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DEVELOPMENT OF A BUILDING WAKE/STACK
HEIGHT NUMERICAL MODELING CAPABILITY

A PROGRESS REPORT

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SUMMARY

We are developing state-of-the-art numerical tools which can be used to provide reliable estimates of potential emissions at various LLNL sites. In particular we have focused our efforts in generating models which can simulate the wind flow and dispersion of airborne pollutants around surface-mounted structures such as buildings or building complexes. To achieve this goal, we have adopted two different but complementary approaches in the modeling of this complex problem. The first approach employs a Reynolds-averaged set of equations whose solution results in a description of the mean flow and concentration pattern. In the second approach, we are developing a more advanced model based on the large eddy simulation (LES) concept. The building flow calculations made with an LES model will provide more detailed information on the time-dependence of the mean flow along with the local turbulent fluctuations.

In this report, we describe the progress in the development of the two approaches. We begin by discussing the calculational procedure which has been chosen for the Reynolds-averaged model, namely: (i) Prediction of the mean flow via a turbulent flow model, and; (ii) Employment of the calculated flow field to drive a particle-in-cell transport and diffusion model (ADPIC). The performance of this model is benchmarked against experimental data obtained for flow over a backward-facing step. The backward-facing step problem can be viewed as a simplification of a rectangular-shaped surface mounted obstacle. Some results for the more practical case of simulating flow and dispersion over an idealized three-dimensional building are also presented.

We next include a brief description of the LES method, the continuum and discretized LES equations, the numerical methodology, and some preliminary flow calculations. As with the Reynolds-averaged model, the backward-facing step is used to benchmark the LES model development. The first set of calculations are the result of exercising the existing code for laminar flow over the step for the purpose of method and code verification without the complication of a turbulence model. Preliminary LES results have also been generated for a simplified subgrid-scale model. The results are in agreement with the calculations of other researchers. We conclude by discussing several improvements which will be considered as we continue the development of both the Reynolds-averaged and the LES models.

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1. INTRODUCTION

Prediction of the transport and dispersion of air pollutants around structures is of interest in environmental applications ranging from the assessment of roadway emissions within street canyons to the siting of containment enclosures for limiting the spread of accidental releases of hazardous gases. However, the fate of the pollutants within these settings is greatly complicated by the presence of multiple obstructions such as buildings, trees and wall barriers. Estimates of the concentration patterns are usually obtained by either collecting field samples of the air pollutants, physical modeling in wind tunnels, or, by numerical modeling. While the first two experimental procedures have been employed extensively, in recent years, numerical models have been used increasingly in extending experimental results, or in many instances, in place of experiments. For the past 10 to 12 years, the mesoscale and fluid dynamics modeling group in G-Division has been developing finite-element-based numerical models to simulate three-dimensional spills of dense gases and atmospheric boundary layer flows over complex terrain. In addition, the division has developed an operational capability (ARAC) whereby a time-varying wind field can be used to drive a particle-in-cell-based transport and diffusion model (ADPIC) to predict the fate of pollutants that are released into the atmosphere. The maturity of these numerical tools are at a level that, with modifications, they can be applied to problems associated with building wakes and stack heights as they influence pollutant transport.

Perhaps the most widely used models for estimating pollutant transport and diffusion are Gaussian-type dispersion models. They are simple to use and there are many years of experience supporting these particular techniques. The development of Gaussian-type dispersion models has reached a level of sophistication such that they are now routinely used as assessment tools for regulatory agencies as well as for many industries. Although these simplified models can be applied with reasonable confidence to pollutant transport within unidirectional flows (such as those over relatively flat terrain), they are less useful for situations where the flows are more complicated. For example, flows over complex terrain or separated flows around obstructions and building wakes are situations where Gaussian dispersion models cannot be applied. In this project, we are focusing our attention on developing the advanced modeling tools which are useful for predicting transport and diffusion for this class of flows.

2. PROJECT GOALS

This modeling effort is motivated by the increase in concern about environmental safety and health issues both on a local and national level. We anticipate a growing need for having in place validated models which can be used to respond quickly to environmental questions, much like the manner ARAC responds to emergencies related to nuclear accidents. Our purpose in this project is to develop such modeling tools.

There are two major goals which we wish to accomplish with this project. First, we will develop a capability, via state-of-the-art numerical tools, which can provide accurate estimates of potential emissions at various LLNL sites. Secondly, we will use this capability to develop

a database for benchmarking simpler models such as Gaussian dispersion models. Although these Gaussian dispersion models are used routinely, we know that they can provide reasonable assessments in only a limited number of situations. We hope to use the advanced models we are developing to provide some insight as to what class of problems the simple models can be applied to and for what problems the advanced models are required.

3. MODELING APPROACH

One of the major challenges of the building wakes project is to accurately model atmospheric flows around buildings. The flow pattern around an arbitrarily-shaped building is very complicated and may require extremely fine resolution for modeling of the flow field. For purposes of testing our models and to build an expertise in modeling this class of problems, we have chosen to first simulate the flow and dispersion over structures which are represented by simple, isolated, rectangular blocks. Even these relatively simple structures depict flow patterns that are turbulent and filled with unsteady motion that are relatively difficult to calculate. To illustrate the complexity of such flows, Figure 1a shows perhaps the simplest pattern within this class of fluid motion which is given by a two-dimensional (2D) laminar steady-state flow pattern over a rectangular infinitely long block. One can think of this as a crude analog of a 2D building. The flow is reasonably complicated with a small corner vortex at the upwind face, a separation streamline starting at the upwind edge, and a recirculating zone terminating with a reattachment point behind the block. Because the flow is 2D, fluid particles which originate from within the recirculating zone cannot move across the separation streamline and are confined to move in closed paths within the zone. If the speed of the incoming wind is high enough such that the flow becomes turbulent, the motion becomes unsteady and the vortices near the downwind faces peel off the surfaces. These vortices are transported downwind forming a turbulent wake. Pollutants that are emitted within the turbulent wake reach ground level almost immediately due to turbulent mixing. The flow pattern for a 3D cubical block is even more complicated (Figure 1b). Separation zones can be present on all surfaces with a main cavity zone exhibited behind the block. Fluid particles within the separated zones no longer move in closed paths but spiral around in corkscrews and the upwind faces of the block generate vortex systems which persists far downstream of the block. The 3D wake pattern is significantly more complicated than its 2D analog. When the flow involves multiple blocks, multiple eddies are formed which will interact with each other within the wake region.

Figure 2 depicts schematically how these types of flow patterns can significantly influence the transport and dispersion of pollutants which are generated in its vicinity. Depending on the height of the plume, it may proceed downwind as though there is no wake present. It may drift to a level in which the trajectory is deflected but not yet entrained into the wake. In another situation, the plume may be partially or completely entrained into the wake. The final case is one in which the pollutants will be transported to ground level in the immediate vicinity of the source. In these types of worse case scenarios, it is extremely important that the recirculating eddies associated with the wake region be simulated as accurately as possible. Moreover, it is unlikely that Gaussian-type dispersion models can predict realistically the concentration pattern

resulting from such a flow.

We have adopted two different but complimentary approaches to the modeling of this complex flow and dispersion problem. To achieve the near term goal of providing a usable model for assessment purposes, we modified and extended a standard Reynolds-averaging formulation which was developed for simulating atmospheric flows and dispersion of pollutants over complex terrain. This model has been developed and is currently being benchmarked against results of other models as well as experiments. Although this standard approach is widely used and has been successfully applied to a variety of engineering and atmospheric applications, there are a few limitations which must be considered. For example, the temporal-averaging procedure, which forms the basis for the Reynolds-average approach, precludes detailed information concerning instantaneous peak-to-peak values of the time-varying fields (e. g., concentrations) which may be one of the important determining factors regarding health effects. Such instantaneous (intensely fluctuating) data can only be obtained from more advanced turbulence modeling based on either a direct approach (i.e., calculating all scales of turbulence directly without resorting to any turbulence models) or Large-Eddy Simulation (LES) approach (simulating large eddies directly with subgrid-scale processes modeled). Of the two approaches, LES is the only one which is computationally feasible for the practical problems of interest here and is the one which we are actively pursuing. In conjunction with the Reynolds-averaged model, we have proceeded to develop an advanced turbulence model based on an LES formulation. Although this model is expected to be computationally expensive and cannot be used routinely for assessment calculations, we plan to exercise the model for special situations where important physics need to be understood or when fine details of the turbulence structure must be simulated. We also plan to use the model for benchmarking studies and to provide a testbed for developing improved turbulence models for the computationally simpler Reynolds-averaged formulation.

