1. INTRODUCTION

There has been recent interest in details of dispersion in urban settings (NRC 2003). To that end, there have been numerous field and modeling studies of dispersion of material in urban situations. It has been shown that flow, and the resulting dispersion of an effluent, is modified in the building wake (Cowan, et al. 1997; Moon, et al. 1997; Palmer, et al. 2003). Specific building features, however, are likely to make a large difference in dispersion. The building is expected to have its own boundary layer immersed in the atmospheric boundary layer and separation occurs in the lee of building. Very refined modeling is necessary to capture such effects. Several investigators have suggested that high fidelity CFD modeling may be nearing the landmark of rivaling the accuracy of wind tunnel experiments (Cowen, et al. 1997, Richards, et al. 2005).

The goal of this study is to best practices high fidelity modeling of computation fluid dynamics (CFD) to model the essential flow about a building. Such a study indicates the type of dispersion to be expected about that structure. The simplest type of building is chosen for this study – a cubical structure – because flow about this type of structure has been well documented and because it includes the essential elements of separation and boundary layer formation that impact the dispersion. The features of our high fidelity study include using a realistic atmospheric boundary layer as an initial condition, using a very fine mesh to resolve boundary layers, and employing detached eddy simulation (DES) methods in the regions of separation. Such methods blend the best of both Reynolds Averaged Navier Stokes (RANS) models with Large Eddy Simulations (LES).

The case of a surface mounted square cylinder is very well documented. Several experimental studies in particular are of great importance for the verification of numerical simulation results. One physical modeling study widely used for the validation of numerical results is the experimental characterization of three dimensional flow around surface mounted prismatic obstacles performed by Martinuzzi and Tropea (1993). Flow around obstacles was investigated in both water and air channels, and static pressure measurements, laser light sheet, oil-film, and crystal violet visualization techniques were used to record results. The data provided in this study is of limited use for validation of the current work, because the experiments were performed for fully developed channel flow at lower Reynolds numbers (Re) ($4 \times 10^4$ and $1.2 \times 10^5$). Comparison CFD studies showed the ability of RANS models to match the major features.

Richards, Hoxey, and Short (2001, 2005) investigated full scale, high Reynolds number ($4 \times 10^5$), flow around a 6m cube at the Silsoe Research Institute, producing pressure data for vertical and horizontal centerlines around the cube. Further investigation produced unsteady flow velocity data along the sides of the cube (Richards and Hoxey 2002). These studies provided the case examined in the current paper. Previously, Wright and Easom (2003) used the Silsoe case for a RANS simulation using a non-linear $k-\varepsilon$ turbulence model. They were able to reproduce the pressure distribution on the windward face of
the cube, but had difficulty on the top, side, and leeward faces. It was determined that isotropic turbulence models were inadequate in this case.

The objectives of this present study are to 1) produce a “best practices” simulation of flow about a bluff body at high Re, 2) compare the results to measured data, and 3) to carefully determine which features are not resolved when fidelity in the modeling parameters is relaxed. The final goal is delineating what parts of the physics and modeling choices are most essential to capture the features necessary to well model atmospheric dispersion in the near source region when a building is present.

Section 2 describes our high fidelity runs, including the mesh, model, boundary initialization conditions, turbulence models, use of DES and zonal-DES, and the resulting features of the flow. The results are compared with the environmental data of Richards and Hoxey (2002) in section 3. Conclusions and suggestions for further studies appear in section 4.

2. MODELING APPROACH

2.1 The Mesh

The computational domain consists of a 6m, wall-mounted cube located inside a 106m × 230m × 100m region. The location of the cube within the domain is shown in Figure 1, which also shows the location of the rectangular mesh refinement region around the cube. This refinement region has a height of z = 19m. The grid was a 1.68 × 10^6 node (4.51 million computational elements), unstructured hybrid tetrahedral mesh with near-surface prism layers, and was generated with Ansys Icem CFD. Prism layers in a hybrid mesh allow for better modelling of near-wall physics than tetrahedras alone. Twenty one prism layers were extruded from both the floor and the surfaces of the cube at an expansion ratio of 1.2. The first prism layer’s distance from the wall was 0.004m, corresponding to a \( y^+ = 75 \).

2.2 The CFD Model

We use the commercial flow code, AcuSolve\textsuperscript{TM}, from ACUSIM Software, Inc. as our computational engine (see the AcuSolve\textsuperscript{TM} manual, 2005). ACUSIM Software Inc. is a developer of robust, fast and accurate finite element flow solvers that can be seamlessly used by all levels of expertise, both as a standalone computational fluid dynamics flow solver and as an embedded CFD component integrated into customer specific engineering and scientific applications.

AcuSolve\textsuperscript{TM} offers a number of turbulence modeling options. Detached-eddy simulation (DES) and Spalart-Allmaras (SA) RANS models are used in this work. DES is a simulation methodology that provides LES-like solutions for massively separated flows like the urban environment. The SA RANS model is a popular contemporary one-equation turbulence closure that yields reliable turbulence statistics for broad classes of turbulent flows.

2.3 Initial Boundary Layer

Measurements at the Silsoe test site have shown that the approach flow velocity profile is a simple logarithmic function of height above the surface, \( z \):

\[
U(z) = \frac{u_*}{\kappa} \ln\left(\frac{z}{z_0}\right)
\]  

(3)
The roughness length $z_0 = 0.01\text{m}$ and von Karman’s constant $\kappa = 0.4$ (Richards et. al. 2000). Additional properties of the approach flow, including turbulence intensities and turbulence length scale, are available (Richards et. al. 2001).

