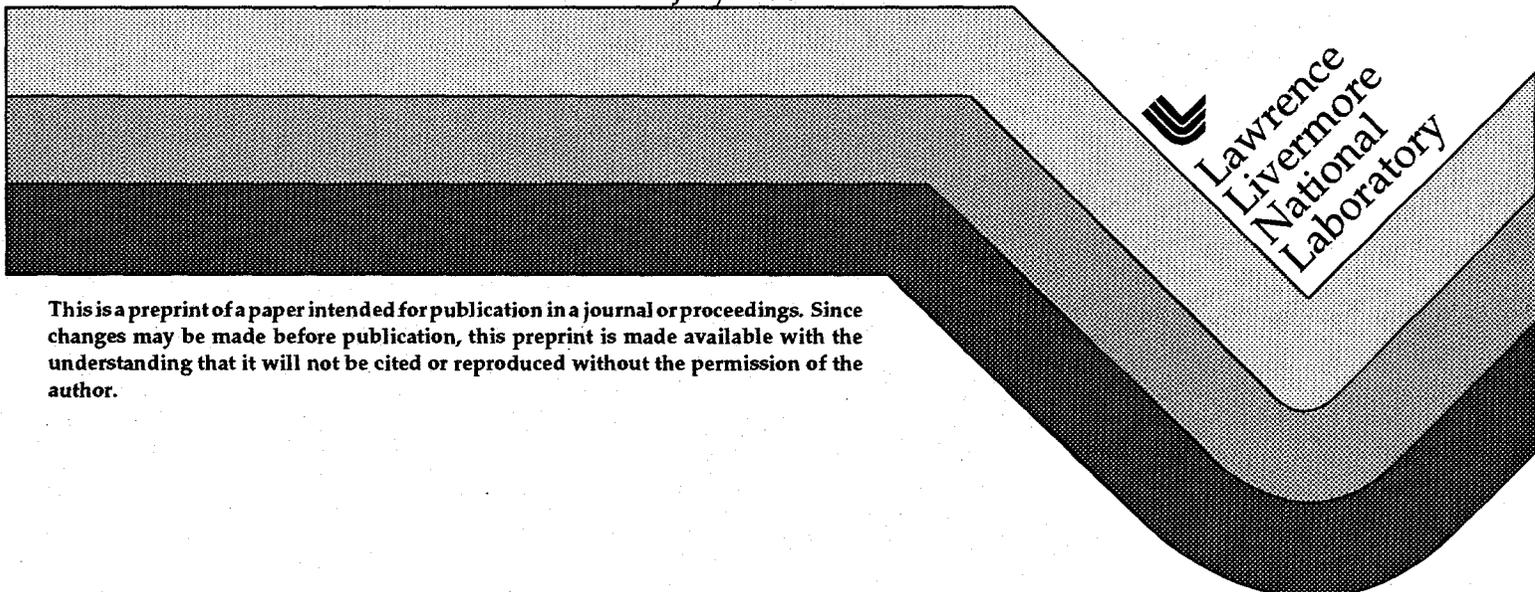


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NUMERICAL SIMULATIONS OF TURBULENT DISPERSION AROUND BUILDINGS VIA A LAGRANGIAN STOCHASTIC PARTICLE MODEL

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ABSTRACT

This paper describes a numerical modeling approach that can be used to provide estimates of air concentrations due to emissions at industrial sites or other sites where buildings may have an important impact on the dispersion patterns. The procedure consists of two sequential steps: (i) Prediction of mean flow and turbulence fields via a turbulent flow model; and, (ii) Employment of the calculated flow and turbulence fields to drive a Lagrangian Stochastic Particle Model. Two flow scenarios in which the approaching mean wind is assumed to be at 90° and 30° to the building complex are used as input to the Lagrangian model. The first calculation is based on an earlier transport and diffusion simulation that employed an existing particle-in-cell flux-gradient dispersion model. The second simulation is used to demonstrate the strong spatial variations that the concentration field exhibit within the highly complex separation zones of building wakes. The relationship between concentration levels and toxic load are discussed for the case of a chemical spill.