A majority of the numerical models which are developed for calculating turbulent flows over surface-mounted obstacles are based on finite volume or finite-difference techniques (Paterson and Apelt 1990, Murakami 1990). In contrast, the Reynolds-averaged and LES flow models that we are developing use a modified finite element method (FEM). The mesoscale modeling group of G-Division is one of the leading groups in the application of finite element techniques to atmospheric flows. Over the past 15 years we have exploited the accuracy and flexibility of this numerical technique to develop a suite of models ranging from simulating the dispersion of heavier-than-air gases (Chan 1984) to complex terrain flows within the atmospheric boundary layer (Lee and Leone 1988). In the next sections, we will discuss details of our approaches for the Reynolds-averaging and for the LES models.

4. FLOW AND POLLUTANT TRANSPORT MODELING

4.1. The Reynolds-averaged Model

The calculational procedure which we have chosen for the Reynolds-averaged model consists of two separate steps, namely: (i) prediction of the turbulent wind field and (ii) employment of the calculated wind field to drive a transport-dispersion model. It is well known

that external flow past non-streamlined bodies is usually very complex, exhibiting separation and reattachment regions, high pressure gradients and turbulence levels, and unsteadiness. The flow can be simulated on the computer by numerically solving the incompressible Navier-Stokes/Boussinesq equations using any of a variety of parameterizations to represent turbulence. The approach which we employed is to solve the Reynolds-averaged Boussinesq equations with turbulence represented via a k-ε formulation (Ferziger 1990). This particular turbulence model has been applied extensively to many classes of flows including those which are influenced by buoyancy, stratification, and rotation effects. It has a good reputation for reliability and is also computationally economical compared to more complex models. The flow model is identical in algorithms to our FEM Planetary Boundary Layer model except that two additional equations are required for the turbulence model and a "building-block" specification is used to represent structures for computational efficiency.

Since pollutant releases near building structures often involve relatively concentrated multiple sources (e.g., point sources), it is important that the transport and dispersion model be able to treat this class of releases. The Atmospheric Diffusion Particle-in-Cell (ADPIC) model which was developed as part of the U.S. Department of Energy's Accidental Release Advisory Capability (ARAC) for emergency responses to accidental pollutant releases is used for the transport-dispersion phase of the calculations. This mathematical model is based on the particle-in-cell technique with the concentration represented statistically by Lagrangian marker particles imbedded in an Eulerian mesh (Lange 1978). The code was originally developed for studying instantaneous or continuous releases over regional scales from 10 to 200 km but has been adapted to the smaller scale problems of interest here. We next summarize briefly the two numerical models which, in concert, form our predictive system.

4.1.1. FEMTKE, The Flow Model

The Continuum Equations. The partial differential equations which are employed in the flow model are the incompressible, Reynolds-averaged, Boussinesq equations with turbulence modeled via a k-ε formulation. These equations are given in the form:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(K_t \frac{\partial u_i}{\partial x_j} \right) + g_i [1 - \beta(\theta - \theta_p)]; \quad i, j = 1, 2, 3 \quad (4.1.1)$$

$$\frac{\partial u_j}{\partial x_j} = 0, \quad (4.1.2)$$

$$\frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{K_t}{\sigma_T} \frac{\partial \theta}{\partial x_j} \right), \quad (4.1.3)$$

$$\frac{\partial k}{\partial t} + u_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{v_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) + v_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} - \epsilon, \quad (4.1.4)$$

$$\frac{\partial \epsilon}{\partial t} + u_j \frac{\partial \epsilon}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{v_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_j} \right) + c_1 \frac{\epsilon}{k} v_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} + c_1 (1 - c_3) \frac{\epsilon}{k} \frac{v_t}{\sigma_T} \frac{\partial \theta}{\partial x_i} g_i - c_2 \frac{\epsilon^2}{k}, \quad (4.1.5)$$

where u_i is the i^{th} component of the velocity vector, θ is the temperature, k and ϵ are the turbulent kinetic energy and viscous dissipation, respectively. For buoyancy-induced flows, the additional parameters are gravity (g_i), volumetric expansion coefficient (β) and mean temperature (θ_p). In the above equations, the "pressure" P , K_t , and turbulent diffusivity v_t are defined by:

$$P = \frac{p}{\rho} + \frac{2}{3} k, \quad K_t = \nu + v_t, \quad v_t = c_\mu \frac{k^2}{\epsilon},$$

with p being the dynamic pressure, ρ the density, and ν the laminar diffusivity. For the present calculations, c_μ , c_1 , c_2 , c_3 , σ_k , σ_ϵ and σ_T are set to 0.09, 1.44, 1.92, 0.8, 1.0, 1.3 and 0.9, respectively.

Boundary Conditions. In typical problems simulated by this model, the boundary layer flow of interest is "semi-confined" whereby the lower boundary is a solid wall with obstacles protruding out from the surface. The remaining lateral and top surfaces can exhibit inflow and/or outflow through their boundaries. In accordance with the normal practice of not attempting to resolve the laminar wall layer, the computational domain is displaced a short distance, h , away from all solid walls. The "slip" tangential velocity along the wall boundaries is computed by applying the following conditions:

$$u_n = 0, \quad K_t \frac{\partial u_{\tau 1}}{\partial x_n} = \frac{u_{\tau 1}}{|u|} u_*^2, \quad \text{and} \quad K_t \frac{\partial u_{\tau 2}}{\partial x_n} = \frac{u_{\tau 2}}{|u|} u_*^2 \quad \text{for the velocities}$$

$$\text{and} \quad \frac{\partial k}{\partial n} = 0 \quad \text{and} \quad \epsilon = \frac{(c_\mu^{1/2} k)^{3/2}}{\kappa h} \quad \text{for the turbulence quantities}$$

where x_n , $x_{\tau 1}$, $x_{\tau 2}$ and u_n , $u_{\tau 1}$, $u_{\tau 2}$ are the coordinates and velocity components normal and tangential to the wall boundary (κ is the Von Karman constant and $|u|$ is the magnitude of the velocity). The friction velocity u_* is obtained from the log-law velocity profile:

$$u_{\text{wall}} = \frac{u_*}{\kappa} \ln \left[9 \frac{h (c_\mu^{1/2} k)^{1/2}}{\nu} \right].$$

The values of u , k , and ϵ are specified at the inflow plane with zero normal gradient and/or no-penetration conditions applied where appropriate at the lateral boundaries. At outflow

boundaries, a finite-element-based "traction" outflow condition is used which permits the flow to leave the computational domain smoothly (Lee and Leone 1989).

