A SIMPLIFIED CFD APPROACH FOR MODELING URBAN DISPERSION

Stevens T. Chan*, Tom D. Humphreys, and Robert L. Lee Lawrence Livermore National Laboratory Livermore, California 94551, USA

1. INTRODUCTION

Recently we have developed and demonstrated the utility of a building scale CFD (Computational Fluid Dynamics) model, FEM3MP (Chan and Stevens, 2000), for simulating flow and dispersion of chemical/biological agents released in the urban environment. Physics of the model include aerosols, UV radiation decay, surface energy budget, canopies, and turbulence, etc. The model has been extensively validated, using data from both wind tunnel and field dispersion experiments, by Chan, et al. (2001, 2002, 2003), Calhoun, et al. (2002), Lee, et al. (2002), and Humphreys, et al. (2003).

While high-resolution CFD models are very useful for emergency planning of special events, vulnerability analyses, post-event assessments, and development of mitigation strategies, such models generally require excessive computer resources and long turnaround time, and thus are unsuitable for emergency response situations. To meet such needs, we are developing a simplified CFD approach for potential integration into the operational modeling system of the DOE National Atmospheric Release Advisory Center (NARAC). With the new approach, only targeted buildings are explicitly treated with fine grid resolution and the remaining buildings are represented as drag elements (or virtual buildings) with coarser grid resolution, thus making the model far more cost-effective. Additional advantages of such an approach include easier generation of the computational mesh and the ability to compute on much larger domains to provide improved parameterization (such as form drag) for use in larger scale models.

Flow and dispersion in urban areas are often driven by highly variable wind with turbulent fluctuations sometimes as large as the mean velocity. To account for such effects, we have also developed a capability for imposing time-dependent boundary conditions as a means to enforce unsteady, large scale forcing. The performance of such a capability is also summarized in this paper.

In the following, we first describe briefly the simplified CFD approach, together with numerical results to show the accuracy and efficiency of the approach, then summarize results from three LES simulations using different boundary conditions for one of the Urban 2000 dispersion experiments (Allwine, et al., 2002), and finally offer a few concluding remarks.

2. SIMPLIFIED CFD APPROACH

2.1 The Approach

For convenience of code parallelization and computational speed, the current FEM3MP model employs a structured mesh and buildings in the computational domain are represented as solids blocks with zero values for velocity, pressure, and diffusivities. The main idea of our simplified CFD approach is to treat only a limited number of targeted buildings as solid blocks, with fine grid resolution to adequately resolve the flow around these buildings, and treat the remaining as virtual buildings with much coarser grid resolution, assuming that details of the flow over the virtual buildings are less essential to the accuracy of the flow around the targeted buildings.

The virtual buildings are modeled as drag elements in a way similar to the treatment of a forest canopy (see, for example, Chan, et al., 2002). The drag elements are composed of all the mesh points representing the virtual buildings and, at such locations, a drag term in the form of C_d lul U_i where C_d is a drag coefficient, lul is the local wind speed, and \textbf{U}_i is the i^{th} velocity component, is added to the momentum equations. Based on considerations of accuracy and computational speed from a number of numerical experiments for the cube problem presented below, a value of 50 was selected for the drag coefficient. For computational efficiency, the drag term is linearized and treated implicitly in the time integration of the momentum equations. In addition, values of diffusivities for the virtual buildings are set equal to the molecular diffusivity of air so as to avoid numerical instability and also to minimize unwanted diffusion.

2.2 Numerical Examples

Two numerical examples are presented below to demonstrate the effectiveness of the simplified CFD approach. In the first example, the flow and concentration fields around a cube were predicted in two simulations, with the cube represented as a solid and a virtual building, respectively. A computational domain of 8H x 6H x 2H, H being the cube height, was used in both calculations, with a graded mesh of 43x33x15 grid points. A logarithmic velocity profile, with U=0.6 m/s at H, was specified on the inlet plan. In each case, a steady state velocity field was first established and then followed by the dispersion simulation associated with a ground level tracer continuously released in front of the cube.