INTRODUCTION

There is a growing awareness that the traditional approaches to transport and diffusion modeling have limited application in complex situations (Barr and Clements, 1984). Typical examples are problems that involve dispersion around structures, topography, and difficulties in modeling turbulence over a wide range of atmospheric conditions. Perhaps the most widely used approach to dispersion modeling is the solution of an Eulerian advection-diffusion equation, in which the diffusion term is formulated from flux-gradient assumptions. The simplest of these dispersion models, the Gaussian plume models, are based on analytical solutions of this equation

assuming constant diffusion coefficients. Applications of these models are limited to rather idealized meteorological conditions. To overcome these restrictions numerical grid-based techniques have been widely used to solve the partial differential equations represented by the dispersion equations under a variety of environmental factors. However, other problems arise when such solution techniques are applied. They are exhibited in the form of artificial diffusion and uncertainties in the parameterization of subgrid-scale processes. It is well known that even the best numerical grid-based schemes deteriorate quickly as the pollutant sources become much smaller than the finest resolvable grid.

Particle models have become viable alternatives to Eulerian (grid) models for simulating transport and diffusion. This is a direct result of the increasing interest in the development of Lagrangian approaches for calculating turbulent dispersion (Lamb, 1980). Lagrangian models overcome some of the problems related to artificial diffusion, treatment of point sources and even the difficult closure problem that is inherent in Eulerian models. In a Lagrangian simulation, dispersion and concentration statistics are calculated by following the advection and diffusion of marker particles within a mean velocity field that is usually defined on an Eulerian grid. While the trajectories of the particles due to advection are determined from the specified velocity field, the diffusion portion of the particle motion can be computed by either deterministic or statistical formulations. The ADPIC model (Lange, 1978) uses a gradient-diffusion "K-theory" representation to define a pseudotransport velocity from the diffusion term that uniquely determines the positions of the particles at a given time. Alternatively, diffusion can be represented as stochastic processes and modeled by a Monte Carlo technique (Hall, 1975). Here, the trajectory of each particle is composed of a

random steps resulting from turbulent motion, with the mean distribution obtained by averaging over a suitable ensemble of paths. Of the two approaches, the gradient-diffusion model has the disadvantage that subgrid parameterizations must be used to calculate concentration gradients when the pollutant distribution cannot be resolved by the chosen grid. In contrast, the stochastic approach is essentially grid-independent and could be easily adapted to more complicated grid structures such as those that conform to complex terrain.

In this paper we discuss applications of a Lagrangian stochastic particle model to turbulent dispersion around buildings. The velocity field around a two-building complex is simulated by solving the Navier-Stokes equations containing a two-equation (k - ϵ) turbulence model. The resulting flow and turbulence field is used as input to a Lagrangian stochastic particle model. Such a modeling approach was reported in an earlier paper (Lee, 1994) except that a "K-Theory" gradient transport diffusion model was used. Differences in the results from the two modeling approaches are discussed.

THE FLOW MODEL

The governing equations for the flow model, FEMTKE, are based on the incompressible, Reynolds-averaged, Navier-Stokes equations coupled with a k - ϵ formulation for turbulence. The set of equations can be written in cartesian tensor form as:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(K_{\epsilon} \frac{\partial U_i}{\partial x_j} \right), \quad (1)$$

$$\frac{\partial U_j}{\partial x_j} = 0, \quad (2)$$

$$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_i} \left(\frac{K_{\epsilon}}{\sigma_k} \frac{\partial k}{\partial x_i} \right) + S - \epsilon, \quad (3)$$

$$\frac{\partial \epsilon}{\partial t} + U_j \frac{\partial \epsilon}{\partial x_j} = \frac{\partial}{\partial x_i} \left(\frac{K_{\epsilon}}{\sigma_{\epsilon}} \frac{\partial \epsilon}{\partial x_i} \right) + C_1 \frac{\epsilon}{k} S - C_2 \frac{\epsilon^2}{k}, \quad (4)$$

$$S = K_{\epsilon} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j}, \quad (5)$$