The Finite Element Procedure. Equations (4.1.1) through (4.1.5) are spatially discretized by the finite element technique in conjunction with the Galerkin method of weighted residuals. The dependent variables are approximated as:

$$f(x,y,z,t) = \sum_{k=1}^n \phi_k(x,y,z) f_k(t) \quad \text{with } f = u, v, w, \theta, k, \text{ or } \epsilon$$

$$P(x,y,z,t) = \sum_{k=1}^m \psi_k(x,y,z) P_k(t),$$

where in the discretized domain there are n nodes for the prognostic variables (u , θ , k and ϵ) and m nodes for the diagnostic variable P . The basis functions $\phi_k(\mathbf{x})$ and $\psi_k(\mathbf{x})$ are piecewise polynomials. For simplicity, ϕ is chosen to be tri-linear (in three dimensions) and Ψ is piecewise constant. A coupled set of first-order ordinary differential equations is generated by premultiplying each prognostic equation with the appropriate basis functions and integrating the pressure terms by parts. For numerical convenience, the continuity equation is replaced with a consistent Poisson equation for pressure. Thus the resulting system of matrix equations which has to be solved are given by:

$$M\dot{u} = -CP - [N(u) + K]u + f,$$

$$(C^T M^{-1} C)P = C^T M^{-1} \{ -[N(u) + K]u + f \},$$

$$M_s \dot{\theta} = -[N_s(u) + K_s^\theta] \theta + S_\theta,$$

$$M_s \dot{k} = -[N_s(u) + K_s^k] k + S_k - M_s \epsilon,$$

$$M_s \dot{\epsilon} = -[N_s(u) + K_s^\epsilon] \epsilon + S_\epsilon - \alpha M_s \frac{\epsilon}{k},$$

where u is a vector containing all velocity components, M , K , and N are the lumped-mass diffusion and advection matrices, C is the pressure gradient matrix with its transpose C^T denoting the divergence matrix, and the remaining vectors represent the various source terms. The subscript "s" denotes an appropriate submatrix associated with the scalar variables. More details of the formulation together with the form of several of these matrices can be found in Gresho, et al (1984).

The time-integration scheme used for integrating the prognostic equations is the explicit forward Euler method, except for the pressure, which must be computed implicitly. The pressure

solutions are calculated by doing an LU factorization of the pressure matrix, $C^T M^{-1} C$, once and performing a forward-reduction and back-substitution with a new right-hand-side whenever a new pressure is required. Rather than computing the pressure solution at every timestep, a calculational procedure has been developed whereby the pressure is only occasionally updated based on a preset time truncation accuracy requirement. This method of pressure subcycling is very cost effective especially for 3D solutions developing towards steady-state conditions.

Numerical Aspects Of The Turbulence Model. It is well known that solutions of k and ϵ often exhibit negative values in conjunction with numerical oscillations. Such oscillations typically occur when the grid Reynolds number is large (resulting in steep field gradients) or when turbulence levels are low (when k and ϵ values are near zero). In addition to being unphysical, even very small negative values of k and ϵ can lead to an unstable solution in time since negative turbulence diffusivities may be generated.

To avoid numerical instabilities, a "clipping" procedure which readjusts the values of k and ϵ is introduced in the model. More specifically, the negative (or near zero) values are clipped whenever they are found to be less than one-thousandth of the maximum field values at each timestep. Also, unrealistically large K_t 's are eliminated whenever a preset maximum value is exceeded by readjusting ϵ . This particular clipping strategy has been employed successfully in a widely-used finite-element-based model called FIDAP (Haroutunian and Engleman 1989). Finally, the time-integration algorithm is further stabilized by treating the source terms in the k and ϵ equations implicitly. The source terms can be made implicit by simply linearizing and grouping the coefficients with the appropriate lumped-mass vectors thus requiring effectively no increase in computational costs.

4.1.2. The Dispersion Model

The Interface Utility. Because of the differing grid structures in ADPIC, the dispersion model, and the finite element wind field model, it was necessary to develop a utility program to act as an interface between the two models. The function of this program is to read in output information from the finite element model and to construct the appropriate input data for ADPIC. The input data includes a definition of a grid, a description of the terrain within this grid (ADPIC treats buildings as terrain), and wind components at each of these ADPIC grid points.

The ADPIC grid is constructed by first specifying a rectangular volume which may be a subdomain of the finite element computational domain. This volume is then divided into $(n_x \times n_y \times n_z)$ equal-sized cells with a subset of these being used to define the building. The cells representing the building are marked as impenetrable for the dispersion calculations.

Once the ADPIC grid is defined, the utility interpolates the FEM-generated wind fields onto the ADPIC grid. The standard finite element tri-linear basis functions are used for the interpolation calculation. Each above ground ADPIC node, (x_a, y_a, z_a) , is identified within the finite element grid in terms of the element E_a which contains it and its local coordinates (ξ_a, η_a, ζ_a) . The local coordinates are calculated by employing Newton's method to invert the tri-

linear isoparametric mapping:

$$x_a = \sum_{i=1}^8 \phi_i x_i, \quad y_a = \sum_{i=1}^8 \phi_i y_i, \quad \text{and} \quad z_a = \sum_{i=1}^8 \phi_i z_i$$

$$\text{where } \phi_i(\xi_a, \eta_a, \zeta_a) = \frac{1}{8}(1 + \xi_a \xi_i)(1 + \eta_a \eta_i)(1 + \zeta_a \zeta_i)$$

and the subscript i denotes evaluations at node i. With the element number and local coordinates of each ADPIC grid point known, the interpolated velocity field is calculated via:

$$u(x_a, y_a, z_a) = \sum_{i=1}^8 \phi_i(\xi_a, \eta_a, \zeta_a) u_i, \quad \text{where } u = (u, v, w).$$

For consistency, all velocities at grid points which are below terrain are assigned the value zero.

ADPIC. The Atmospheric Diffusion Particle-in-Cell (ADPIC) model is a three-dimensional, cartesian, particle-diffusion code capable of simulating the time-dependent distribution of air pollutants. The model solves the three-dimensional advection-diffusion equation in flux-conservative form. The solution method is based on the Particle-in-Cell technique with the pollutants represented by Lagrangian marker particles which are moved within a fixed Eulerian grid via the pseudo-velocity technique (Lange 1978).

The pseudo-velocity method is based on the following solution approach. Given the conservative form of the nonlinear transport-diffusion equation

$$\frac{\partial \chi}{\partial t} + \nabla \cdot (U_A \chi - K \nabla \chi) = 0,$$

where χ is a scalar concentration, K is the turbulent diffusion coefficient, and U_A is the advection velocity derived from the dynamic model, a pseudo-transport velocity U_P can be defined to be

$$U_P = U_A + U_D \quad \text{where} \quad U_D = -\frac{K}{\chi} \nabla \chi \quad \text{is a diffusion velocity.}$$

Thus, the equivalent equation which has to be solved is given by

$$\frac{\partial \chi}{\partial t} + \nabla \cdot (\chi U_P) = 0.$$

The ADPIC model employs an Eulerian grid of equal-sized cells with the concentration, χ , defined at the cell centers and the velocities, U_A , U_D , and U_P defined at the cell corners. The solution is advanced in time via the following steps:

- 1) An Eulerian step - for each cell corner, using the cell-centered concentration to calculate

- 2) U_D . The velocity U_D is added to U_A to obtain U_p .
 A Lagrangian step - for each Lagrangian particle its new coordinates are calculated via

$$R_{t+\Delta t} = R_t + U_p \Delta t$$

where R is the particle position vector and U_p is derived by linearly interpolating the cell corner values. A particle which has impacted a boundary during this step is reflected back into the domain if the boundary is solid. Otherwise, it is annihilated if the boundary is open.

- 3) The new cell-centered concentrations are calculated.
 4) If the final time has been reached the integration is terminated, otherwise we return to step 1 to repeat the process.

4.1.3. Benchmark Calculations in 2D

Our first attempt to evaluate the accuracy of the k- ϵ model (FEMTKE) was to perform calculations for turbulent flow over a 2D backward-facing step. This flow has been extensively simulated over the past two decades and excellent experimental data sets are available for comparison with numerical computations. Although the resulting flow pattern is not overly complicated, it nevertheless exhibit many features that are present within building wakes such as separation, reattachment, and recirculations. The flow geometry chosen for our calculations are based on the channel flow experiments of Kim (1980) with a developing channel flow approaching a step. The ratio of the upstream channel width to step height (H_c/H_s) is 2.0 (Figure 3). The Reynolds number based on the step height (H_s) and inlet maximum velocity (u_p) is 4.5×10^4 . The computational domain extends from three step-heights upstream of the step to 21 step-heights downstream. All domain boundaries are displaced 0.025 step-heights away from the solid boundaries to allow for imposition of the wall models. A fully-developed turbulent profile with values that matched Kim's experiments is assumed at the inlet plane. The model was integrated for 17500 timesteps at which time an approximate steady-state condition was reached.

