian grid volume (P') and its Lagrangian counterpart (P) are

$$P'(x_\ell, x_i) = \begin{cases} \exp\left\{-0.5\left[\dfrac{x_\ell - x_i}{\alpha\Delta x}\right]^2\right\} & \text{for } |x_\ell - x_i| \le \Delta x \\ 0 & \text{otherwise} \end{cases} \qquad (6)$$

$$P(x_\ell, x_i) = \begin{cases} \exp \left\{ -0.5 \left[\dfrac{x_\ell - (u\Delta t + x_i)}{\alpha \Delta x + \beta(\xi_i^+ + \xi_i^-) \Delta t} \right]^2 \right\} & \text{for } \ell = i-1, i \text{ and } i+1 \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

where α and β are constants relating the standard deviation of the Guassian distribution to the grid length and the displacement due to diffusion. These constants will be determined by calibrating the model against the analytical solution of pollutant dispersion from a continuous point source in a uniform flow. The time increment, Δt, should be determined with the criterion that the total displacement of pollutant element in one time step is smaller than the grid length as required in most of the numerical simulations. This constraint simplified computations by distributing the pollutant in the Lagrangian puff to only a few of the Eulerian grid points which surround the Eulerian grid point from which the Lagrangian puff originated. The pollutant concentration from the Lagrangian puff corresponding to the Eulerian grid is distributed according to the Gaussian weighting function to the Eulerian grid points i-1, i, and i+1 by

$$\Delta C^{t+1}(x_\ell, x_i) = \frac{P(x_\ell, x_i)}{\sum_{j=i-1}^{i+1} P(x_j, x_i)} C^t(x_i), \qquad \text{for } \ell = i-1, i \text{ and } i+1. \quad (8)$$

The final pollutant concentration at a point of interest, x_ℓ, is simply the sum of the contribution from the Lagrangian puffs, i.e.,

$$C^{t+1}(x_\ell) = \sum_{i=1}^{N} \Delta C^{t+1}(x_\ell, x_i) \qquad \text{for } \ell = 1, \ldots, N, \quad (9)$$

where N is the total number of Eulerian grid points.

The results of the numerical prediction for various combinations of α and β show that the set $\alpha = 0.5$ and $\beta = 0.6$ gives the best approximation to the analytical solution. The relative numerical and analytical concentration profiles at various time steps of the integration are shown in Figure 2. Since the plume is symmetric about its center line, only half of the profiles are presented. The results show that excellent agreement has been achieved.

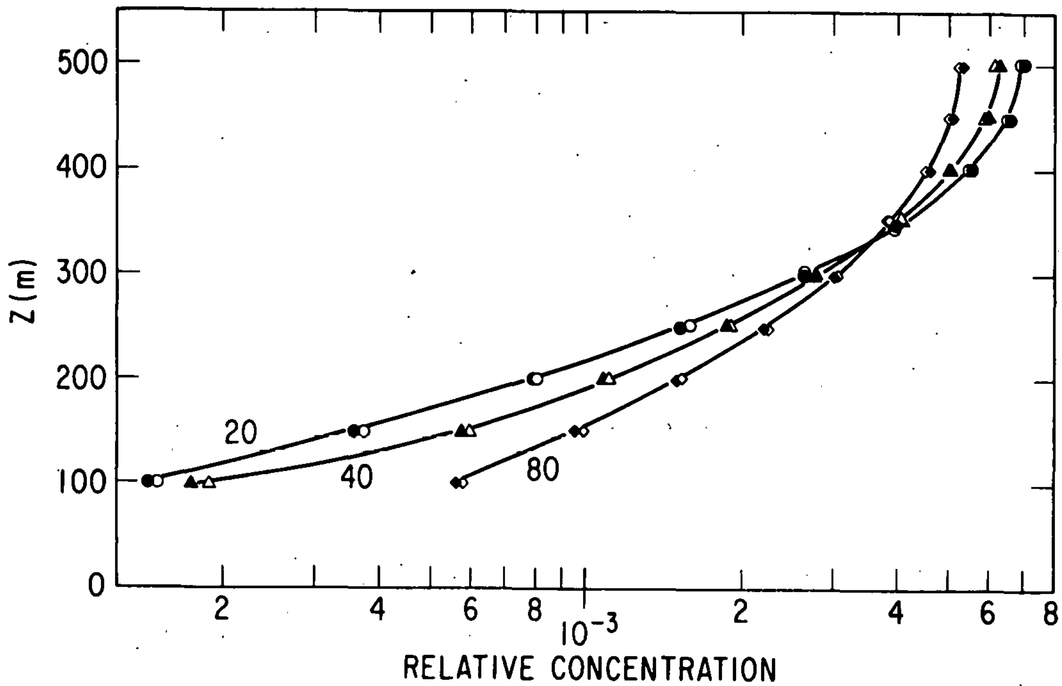

FIG. 2.--Comparison of the concentration profiles of the analytical results (solid) and the numerical predictions (open) of the optimal case $(\alpha, \beta) = (0.5, 0.6)$ at various time steps. (ANL neg. 149-76-177)

References

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