$$K_{\epsilon} = C_{\mu} \frac{k^2}{\epsilon}, \quad (6)$$

where U_i is the velocity, k the turbulent kinetic energy and ϵ the viscous dissipation. In the above equations, $P = p/\rho + 2/3k$ is the "pressure", with p being the dynamic pressure and ρ the density, $K_{\epsilon} = \nu + K_{\epsilon}$ is the effective diffusivity, and ν and K_{ϵ} are the laminar and turbulent diffusivities. The constants of the k - ϵ model C_{μ} , C_1 , C_2 , σ_{ϵ} , and σ_k are set to the standard values of 0.09, 1.44, 1.92, 1.0, and 1.3, respectively.

The FEMTKE model was developed specifically to simulate turbulent flows over surface-mounted obstacles. It uses a modified finite element technique to provide great flexibility in arbitrary grading of the mesh in order to economize on computational costs. While the standard Galerkin finite element formulation can be easily applied to very general meshes, it is also computationally expensive to use. In FEMTKE we employ a number of simplifications to the traditional finite element method to permit the code to be computationally affordable for three-dimensional problems.

Rather than solving the coupled set of momentum and continuity equations, the model uses a segregated approach in which the system is decoupled by using a consistent pressure Poisson equation in lieu of the continuity equation. The overall solution scheme begins with advancing the velocities in time (with the pressure gradient term omitted) via a forward-Euler algorithm to obtain a provisional velocity field. The provisional velocities are used in the Poisson pressure equation to calculate a time-consistent pressure field. To complete the cycle, the computed pressure field is evaluated with all other forcing terms in the momentum equations to generate the fully updated velocity field. This semi-implicit time integration scheme was first proposed and analyzed by Chorin (1968) and many variants of this algorithm have been used in the computation of incompressible flows.

A number of simplifications have been adopted in order to render the finite element approach more computationally cost-effective relative to competing finite difference approaches. More specifically we use: (i) Mass-lumping of the time derivatives; (ii) One-point quadrature in evaluations of the finite element integrals; and (iii) Pressure sub-cycling in which the pressure field is updated, based on stability and accuracy requirements, once every few timesteps. The numerical algorithms employed in the solution of the k - ϵ equations in the turbulence model are relatively standard. We use a forward-Euler scheme to update the turbulence field except for the source terms for the ϵ equation which are treated implicitly. In addition, a "clipping" algorithm is invoked to eliminate unrealistic values of the turbulence quantities and a wall layer is applied at solid boundaries. More details regarding the numerical procedures contained in FEMTKE can be found in Gresho, et al. (1984) and Lee (1994).

THE TRANSPORT AND DIFFUSION MODEL

The Lagrangian stochastic particle model (LSPM) is based on the Langevin equation which, in three dimensions, takes the form

$$du_i = a_i(x, u, t)dt + b_{ij}(x, t)dW_j, \quad (7)$$

$$dx_i = u_i dt \quad (8)$$

where x and u are the particle position and velocity; a is a function of x , u and t ; b is a function of x and t ; and dW_j are the increments of a vector-valued Wiener process with independent

components (Thomson, 1987). The increments dW_j are Gaussian with zero mean and variance dt ; increments dW_i and dW_j occurring at different times, or at the same time with $i \neq j$, are independent. The a_i and b_{ij} are determined by the following formulas:

$$a_i = -\left(\frac{C_0 \varepsilon}{2}\right) \delta_{ij} \Gamma_{jk} (u_k - U_k) + \frac{\phi_i}{g_a} \quad (9)$$

$$b_{ij} = (C_0 \varepsilon)^{1/2} \delta_{ij} \quad (10)$$

where $C_0 (= 5.7)$ is the universal constant associated with the Lagrangian structure function (Rodean, 1991); δ_{ij} is the Kronecker delta; Γ_{jk} is the tensor inverse of the Reynolds stress tensor component τ_{jk} . Thompson (1987) derived a functional form of ϕ_i/g_a that meets the well-mixed criteria but the formulation, in its expanded form, results in a total of 63 terms for each component.