Results of the simulations are shown in Figures 4 and 5. Figure 4 depicts the important field variables in the form of velocity vector plot and contour plots of k and ϵ . These are in close agreement with similar results from other numerical models. The steady-state streamline pattern is shown in Figure 5 in conjunction with a closeup view of the recirculation zone behind the step. Table 1 compares the dimensionless reattachment length x_R/H_s from the present calculation with those from several recent calculations and with Kim's experiment. We note that, whereas typical k- ϵ models exhibit reattachment lengths that are consistently below that from experiments, FEMTKE predicted a reattachment length of 7.0 which matched exactly with the average of the experimental results.

4.1.4. Computations of Flow and Dispersion over a 3D Building

Numerical simulations of the flow and dispersion over an isolated, three-dimensional,

rectangular building are presented here as an example of a practical application of the model. A building, with dimensions ($\ell_x \times \ell_y \times \ell_z$) of 50m $\times$ 100m $\times$ 20m is located within a computational domain 450m $\times$ 300m $\times$ 150m as shown schematically in Figure 6. The finite element mesh of 35 $\times$ 36 $\times$ 20 cells is graded such that the finest resolutions are located adjacent to the solid boundaries. A steady wind which is calculated from a power-law profile given by $u = u_o (y/y_o)^\alpha$ where u_o , y_o , and α are 5 m/s, 20m, and 0.1, respectively, approaches the building from the left. The free-stream Reynolds number based on the building height is approximately 6.7×10^6 and the atmosphere is assumed to be neutrally stable. At the inflow boundary, the profiles of k and ϵ are prescribed by the formulae $k = c_\mu^{-1/2} [\ell_m \partial u / \partial y]^2$ and $\epsilon = c_\mu k^2 [\ell_m \partial u / \partial y]^{-1}$ where $\ell_m = \min [ky, \kappa h_s]$, with h_s the height of the surface layer taken to be 50m. Slip-wall boundary conditions are used at all solid surfaces (with the grid standoff distance $h = 2.5$ m), a no-penetration boundary condition is applied at the top and lateral boundaries, and zero traction conditions are used at the outflow. The initial flow field is calculated by "mass-adjusting" (Gresho et al 1984) the one-dimensional power-law velocity field within the domain containing the building.

Figure 7a shows projections of the velocity vectors onto cross-sectional planes at the centerline and mid-height of the building after integrating 2000 timesteps ($\Delta t = 0.2$ s) at which time steady-state conditions are approximately established. The main features of the flow are the separation and recirculation zones immediately forward, above, and aft of the structure, and the symmetrical wake region which is developed downstream toward the outflow. Although the upwind recirculation cavity is relatively small, its downstream counterpart extends to a distance of over 8 building heights behind the building.

The computation of the dispersion from a source requires the FEM velocity field to be interpolated onto an equally-spaced ADPIC mesh with the building represented as terrain. The ADPIC mesh employed here has 40 $\times$ 37 $\times$ 20 rectangular cells within a somewhat smaller computational domain of 400m $\times$ 296m $\times$ 80m. The interpolated ADPIC velocity field for the cross-sectional planes at approximately halfway up the building height and the centerline is shown in Figure 7b. A near-surface source with a constant release rate of unity is placed at (20m, 148m, 7m), based on the ADPIC mesh coordinates, with particles released continuously throughout the integration period. As a first approximation, the K 's are derived from formulas which involve the horizontal (σ_h) and vertical (σ_z) standard deviations of the plume dimensions with values based on the Pasquill-Gifford curves (Slade 1968). In the absence of turbulence measurements, the Pasquill-Gifford prescription has been used extensively in many atmospheric diffusion models. The end (a), side (b), and top (c) views of the particle concentrations at 1 and 5 minutes after initiation of the release is depicted in Figures 8 and 9. At early time (1 minute), the particles are clearly seen to concentrate in the area near the forward stagnation point with a fraction of the total number being pushed up and above the top face of the building. At 5 minutes, the major part of the plume has already dispersed past the end of the domain but the particles which are caught within the back recirculation region are advected toward the backside of the building.

In the next example, the flow is assumed to approach the building at a 26 degree angle. For this simulation the wind enters the domain from *both* the left and rear lateral boundaries

while outflow occurs at the right and front lateral boundaries. The source location is now located at (25m, 225m, 7m), near the inflow corner. The same cross-sectional views for the flow and particle dispersion is depicted in Figures 10 and 11. In this case, the flow generated two relatively large recirculation zones at the rearward faces of the building (Figure 10a). Also, the unsymmetrical splitting of the flow due to the oblique wind direction resulted in a particle dispersion pattern which is quite different than that of the previous simulation. Here, the particles are dispersed over a somewhat wider area than when the approaching wind is perpendicular to the building.

4.2. The Large-Eddy Simulation Flow Model

4.2.1. Objective and Scope of Work

The wind flow around buildings is very complex and dependent on the building geometry, orientation, and proximity to other flow obstacles (e.g., trees and other buildings). Streamwise vortices are generated by flow obstacles and will shed and propagate downstream resulting in an unsteady flapping wake. The wakes from buildings in close proximity may interact increasing or decreasing the length or spread of a wake. In predicting the dispersion of airborne pollutants, around buildings, the critical and most difficult physics to model is the wind flow. The dispersion modeling is straightforward relative to the wind flow modeling. Accurate modeling of the wind flow is required if one wishes to determine the distribution and magnitude of pollutant concentration, including the maximum and minimum concentrations (i.e., concentration fluctuation) along with mean quantities. Accurate flow modeling is also required to determine with certainty the degree of plume spread or mixing. Thus, we are developing an advanced turbulence modeling approach which uses the large-eddy simulation (LES) method. With the LES method, the large eddies are directly simulated and the small eddies are modeled (i.e., approximated by semi-empirical/analytical relations). Some experts believe that the LES concept is the preferred approach for developing a more general application model (e.g., Ferziger 1990 and Wyngaard 1984). It provides a high degree of accuracy with a minimum of empiricism. The LES method should be capable of accurately predicting the flow for all building geometries and orientation and upstream flow conditions without the manipulation of parameters. The building flow calculations made with an LES model will show the time dependence of the mean flow (e.g., flapping of the building wake) along with local velocity fluctuations.

An LES model is being incorporated into an existing laminar, incompressible flow code that uses a finite element numerical approach. Unique to this research is the use of an LES model in conjunction with the use of a finite element numerical scheme. Most LES modeling has been performed with finite difference or spectral schemes. Thus, part of this research will require development of the finite element approach to insure the most efficient use of numerical resources.

As with the Reynolds-averaged approach, the backward-facing step (Figure 3) will be used as the benchmark problem for the LES model development.

In summary, the tasks to be completed in this research are:

- the development of an efficient and accurate finite element scheme for use with a large-eddy simulation and implementation into an existing laminar finite element code,
- application of current subgrid-scale models and possible improvements (described in Section 4.2.4),
- implementation (with some possible development) of wall models for three-dimensional separating flow (described in Section 4.2.5),
- verification and testing of the model for the case of a backward-facing step, and
- prediction of flow past a generic building (a cube).

The modeling schemes will be tested and verified by comparison to experimental data and other numerical predictions.

4.2.2. Method Description

Turbulent flow is stochastic (i.e., nondeterministic), three-dimensional, time-dependent, and contains structures called eddies with a wide range of scales (eddy sizes). These eddies are viewed as swirls of flow. The eddy sizes can range from the size of the computational domain to many orders of magnitude smaller and the spectrum of eddy sizes is continuous (Figure 12). The large eddies are responsible for energy transport. They are nonhomogeneous, anisotropic, and geometry dependent. The small eddies are responsible for energy dissipation. They are homogeneous, isotropic, and not geometry dependent and thus, are more universal. The term small eddies used here will imply all the eddies below a cutoff eddy size that display the characteristics of being homogeneous, isotropic, and not geometry dependent.