The inflow boundary condition was set to match this profile. In addition, a profile for eddy viscosity was also specified. Additionally, the turbulence intensities and length scales were used to produce an inlet eddy viscosity profile for the S-A model. This was done to establish an equilibrium boundary layer.

2.4 Detached Eddy Simulation

Detached Eddy Simulation (DES) is a response to the high computational costs of LES, and the low accuracy of RANS turbulence models in massively separated turbulent flows. In general, DES compares the grid spacing, $\Delta$, to the flow turbulence length-scale, $\delta_t$, and runs in an LES mode where $\Delta \ll \delta_t$ and a RANS mode elsewhere (Strelets 2001).

The RANS Spalart-Allmaras turbulence model is modified for DES by replacing the distance to the closest wall, $d$, with a length proportional to $\Delta$. This length is defined by

$$d = \min(d, C_{DES}\Delta), \quad (4)$$

where $C_{DES}$ is an adjustable constant and $\Delta \equiv \max(\Delta x, \Delta y, \Delta z)$. For $d \ll \Delta$ the model will behave like the S-A turbulence model; For $d >\!\!> \Delta$ it will behave like an subgrid scale model (Spalart, et al. 1997).

2.5 Full Scale Flow Features

Several flow features have been described for the full scale atmospheric case as measured by Hoxey, et al. (2005). The stagnation point on the front face of the cube has been observed above mid height. There is a detached recirculation zone on the top of the cube that reattaches, on average, between 0.5 and 0.83 cube heights downstream from the front face. The reattachment length behind the cube is 1.9 cube heights downstream from the front face. Finally, weak shedding with a frequency ($n$) of 0.154 Hz and a Strouhal number ($St=nh/U$) of 0.14 was observed for a reference velocity ($U$) of 6.8 m/s and cube height ($h$) of 6 m (Hoxey, et al. 2005).

3. RESULTS COMPARISON

We have been able to reproduce the flow features expected for flow about a cube. The general characteristics of the time average flow around a surface mounted cube are described by Ferziger and Milanovich (1999). Incoming flow reaches a stagnation point near the ground upstream from the cube and flows around the sides of the cube as seen in our ZDES simulation in Fig. 2. Further above the ground, flow hits the front face of the cube and some of it moves down the face and into a region of reversed flow. One goal is to determine this stagnation point on the face of the cube. Figure 3 shows this feature at above the halfway point as expected from the measurements. Just upstream from the front face of the cube and along the lower surface, there is a separation zone, which is the head of a horseshoe vortex. This horseshoe vortex extends along the sides of the cube. This is evident in both Figs. 2 and 3. The top view (Fig. 3) shows the horseshoe vortex in roughly the correct location. It shows up as a vortex recirculation zone in Fig. 3. A secondary horseshoe vortex in front of the primary one is also evident.

Figure 2. Time averaged streamlines for a short time as modeled by ZDES and viewed from above. The streamlines are plotted at 1.1 above the ground.
On the top surface of the cube there is a recirculation zone, which is evident in the wind vectors of Fig. 4. In the wake behind the cube, there is an arch vortex that appears as the upper vortex in the lee of the cube in Fig. 3 and also evident in Fig. 5 in the streamlines as viewed from behind the cube. Further downstream there is a reattachment line where the wake ends, evident in Figs 2 and 3.

Some of these features, as well as the details of the flow are visualized using additional variables. Figure 6 plots the streamwise velocity magnitude at 1 m above the ground. The fine scale details are evident – the primary and secondary horseshoe vortices in front of cube, the separation along the sides of the cube, and the vortex shedding in the lee of the cube. Figure 7 is similar, but depicts the wind vectors colored by the vertical component of vorticity. The fine scale circulations are well modeled and we see a bifurcation of the vortices in the lee of the cube.

Figure 6. Streamwise velocity at 1 m above the ground.

Figure 7. Wind vectors in the immediate vicinity of the cube as viewed from above. Vectors are colored by the vertical component (out of the page) of vorticity.

Figure 8 shows the streamwise velocity on a plane cut longitudinally through the cube. One can see the fine-scale features and recirculation zones in the lee of the cube. Figure 9 depicts three dimensional streamlines around the cube, demonstrating a complex vertical flow field that is largely altered by the presence of the structure. Finally, Fig. 10 is an isosurface of vorticity colored by the helicity

$$\left(\frac{\tilde{\omega} \cdot \tilde{V}}{||\tilde{\omega}||} \right),$$

where $\tilde{\omega}$ and $\tilde{V}$ are the three dimensional vorticity and wind vectors, respectively. This view give a good feel for the three dimensional structure to the flow. These single time vorticies show a very complex shedding structure in the lee of the cube.
A time dependence to the flow is evident in these figures that is largely due to the LES features of this ZDES simulation.

This study is a first step in a more detailed study to delineate which features of the flow are dependent on the highest fidelity grids and most accurate modeling implementations.

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REFERENCES


3. DISCUSSION

This work has demonstrated that very fine scale structure can be modeled using CFD and a Detached Eddy Simulation. The zonal implementation emphasized here give very realistic time dependent features to the flow. The time averaged streamline plots demonstrate that the flow features are those expected while the single time plots depict the very detailed time dependent structure to the flow. We can observe vortex shedding, recirculation zones, coherent vorticies, and very detailed structure in the flow.