This is clearly a nontrivial complication in the implementation of the three-dimensional Langevin model. To overcome this difficulty, we used a method of transforming the equations to a local streamline coordinate system as described in Näslund et al. (1994). This transformation simplifies Equation (9) into a form with substantially fewer number of terms and calculations can be more readily performed for three-dimensional problems.

The fields calculated by FEMTKE (mean wind - U, V, W ; turbulent kinetic energy - k and turbulent dissipation - ε) are all used as input to LSPM. However, since the Lagrangian particle model requires information on Reynolds stresses rather than the turbulent kinetic energy, the stresses are recovered from the mean fields using the following formulas;

$$\tau_{ij} = K_{te} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad (12)$$

$$\tau_{ii} = \frac{2}{3} k \quad (13)$$

where $K_{te} = C_{te} k^2 / \varepsilon$ is the eddy diffusivity defined according to the k - ε turbulence model.

It is important to note that the same grid system was employed in both the flow and dispersion calculations. In FEMTKE, like in most fluid dynamics calculations, variable gridding is used to resolve locations where strong gradients occurred. A variable grid algorithm has also been implemented in the dispersion calculations to move particles within a graded mesh. The computational cost for this more general "particle-pushing" algorithm is somewhat higher than that for a uniform mesh because a more complicated search strategy must be used in order to determine what subset of grid points must be used when a particle is moved.

In the paper by Lee (1994) the fields were interpolated to a regular grid as required by the particle-in-cell model, ADPIC (Lange, 1978). This leads to a loss of some fine details in the

fields which, as we will discuss later, can be crucial particularly in the regions where the distribution of particles are strongly influenced by the presence of fine-scale flow structures.

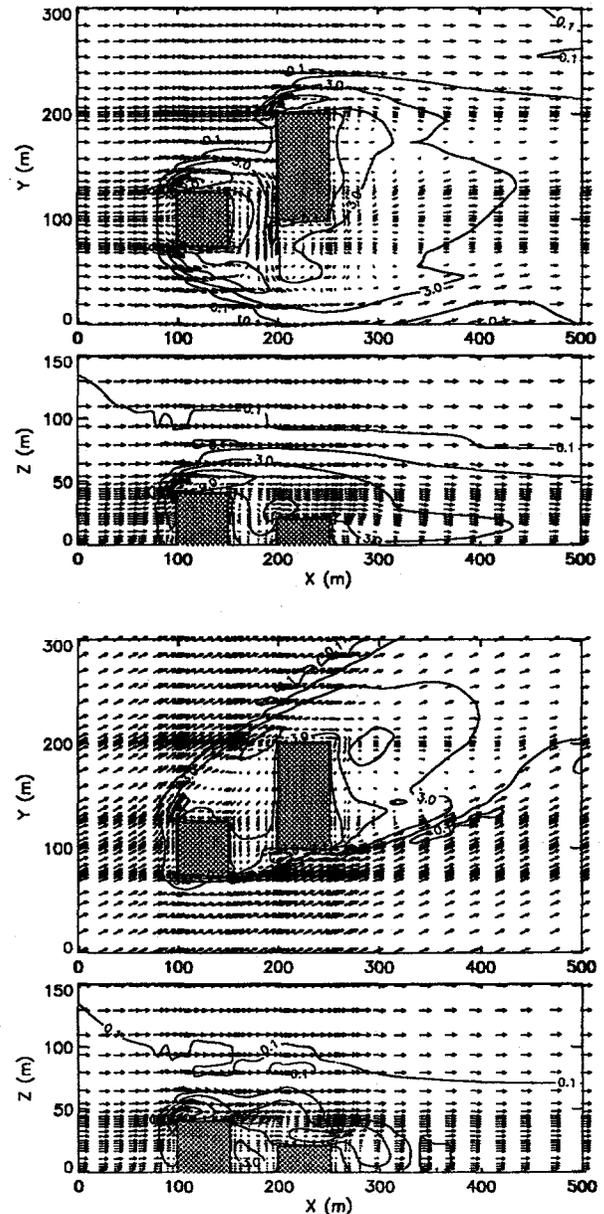


FIGURE 1: Velocity fields on the FEMTKE mesh. The two uppermost figures show velocity vectors for the 90° case while the two lower figures show the 30° case, both at two cross-sectional planes: $z = 10$ m (upper) and $y = 112$ m (lower). Contours plots for the turbulent kinetic energy at those planes are also displayed.