The LES approach is designed to take advantage of this turbulent flow characteristic. In an LES, the large eddies are resolved and the small ones are modeled. By restricting the averaging to small spatial regions, only the information on the small-scale fluctuations is removed. Thus, instantaneous results along with averaged results can be generated. (The averaged results are computed using the LES instantaneous results.)

The LES average can be regarded as a short-range filter (whereas the Reynolds average is a long-range filter). The large-scale motions which are solved for explicitly are called the resolved field and the small-scale motions which are modeled are called the subgrid-scale motion or residual field. The term subgrid scale comes from the grid-based method approach where the modeled small-scale motion is smaller than the grid size.

In theory, with the finite element method, various filtering schemes can be used, however, cell volume-averaging (or top-hat filtering) will exclusively be used here. (See McCallen 1991 for review of filtering options and justification for the top-hat filter choice).

With cell volume-averaging, the resolved field is defined by

$$\bar{f}(x,y,z,t) = \frac{1}{\Delta x \Delta y \Delta z} \int_{x-\frac{1}{2}\Delta x}^{x+\frac{1}{2}\Delta x} \int_{y-\frac{1}{2}\Delta y}^{y+\frac{1}{2}\Delta y} \int_{z-\frac{1}{2}\Delta z}^{z+\frac{1}{2}\Delta z} f(\xi,\eta,\zeta,t) d\zeta d\eta d\xi$$

where Δx , Δy , and Δz defines the size of the volume averaging over. Thus, using cell volume-averaging, the variable f can be decomposed into a resolved field, $\bar{f}$, and an SGS field, f' ;

$$f = \bar{f} + f'.$$

However, $\overline{f'} \neq \bar{f}'$, unless $f = \text{constant}$, and $\overline{fg} \neq \bar{f} \bar{g}$. It should also be noted that in general, $\bar{f'} \neq 0$.

4.2.3. Formulation of the Continuum Equations

For an incompressible flow with constant molecular viscosity the LES governing equations are

$$\begin{aligned} \frac{\partial \bar{u}_\alpha}{\partial x_\alpha} &= 0 \\ \frac{\partial \bar{u}_\alpha}{\partial t} + \frac{\partial}{\partial x_\beta} \overline{u_\alpha u_\beta} &= -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_\alpha} + \nu \frac{\partial^2}{\partial x_\beta^2} \bar{u}_\alpha \end{aligned}$$

where u_α is the instantaneous velocity field that has been decomposed into a resolved field, $\bar{u}_\alpha$, and a subgrid-scale (SGS) field, u'_α ($u_\alpha = \bar{u}_\alpha + u'_\alpha$), and $\bar{p}$ includes the gravitational body force potential.

For the velocity product we have, in expanded form,

$$\overline{u_\alpha u_\beta} = \overline{\bar{u}_\alpha \bar{u}_\beta} + \overline{\bar{u}_\alpha u'_\beta} + \overline{u'_\alpha \bar{u}_\beta} + \overline{u'_\alpha u'_\beta}.$$

The first term on the right can actually be explicitly computed (by using the solution from the previous time step), but it is commonly modeled. The last three terms in the velocity product

involve the residual field and must be modeled. Various ways of modeling these terms are briefly discussed below.

The equations of motion for the large-scale eddies are then

$$\frac{\partial \bar{u}_\alpha}{\partial x_\alpha} = 0 \quad (4.2.1)$$

$$\frac{\partial \bar{u}_\alpha}{\partial t} + \frac{\partial}{\partial x_\beta} \bar{u}_\alpha \bar{u}_\beta = -\frac{1}{\rho} \frac{\partial \bar{P}}{\partial x_\alpha} - \frac{\partial}{\partial x_\beta} (L_{\alpha\beta} + C_{\alpha\beta} + R_{\alpha\beta}) + \nu \frac{\partial^2 \bar{u}_\alpha}{\partial x_\beta^2} \quad (4.2.2)$$

where

$$\begin{aligned} \bar{P} &= \bar{p} + \frac{1}{3} \rho \delta_{\alpha\beta} \overline{u_\alpha u_\beta} \\ L_{\alpha\beta} &= \overline{\bar{u}_\alpha \bar{u}_\beta} - \bar{u}_\alpha \bar{u}_\beta \\ C_{\alpha\beta} &= \overline{u_\alpha \bar{u}_\beta} + \overline{\bar{u}_\alpha u_\beta} \\ R_{\alpha\beta} &= \overline{u_\alpha u_\beta} - \frac{1}{3} \delta_{\alpha\beta} \overline{u_\gamma u_\gamma} \end{aligned}$$

The modeling of nonclosed terms, $C_{\alpha\beta}$ and $R_{\alpha\beta}$, will be discussed in the following section. This form for the LES momentum equations is quite common, and is used for the calculations shown in Section 4.2.7 with a simplified SGS model (i.e., $L_{\alpha\beta} + C_{\alpha\beta} = 0$ and $R_{\alpha\beta}$ modeled).

An alternate form of the momentum equations (which will also be implemented in the code along with an improved SGS modeling approach discussed in the Section 4.2.4) is

$$\frac{\partial \bar{u}_\alpha}{\partial t} + \frac{\partial}{\partial x_\beta} \overline{\bar{u}_\alpha \bar{u}_\beta} = -\frac{1}{\rho} \frac{\partial \bar{P}}{\partial x_\alpha} - \frac{\partial}{\partial x_\beta} (\overline{u_\alpha \bar{u}_\beta} + \overline{\bar{u}_\alpha u_\beta} + \overline{u_\alpha u_\beta}) + \nu \frac{\partial^2 \bar{u}_\alpha}{\partial x_\beta^2} \quad (4.2.3)$$

where the term $\overline{\bar{u}_\alpha \bar{u}_\beta}$, has been brought over to the left side and has the form of a filtered advection term. Leonard (1974) showed that this advection term removes significant energy from the resolved scales and thus, it should not be lumped with the SGS terms (as is done with equation 4.2.2). This form of the momentum equation is consistent with the SGS modeling approach developed by Bardina et al. (1983) described in the following Section. The discretized form of this formulation will be described in Section 4.2.6.

4.2.4. Subgrid-Scale Models

By filtering the Navier-Stokes equation, we are discarding information and as a result, the filtered equations are not closed. The filtered advection term includes the SGS motion, u'_α , for which we have no closed equation. Thus, the SGS motion must be modeled (approximated).

Even though twenty years have passed since Deardorff's (1970) first LES modeling of a channel flow, very few advances in SGS modeling have occurred. Deardorff (1970) and Schumann (1975) applied the Reynolds-averaging assumption

$$\overline{u'_\alpha u'_\beta} - \overline{u_\alpha u'_\beta} + \overline{u'_\alpha u_\beta} + \overline{u_\alpha u_\beta} = 0$$

which effectively reduces the velocity product to

$$\overline{u_\alpha u_\beta} = \overline{u_\alpha u_\beta} + \overline{u'_\alpha u'_\beta}$$

Rogallo and Moin (1984) criticize this approach for the channel flow problem because the Reynolds-averaging assumption is applicable only to cell volume-averaging that is uniform over an unbounded homogeneous space. The assumption should not be applied to averages over bounded domains (Monin and Yaglom 1971, Leonard 1974). However, the resulting approximation is still used in current LES calculations (e.g., Murakami et al. 1987). As described below, this approximation is a simplified approach and easy to implement into the laminar code, but it has been shown by others to give results that compare well with experiment. The results shown in Section 4.2.7 apply this Reynolds-averaging assumption.

In using the Reynolds-averaging assumption, the only term that requires modeling is the SGS term, $\overline{u'_\alpha u'_\beta}$ (or $R_{\alpha\beta}$ in equation 4.2). We model this nonclosed term using the model of Smagorinsky (1963)

$$\overline{u'_\alpha u'_\beta} - \frac{1}{3} \delta_{\alpha\beta} \overline{u'_\gamma u'_\gamma} = -2 \nu_T S_{\alpha\beta} ,$$

where

$$S_{\alpha\beta} = \frac{1}{2} \left(\frac{\partial \overline{u}_\alpha}{\partial x_\beta} + \frac{\partial \overline{u}_\beta}{\partial x_\alpha} \right) ,$$

$\nu_T = (c\Delta)^2 (2 S_{\alpha\beta} S_{\alpha\beta})^{1/2}$, $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$, and c is a constant.

The Smagorinsky model is an eddy-viscosity model. The use of an eddy-viscosity model for the SGS terms usually produces the correct average energy removal from large eddies but poorly represents the effects of small eddies on large eddies. This random nonlinear interaction of the small eddies on the large eddies is called stochastic backscatter.

After completing the calculations with the Smagorinsky model, the improved but more complex model developed by Bardina et al. (1983) will be implemented. Bardina et al. (1983) include a separate model for the cross terms, $C_{\alpha\beta} = C_r (\bar{u}_\alpha \bar{u}_\beta - \bar{\bar{u}}_\alpha \bar{\bar{u}}_\beta)$, along with the Smagorinsky model for $R_{\alpha\beta}$;

$$\overline{u'_\alpha u'_\beta} + \overline{u'_\alpha \bar{u}_\beta} + \overline{\bar{u}_\alpha u'_\beta} = C_r (\bar{u}_\alpha \bar{u}_\beta - \bar{\bar{u}}_\alpha \bar{\bar{u}}_\beta) - 2 \nu_T S_{\alpha\beta}$$

The model for $C_{\alpha\beta}$ is based on the assumption that the modeled scales are structurally similar to the smallest resolved scales. We will use Bardina's model with the advection term explicitly calculated.

In summary, preliminary calculations have been performed with the Smagorinsky model and the Reynolds-averaged assumption, because of its reduced complexity and reduced computational requirements. Improvements will be made by incorporating Bardina's model and the explicit solution of the advection term into the code.

4.2.5. Wall Models and Inflow and Outflow Conditions

Much of the important physics of wall-bounded flows occurs at the wall region. To simulate the wall region 'exactly' requires the specification of a no-slip boundary condition, very fine discretization of the region, and the equations of motion must account for the low Reynolds-number flow close to the wall (e.g., the SGS stresses should asymptotically go to zero at the wall). The Stanford group (Moin et al. 1978, Moin and Kim 1981, Spalart 1988) has simulated wall regions as accurately as possible for simple (nonseparating) flows. They have generated three-dimensional movies of their simulations (Robinson 1989 and Robinson et al. 1989) which display streaks, bursts, and ejections in the flow. However, most researchers that are applying LES to more complicated geometries do use wall models (artificial boundary conditions) to represent the physics in the regions close to the wall (Deardorff 1970, Schumann 1975, Mason and Callen 1986). This is usually done by setting the instantaneous stress at the wall proportional to the tangential velocity at the first grid point away from the wall. The coefficient of proportionality can be described by either a logarithmic, power, or linear law-of-the-wall relation depending on the type of flow simulation and location of the first grid point relative to the wall. The normal velocity component at the wall is set to zero. With an LES, the approximate boundary conditions are applied everywhere on a plane surface parallel to the wall and are time dependent. For the Reynolds-averaged equations only a single averaged value is specified.

For high Reynolds-number flows in three dimensions with separation, it is not clear what wall models to use. The commonly used law-of-the-wall approximations are accurately known only for two-dimensional geometries and then only for attached flows. For example, Ruderich and Fernholz (1986) have shown that the logarithmic law-of-the-wall is not valid in recirculating flow regions. Reynolds (1989) also states that assuming that the law-of-the-wall is satisfied instantaneously is unlikely to be valid.

Some testing of wall models will be part of this research. It may be possible to test wall models in low Reynolds-number cases for the backward-facing step, by comparing experimental or direct simulation results to LES results where the wall region is simulated as accurately as possible. Because of the computational effort required for an LES, high Reynolds number cases will probably require wall models.

Inflow conditions can be specified as the instantaneous flow field of a direct simulation or artificial inflow conditions can be generated with the same mean flow and turbulence intensity characteristics as the experimental or computational results being considered for comparison. Sandham and Reynolds (1987) suggest that for the case of artificial inflow conditions, some randomizing of the inflow conditions may be necessary to represent turbulent flows. Different ways of randomizing the inflow conditions are presently being considered.

For the laminar backward-facing step problem with a finite element code, a zero natural boundary condition (see Section 4.2.5) at the outflow gives accurate results so long as the outlet is reasonably far downstream of the recirculation zone, so that the mean-flow velocity profile displays approximate vertical symmetry. In the discretized LES formulation (Section 4.2.6), however, the natural boundary conditions include the subgrid-scale motion and using zero natural boundary conditions for the LES outflow condition may not be appropriate. The choice of outflow boundary condition for the finite element LES are being investigated as part of this research.

4.2.6. The Discretized Equations

The following includes a brief description of the discretized LES equations (for the continuum equations 4.2.1 and 4.2.3) and the solution approach. Details of the derivation can be found in McCallen (1991).

The method used here is the finite element method. The use of finite element schemes for LES has been far less prominent (scarce, in fact) than the use of finite difference and spectral methods, but several researchers believe it to be the preferred numerical approach for complex geometries of technological interest (e.g., Hutton et al. 1987). In a literature search for LES results computed using the finite element method, only three references were found (Kondo et al. 1986, Findikakis et al. 1978, Findikakis and Street 1980). Even though very few LES researchers have chosen the finite element approach, the past LES developments with the spectral and finite difference methods should be adaptable to the finite element approach. However, the solution methods for the discretized equations may need some development.

As with the Reynolds-average approach, equations 4.2.1 and 4.2.3 are spatially discretized by the Galerkin finite element method. The velocity components $\bar{u}_\alpha$ and pressure $\bar{p}$ are expanded into the appropriate basis functions ϕ_j and ψ_j , respectively, as follows:

$$\bar{u}_\alpha^h(\mathbf{x}, t) = \sum_{j=1}^N \bar{u}_\alpha^j(t) \phi_j(\mathbf{x})$$

$$\bar{p}^h(\mathbf{x}, t) = \sum_{j=1}^M \bar{p}_j(t) \psi_j(\mathbf{x})$$

where N is the total number of basis functions $\phi_j(\mathbf{x})$, and $\bar{u}_\alpha^j(t)$ is the instantaneous value of the resolved velocity, $\bar{u}_\alpha^h$, and M is the total number of basis functions $\psi_j(\mathbf{x})$, with $\bar{p}_j(t)$ being the instantaneous value of $\bar{p}^h$. The superscript h signifies that $\bar{u}_\alpha^h$ and $\bar{p}^h$ are the approximate weak solutions on a mesh of the computational domain (with characteristic element size h). The functions ϕ_j and ψ_j are linearly independent piecewise polynomial basis functions. (Here $\phi_j(\mathbf{x})$ is chosen to be piecewise linear and $\psi_j(\mathbf{x})$ piecewise constant.)

The expansions will also be substituted for $\bar{u}_\alpha$ in the SGS terms and the resulting terms will depend on the chosen SGS model. These terms will be defined for Bardina's model below.