SIMULATIONS OF FLOW AND DISPERSION AROUND BUILDINGS

In this section we discuss simulations of flow and dispersion around a two-building complex using FEMTKE to generate the mean wind and turbulent fields and employing the resulting fields in the stochastic particle model. Two buildings with dimensions $(l_x \times l_y \times l_z)$ of $50\text{m} \times 50\text{m} \times 40\text{m}$ and $50\text{m} \times 100\text{m} \times 20\text{m}$ are staggered 50m apart within a computational domain of $500\text{m} \times 300\text{m} \times 150\text{m}$. A graded finite element mesh of $49 \times 39 \times 23$ was used with fine resolution located near the solid boundaries. The atmospheric stability was assumed to be neutral with a steady mean wind based on a power-law profile given by $U = U_o(y/y_o)^\alpha$ where $U_o = 10\text{ m/s}$, $y_o = 40\text{m}$, and $\alpha = 0.1$.

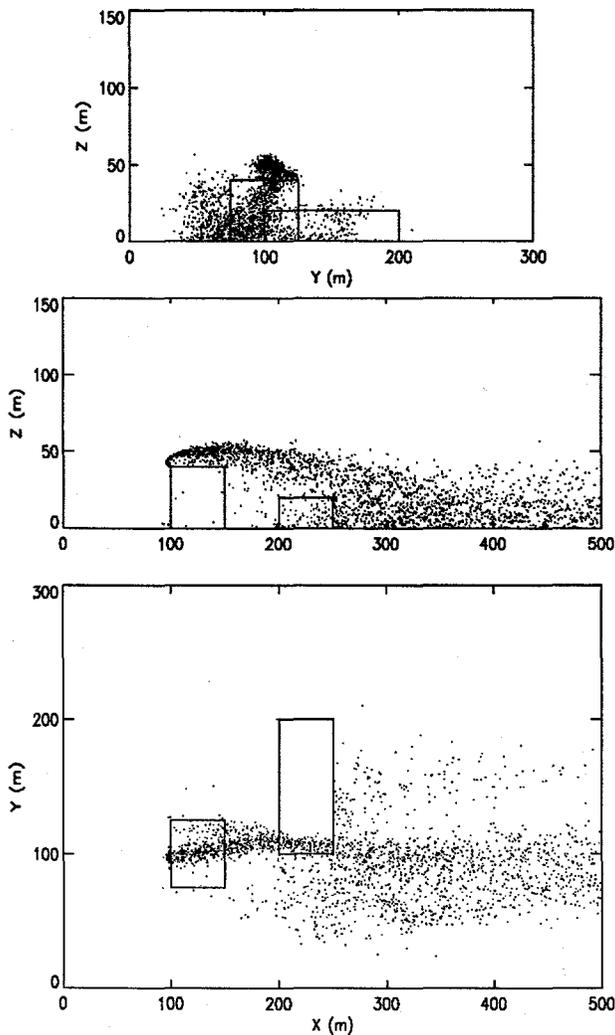


FIGURE 2: Particle concentration pattern 4 minutes after particles are released at source A. End view (upper); Side view (middle); Top view (lower).

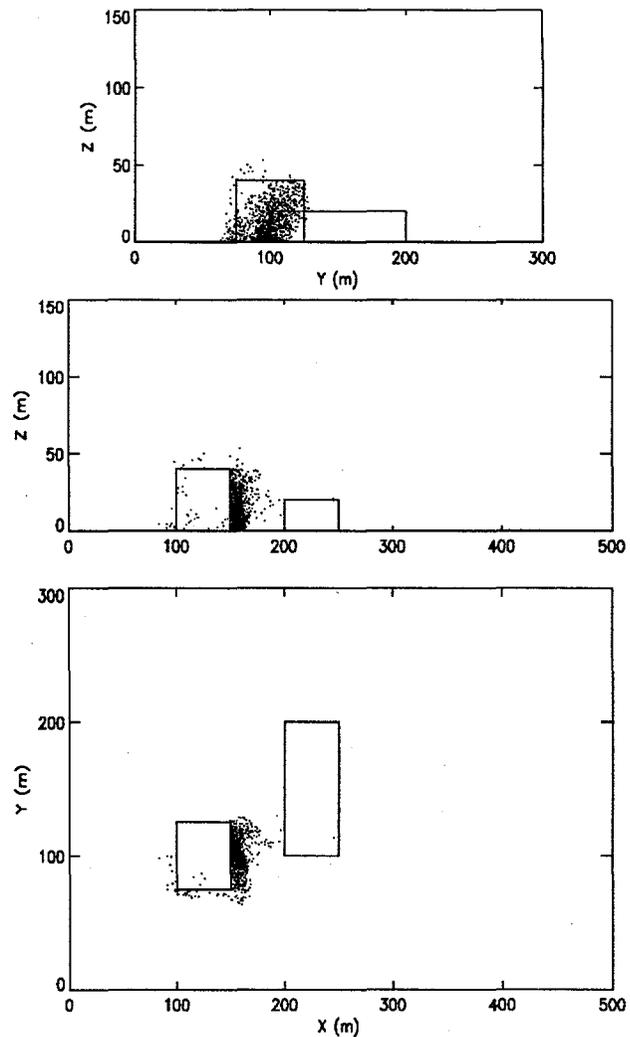


FIGURE 3: Particle concentration pattern 1 minute after particles are released at source B. End view (upper); Side view (middle); Top view (lower).

Two flow scenarios were considered, the first with a fixed incoming mean wind that was perpendicular to the buildings, and the second with the wind at approximately a 30° angle (see Figure 1). In both cases, computations of the flow were terminated when the resulting fields were effectively at steady-state. More details regarding the first flow simulation can be found in Lee (1994). All flow parameters were maintained for the second simulation with the incident mean wind at 30° except that the inflow and outflow boundaries were now specified at the appropriate inflow and outflow faces of the rectangular computational domain. As noted earlier, an important difference between the simulations here and those reported by Lee (1994)