The discretized Poisson equation for pressure is solved in place of the continuity equation so that continuity and momentum are decoupled, and then an explicit time-integration scheme may be used. The final spatially discretized equations in matrix form are

$$\mathbf{C}^T \mathbf{M}^{-1} \mathbf{C} \bar{\mathbf{P}} = \mathbf{C}^T \mathbf{M}^{-1} [(\mathbf{K} + \mathbf{N}(\bar{\mathbf{u}})) \bar{\mathbf{u}} - \mathbf{F}] \quad (4.2.4)$$

and

$$\mathbf{M} \dot{\bar{\mathbf{u}}} + [\mathbf{K} + \mathbf{N}(\bar{\mathbf{u}})] \bar{\mathbf{u}} - \mathbf{C} \bar{\mathbf{P}} = \mathbf{F} \quad (4.2.5)$$

where $\bar{\mathbf{P}}$ is the pressure matrix for $\bar{p}_j / \rho$ and in three-dimensional space

$$\mathbf{M} = \begin{bmatrix} m_{ij} & 0 & 0 \\ 0 & m_{ij} & 0 \\ 0 & 0 & m_{ij} \end{bmatrix}, \quad m_{ij} = \int_{\Omega} \phi_i \phi_j$$

$$\mathbf{K} = \begin{bmatrix} k_{ij(1)} & 0 & 0 \\ 0 & k_{ij(2)} & 0 \\ 0 & 0 & k_{ij(3)} \end{bmatrix},$$

$$k_{ij(1)} = \int_{\Omega} \left[(v + 2 v_T^h) \frac{\partial \phi_i}{\partial x_1} \frac{\partial \phi_j}{\partial x_1} + (v + v_T^h) \left(\frac{\partial \phi_i}{\partial x_2} \frac{\partial \phi_j}{\partial x_2} + \frac{\partial \phi_i}{\partial x_3} \frac{\partial \phi_j}{\partial x_3} \right) \right] + \int_{\partial \Omega} \gamma_{(1)} \phi_i \phi_j$$

$$k_{ij(2)} = \int_{\Omega} \left[(v + 2 v_T^h) \frac{\partial \phi_i}{\partial x_2} \frac{\partial \phi_j}{\partial x_2} + (v + v_T^h) \left(\frac{\partial \phi_i}{\partial x_1} \frac{\partial \phi_j}{\partial x_1} + \frac{\partial \phi_i}{\partial x_3} \frac{\partial \phi_j}{\partial x_3} \right) \right] + \int_{\partial \Omega} \gamma_{(2)} \phi_i \phi_j$$

$$k_{ij(3)} = \int_{\Omega} \left[(v + 2 v_T^h) \frac{\partial \phi_i}{\partial x_3} \frac{\partial \phi_j}{\partial x_3} + (v + v_T^h) \left(\frac{\partial \phi_i}{\partial x_1} \frac{\partial \phi_j}{\partial x_1} + \frac{\partial \phi_i}{\partial x_2} \frac{\partial \phi_j}{\partial x_2} \right) \right] + \int_{\partial \Omega} \gamma_{(3)} \phi_i \phi_j$$

$$\mathbf{N} = \begin{bmatrix} n_{ij}(\bar{u}) & 0 & 0 \\ 0 & n_{ij}(\bar{u}) & 0 \\ 0 & 0 & n_{ij}(\bar{u}) \end{bmatrix}, \quad n_{ij}(\bar{u}) = \bar{u}_{\beta}^k \int_{\Omega} \phi_i \frac{\partial}{\partial x_{\beta}} \overline{\phi_j \phi_k} - \bar{u}_{\beta}^k \int_{\Omega} (\phi_j \phi_k - \bar{\phi}_j \bar{\phi}_k) \frac{\partial \phi_i}{\partial x_{\beta}}$$

$$\mathbf{C} = \begin{bmatrix} c_{ij(1)} \\ c_{ij(2)} \\ c_{ij(3)} \end{bmatrix}, \quad c_{ij(\alpha)} = \int_{\Omega} \frac{\partial \phi_i}{\partial x_{\alpha}} \psi_j$$

$$\mathbf{F} = \begin{bmatrix} f_{ij(1)} \\ f_{ij(2)} \\ f_{ij(3)} \end{bmatrix}, \quad \begin{aligned} f_{ij(1)} &= \int_{\partial\Omega} \phi_i f_1 - \left(\bar{u}_2^j \int_{\Omega} v_T^h \frac{\partial \phi_i}{\partial x_2} \frac{\partial \phi_j}{\partial x_1} + \bar{u}_3^j \int_{\Omega} v_T^h \frac{\partial \phi_i}{\partial x_3} \frac{\partial \phi_j}{\partial x_1} \right) \\ f_{ij(2)} &= \int_{\partial\Omega} \phi_i f_2 - \left(\bar{u}_1^j \int_{\Omega} v_T^h \frac{\partial \phi_i}{\partial x_1} \frac{\partial \phi_j}{\partial x_2} + \bar{u}_3^j \int_{\Omega} v_T^h \frac{\partial \phi_i}{\partial x_3} \frac{\partial \phi_j}{\partial x_2} \right) \\ f_{ij(3)} &= \int_{\partial\Omega} \phi_i f_3 - \left(\bar{u}_1^j \int_{\Omega} v_T^h \frac{\partial \phi_i}{\partial x_1} \frac{\partial \phi_j}{\partial x_3} + \bar{u}_2^j \int_{\Omega} v_T^h \frac{\partial \phi_i}{\partial x_2} \frac{\partial \phi_j}{\partial x_3} \right) \end{aligned}$$

$$\mathbf{C} = [c_{ji(1)} \ c_{ji(2)} \ c_{ji(3)}], \quad c_{ji(\alpha)} = \int_{\Omega} \frac{\partial \phi_j}{\partial x_{\alpha}} \psi_i$$

where

$$v_T^h = (c\Delta)^2 \left(\bar{u}_{\alpha}^m \frac{\partial \phi_m}{\partial x_{\beta}} \left(\bar{u}_{\alpha}^k \frac{\partial \phi_k}{\partial x_{\beta}} + \bar{u}_{\beta}^k \frac{\partial \phi_k}{\partial x_{\alpha}} \right) \right)^{1/2}.$$

These are the global system of differential-algebraic equations. The integrals in the coefficient matrices are computed using 1-point quadrature with a lumped mass matrix.

To avoid solving the linear system of equations and to keep the pressure matrix sparse, $\mathbf{M}$ is diagonalized by 'mass lumping'. Mass lumping decouples the time derivative and simplifies the use of explicit time integration. The mass lumping is done by summing rows at the element level and is frequently used in practice. Mass lumping may reduce accuracy, especially for highly transient advection-dominated flow, but it also reduces run time cost. It requires less work per element and per time step and one can usually maintain desired accuracy by finer discretization (Gresho et al. 1984).

As with the Reynolds-averaged approach, the time integration scheme involves the choice of a direct or iterative solution method for the pressure. More specifically, the pressure Poisson equation is first solved by using either a direct skyline solver or a preconditioned conjugate gradient iterative solver. For the matrix equation 4.2.4 we first compute

$$\begin{aligned} \mathbf{A}^n &\equiv \mathbf{M}^{-1} [(\mathbf{K}^n + \mathbf{N}(\bar{\mathbf{u}}^n)) \bar{\mathbf{u}}^n - \mathbf{F}(\bar{\mathbf{u}}^n)] \\ (\mathbf{C}^T \mathbf{M}^{-1} \mathbf{C}) \bar{\mathbf{P}}^n &= \mathbf{C}^T \mathbf{A}^n \end{aligned}$$

and then solve for $\bar{\mathbf{P}}^n$.

The momentum equations can be solved semi-implicitly or explicitly; however, the implicit scheme in the existing code is only operational for two-dimensional problems, so the explicit scheme will (must) be used for all three-dimensional calculations. Rearranging the momentum equation 4.2.5 to the form

$$\mathbf{M} \dot{\bar{\mathbf{u}}} = -(\mathbf{K} + \mathbf{N}(\bar{\mathbf{u}})) \bar{\mathbf{u}} + \mathbf{F} + \mathbf{C} \bar{\mathbf{P}}$$

and multiplying through by $\mathbf{M}^{-1}$,

$$\dot{\bar{\mathbf{u}}} = \mathbf{M}^{-1} [-(\mathbf{K} + \mathbf{N}(\bar{\mathbf{u}})) \bar{\mathbf{u}} + \mathbf{F} + \mathbf{C} \bar{\mathbf{P}}]$$

and using a forward (explicit) Euler scheme gives

$$\bar{\mathbf{u}}^{n+1} = \bar{\mathbf{u}}^n + \delta t \mathbf{M}^{-1} [-(\mathbf{K}^n + \mathbf{N}(\bar{\mathbf{u}}^n)) \bar{\mathbf{u}}^n + \mathbf{F}^n + \mathbf{C} \bar{\mathbf{P}}^n] ,$$

or

$$\bar{\mathbf{u}}^{n+1} = \bar{\mathbf{u}}^n - \delta t [\mathbf{A}^n - \mathbf{M}^{-1} \mathbf{C} \bar{\mathbf{P}}] .$$