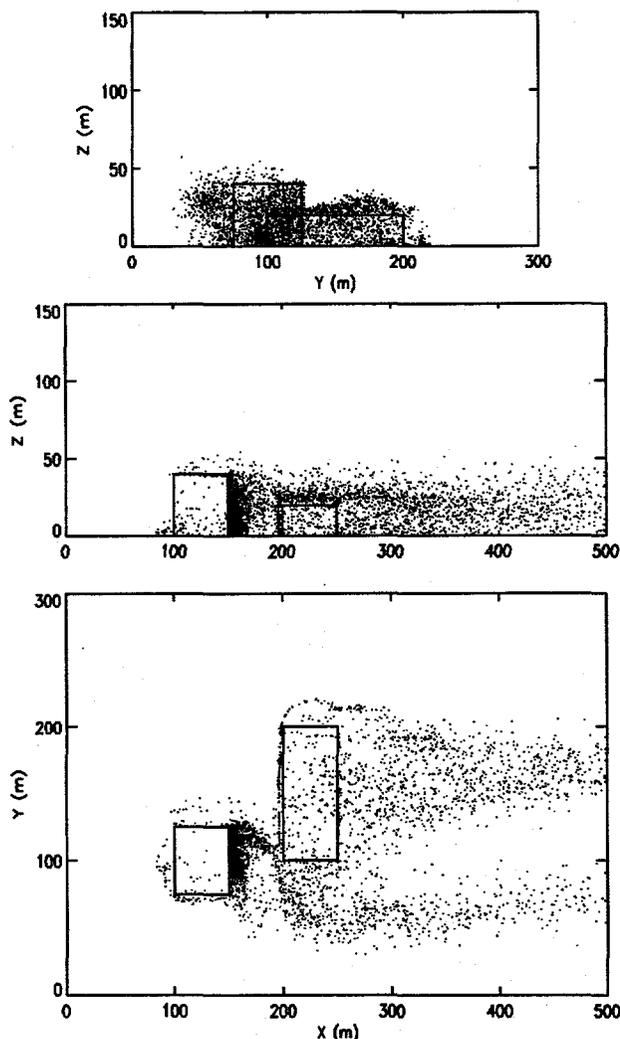


FIGURE 4: Particle concentration pattern 5 minutes after particles are released at source B. End view (upper); Side view (middle); Top view (lower).

is the manner in which the computed winds were transposed into the dispersion calculations. In the earlier paper the wind results were interpolated into a somewhat smaller domain with uniform grid spacing which, while increasing the efficiency of the particle calculations, will result in a smoothing of the fine structures of the computed field. The current calculations employed the original flow grid system in the dispersion computations and the full resolution of the computed wind field was maintained for the stochastic particle calculations.

Two precomputed velocity fields with the mean wind at 90° and 30° were used in the dispersion calculations. For the 90°

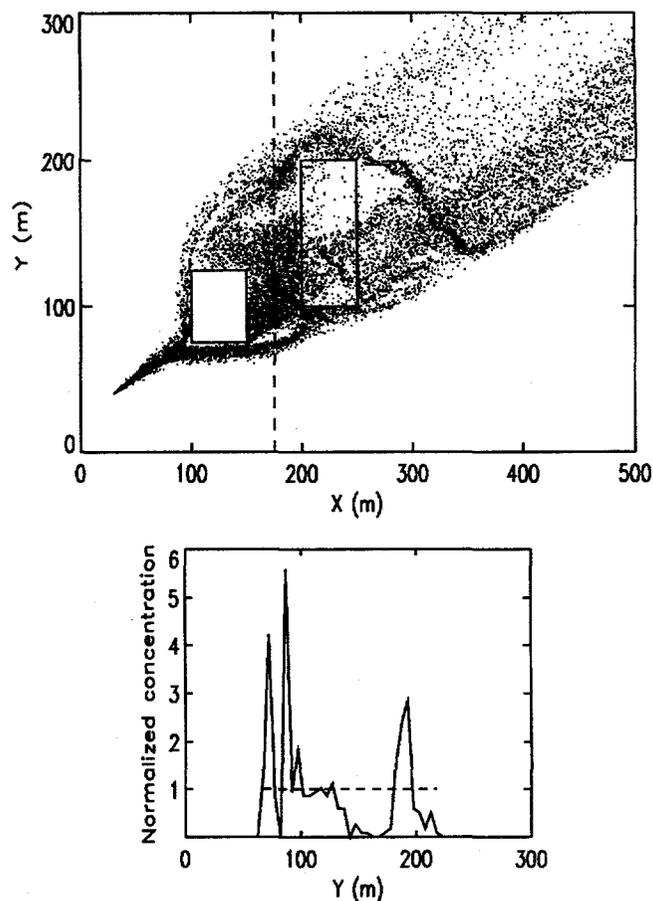


FIGURE 5: Particle concentration pattern 10 minutes after particles are released at source C (upper fig.). The dash line depicts the cross-section where the ground level concentration (shown in lower fig.) is calculated. The average plume concentration is normalized to 1.

case the same source positions as in Lee (1994) were used in order to compare the dispersal patterns between the gradient diffusion and stochastic models. The sources were located at (100m, 100m, 40m), for source A and at (162m, 100m, 4m) for source B. For the 30° case we show results from a single release at source C (30m, 40m, 4m), upwind of the building complex, to illustrate that the resulting concentration pattern can be strongly inhomogeneous within highly complex flow regimes.

Figure 2 shows particle concentration patterns from the 90° case (source A). These patterns are similar to the results presented by Lee (1994) using an interpolated, equally-spaced, grid together with a particle-in-cell model (ADPIC). The main differences are caused by the occurrence of smaller horizontal diffusion near the source. This is not surprising since ADPIC initially uses a Gaussian diffusion distribution near the source location until particles are sufficiently spread out over the grid. Also, in the earlier simulation, diffusion was parameterized via a

gradient-flux formulation whereas, in the current simulation, FEMTKE generated turbulence fields are used in conjunction with the stochastic particle model.

Figures 3 and 4 show particle concentration patterns from release at source B. Here the differences are more pronounced. While Lee (1994) exhibited a pattern where the major part of the plume passed the second building at the south-side the present results depict a significant part of the plume passing over that building. Although this may seem unusual at first, more close inspection of the fine structure of the wind field reveals that there is a recirculation eddy that induced an upwind drift of the particles immediately behind building one. Particles released at source B initially move in southeasterly direction. When these approach building 1 the mean wind veers due to recirculation to a northerly-upwind direction and a large fraction of the particles are "lifted" over building 2. This scenario demonstrates the crucial role that fine structures of the flow play in the dispersion processes and how interpolation of the velocity field can change

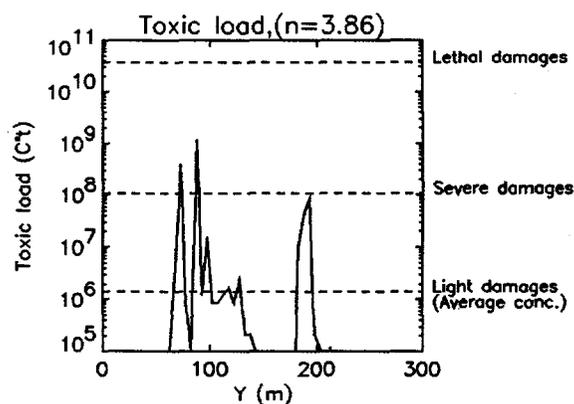


FIGURE 6: Toxic load, (C^t), from a 1 minute integration of the concentration shown in Figure 5. The average plume concentration is assumed to correspond to a level where nitrous gases may cause light damages to a human ($\approx 40 \text{ mg/m}^3$).

the results of the simulation. In some cases this may be of little significance (as in the source A release), whereas in other cases the particle patterns will be quite different.

Figure 5 shows a particle concentration pattern from the 30° case (source C) as well as the calculated ground level concentration at a cross-sectional cut between the buildings. These figures illustrate the significant concentration variations that may occur at a site with non-uniform wind and turbulence. Since the toxic effect on humans is a nonlinear function of concentration, i.e.,

$$\text{Toxic load} = \int C^n dt \quad (14)$$

where n often is a factor larger than 1 (CPR 16E, 1992), the effect of a non-uniform concentration can result in a significant increase in toxic levels. We illustrate this effect by calculating the Toxic Load corresponding to a mixture of nitrous gases (NO , NO_2 , N_2O_4 , etc) which has an exponential factor $n = 3.86$ (Anjemo et al. 1994). Those gases can be generated when nitric acid comes in contact with organic substances and metals. Let us assume that the average plume concentration would give a 5% risk of light damages when a human is exposed to the fumes within the plume for one minute. Figure 6 shows the spatial distribution of the toxic load at a cross-section between the two buildings. We note that, although health risks are minimal at the average plume concentration, peak concentrations that are generated at specific locations can result in toxic loads which are sufficiently high to cause serious damage to humans.

CONCLUSIONS

We have presented simulations of turbulent dispersion around a two-building complex with diffusion modeled by a Lagrangian stochastic particle technique. The dispersion model required velocity and turbulence fields that were generated from a Navier-Stokes flow model. Dispersion patterns from single point sources released at various locations near the complex show strong perturbations that were caused by the bifurcation of the mean flow around the buildings. In particular, fine structures of the mean flow play important roles in the distribution of the particles within the regions of most interests, those being the areas near the structures. We also demonstrate that, in the event of a toxic release, significant variations of concentration levels with consequences on health risks can occur under conditions of non-uniform wind and turbulence.

ACKNOWLEDGMENTS

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