4.2.7. Preliminary Results

The first step was to exercise the existing code for laminar flow over a backward-facing step for the purpose of method and code verification without the presence of a turbulence model. Figure 13 shows the results of two test cases for Reynolds number (Re_h) of 648 and 1000, based on the step height and the average inlet velocity. Plotted are the distances from the step to the point of reattachment of the step recirculation zone (x_1) and the points of separation (x_2) and reattachment (x_3) of the top-wall recirculation zone. Also shown on the plots are the numerical results of Durst and Pereira (1988) and the experimental results of Ghia et al. (1987), Mansour et al. (1983), and Armaly et al. (1983). Our calculations at $Re_h = 1000$ were performed for a 60×200 mesh and agree quite well with the numerical results of Durst and Pereira (1988), however, the numerical results only qualitatively agree with experiment. Our calculations at $Re_h = 648$ were performed for a 30×100 mesh and are not in as good agreement with the results of Durst and Pereira (1988).

Kim and Moin (1985) suggest that the differences between the numerical and measured results are due to three-dimensional effects (i.e., the vertical side walls) that are not considered in the above reported two-dimensional numerical results. Work has begun on three-dimensional calculations for $Re_h = 648$. Preliminary results show that there may also be a discrepancy in the reporting of the experimental results of Armaly et al. (1983). Calculations for a three-dimensional channel with a flat inlet velocity profile predict a lower velocity profile at the step than that reported by Armaly et al. (1983) for $Re_h = 648$. This would suggest that the experimental results need to be shifted to a higher Reynolds number (i.e., the experimental results for $Re_h = 648$ are really those for a higher Reynolds number).

Preliminary LES results have been generated for a simplified SGS model. Snapshots of the instantaneous flow field are shown in Figure 14. The calculations were performed in two-dimensions on a 60×200 mesh with the Smagorinsky SGS model for $R_{\alpha\beta}$ and model simplifications of $L_{\alpha\beta} + C_{\alpha\beta} = 0$ (see equation 4.2.2 for the definitions of terms and Section 4.2.4 for the definition of the Smagorinsky model). The wall region is not approximated with a model, but some additional viscous terms are present at the wall from the SGS model (i.e., $R_{\alpha\beta}$ does not go to zero at the wall). The LES results show vortices forming at the step and upper boundary and then traveling downstream. These results are in agreement with the direct simulation results of Kondoh and Nagano (1989) shown in Figure 15. Kondoh and Nagano also show that the complex instantaneous flow field of shedding vortices reduces to a single recirculation zone after time averaging. Thus, it appears that the LES method is capable of capturing the complex flow field of shedding vortices within the wake of a backward-facing step.

5. Future Work

5.1 The Reynolds-Averaged Model

We have demonstrated a viable approach of coupling a finite-element flow model FEMTKE to a particle-in-cell-based ADPIC model for simulating the transport and dispersion of pollutants from point sources. The initial results for dispersion over isolated rectangular blocks appear very encouraging. We are currently proceeding on further development of the models based on the following near-term and long-term tasks:

Near term

- Perform calculations on multiple buildings.
- Include and test dispersions which are affected by atmospheric stability. Our simulations so far are based on neutrally-stable atmospheric conditions. Since it is clear that atmospheric stability can significantly influence the dispersion pattern of the pollutants, it is important to begin sensitivity tests on the effects of the thermal structure on transport and diffusion processes.
- Provide an alternative to the K-Theory turbulence model option currently employed in ADPIC by using the turbulent diffusion parameters which are calculated via the higher-order-closure FEMTKE model.

- Improve the postprocessing capabilities of ADPIC such that concentration fields for any chosen plane can be displayed at any desired time. Currently, only a predetermined number of selected planes can be displayed after the calculation is made.

Long term

- Validate the model with wind tunnel experiments which have been conducted at U. C. Davis and other institutions.
- Validate the model with field experiments wherever possible.

5.2 The Large-Eddy Simulation Model

Future work on the LES modeling will include the following tasks:

- Completion of the laminar cases (for establishing a baseline case without a turbulence model) for both the two- and three-dimensional calculations.
- Continue work on the LES calculations with the simplified SGS model by implementing into the code
 - the option of calculating the flow statistical quantities (i.e., time-averaging), and
 - a wall model option, which will be compared to cases where the wall has been finely discretised and the SGS model has been allowed to go to zero at the wall.
- Incorporating an improved SGS model with
 - the advection term ($L_{\alpha\beta}$) calculated explicitly and
 - the SGS cross terms modeled along with the SGS stress term ($R_{\alpha\beta}$) using Bardina's model.
- Performing the LES calculations in three dimensions for the backward-facing step.

When possible, the code will be applied to flow over idealized buildings (i.e., flow around a surface-mounted cube). The first cases will be performed with the simplified SGS model after code testing has been completed for the backward-facing step.

Since the LES results are time-dependent and long calculational times are required to obtain statistical results, the process of coupling the flow model with the particle transport model (ADPIC) to obtain dispersion results may not be computationally practical. It may be more efficient to include a particle transport model in the LES flow code. The effort required to incorporate a particle transport model in the existing code will be determined and the method of code modification will be outlined as part of our future work.

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Figure 1. Typical flow patterns around a rectangular block. (a) Streamline pattern at steady-state for a 2D block; (b) Time-averaged schematic of flow around a 3D block.

Figure 2. Effects of atmospheric stability and building wakes on plumes emitted from a stack.

Figure 3. Schematic of 2D Flow over a backward-facing step.

Figure 4. Steady-state results from k- ϵ model (FEMTKE) for turbulent flow over a two-dimensional backward-facing step: (a) Velocity vector; (b) Turbulent kinetic energy (k); (c) Viscous dissipation (ϵ)

Figure 5. Streamline pattern for flow over a 2D backward-facing step.

Figure 6. Computational domain for flow over a building.

(b) Interpolated field

(a) FEM Model Results

Figure 7. Mean flow perpendicular to building.(a) FEM model results; (b) Interpolated results. Velocity vector projections are shown for mid-height plane (top) and centerline plane (bottom). Note that origins for the FEM and ADPIC coordinates are not coincident.

Figure 8. Particle concentration pattern 1 minute after particles are released, 90° wind: (a) End view; (b) Side view; (c) Top view.

Figure 9. Particle concentration pattern 5 minutes after particles are released, 90° wind: (a) End view; (b) Side view; (c) Top view.

Figure 10. Mean flow at 26° to building. Velocity vector projections at:
(a) Mid-height plane; (b) Centerline plane.

Figure 11. Particle concentration pattern 5 minutes after particles are released, 26° wind. (a) End view; (b) Side view; (c) Top view.

MODEL	NUMERICAL METHOD	FORMULATION	MESH	X_R/H_S
KIM	EXPERIMENT	-----	-----	7.0 ± 0.5
TEAM (UMIST)	FINITE VOLUME	STEADY	44×36	5.75
THANGAN & HUR	FINITE VOLUME	STEADY	166×73	6.28
FEMSET-2D (HAROUTUNIAN)	FINITE ELEMENT	TRANSIENT	40×32	6.37
FEMTKE	FINITE ELEMENT	TRANSIENT	54×30	7.0

Table 1. Reattachment lengths for various models compared with Kim's experiment

Figure 12. Plot of turbulent energy spectrum showing a continuous range of eddy sizes.

Figure 13. Comparison of experimental and predicted separation and reattachment points downstream of a backward-facing step.

Figure 14. The LES predicted instantaneous flow field for the backward-facing step with a simplified SGS model.

Instantaneous Velocity at Mid-Span

Time-Averaged Velocity at Mid-Span

Figure 15. Direct simulation results of Kondoh and Nagano (1989) showing their predicted instantaneous flow field and the results of time averaging.

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