^{*}Corresponding author address: Stevens T. Chan, Lawrence Livermore National Laboratory, P.O. Box 808, L-103, Livermore, CA 94551, e-mail: <u>schan@llnl.gov</u>

A comparison of dimensionless concentrations, χ =C*U*H²/Q (C being the calculated concentration, U being the reference velocity at H, and Q being the source rate), and velocity projection on the vertical plane of symmetry and z/H=0.2 plane from the two simulations is presented in Fig.1. The figure shows that, despite some small differences, the virtual building approach reproduces very well the major features of the velocity field, including the stagnation zone in front of the cube, flow separation on the sides and the rooftop, and the large wake region behind the cube. The predicted concentrations on the two planes also agree well, with the virtual building approach reproducing essentially the same horseshoe-shaped plume on the horizontal plane. For concentration on the vertical plane, the agreement is still very reasonable except there is a small amount of tracer seeping through the bottom part of the virtual building.

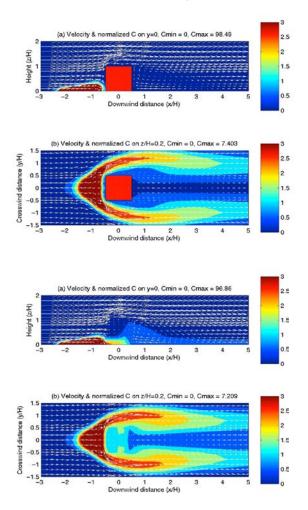


Fig. 1. Predicted velocity and concentrations around a cube with the cube modeled as a solid building (top panels) and as a virtual building (bottom panels).

As a second example, flow and dispersion simulations were performed for a hypothetical tracer gas release in the Salt Lake City downtown area of about 1 km². The prevailing wind was assumed to come from the South, with u=3 m/s at 10 m height and under neutral stability conditions. A continuous source near the south side was released at ground level at the rate of 1 kg/s for 10 min. The scenario was simulated with three different representations of the buildings inside the computational domain: (1) a high resolution, graded mesh of 229x227x35 grid points with all buildings modeled as solid blocks, (2) a hybrid mesh of the same grid resolution but with only eight of the buildings explicitly represented and the rest modeled as virtual buildings, and (3) a mesh of only 101x101x20 grid points with uniform horizontal grid resolution and all buildings modeled as virtual buildings. Incidentally, due to its ease in mesh generation, many more buildings have been included in the last case than the other two cases. Again, in each case, a steady wind field was first established and then followed by the dispersion simulation.

Predicted velocity projection and concentrations on the z=2 m plane at t=10 min the simulations are shown in Figs. 2 and 3, respectively. As seen in these figures, the overall agreement for both the velocity and concentration fields among the three simulations is very good. Results from the hybrid mesh are essentially the same as those from the first mesh, albeit some low level concentrations inside some of the virtual buildings. Despite its use of a much coarser grid, the all virtualbuilding mesh is still able to reproduce the main features of concentration patterns predicted by the other two approaches, but with an order-of-magnitude savings in computational cost. However, as expected, less accurate results are produced inside the virtual buildings near the source, where solid buildings are apparently more appropriate to use.

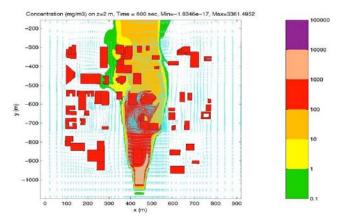


Fig. 2. Predicted velocity and concentrations on z=2 m plane at t =10 min, with all buildings modeled as solid blocks.

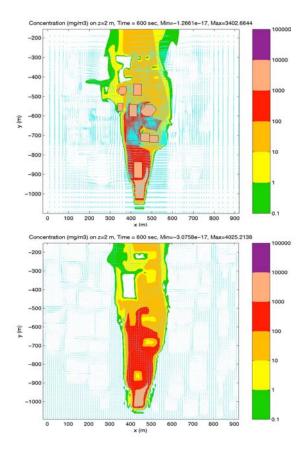


Fig. 3. Predicted velocity and concentrations on z=2 m plane at t =10 min, with buildings modeled as solid blocks and virtual buildings (top panel) and all buildings modeled as virtual buildings (bottom panel).

In Fig. 4, predicted concentrations along the centerline from the hybrid mesh and the all virtualbuilding mesh are compared. Results from the all solidbuilding mesh are almost identical to those from the hybrid mesh and thus are not presented here. Despite a slight under-prediction of certain peak values, the all virtual-building approach has yielded very reasonable results as compared with those from the more rigorous, expensive approaches.

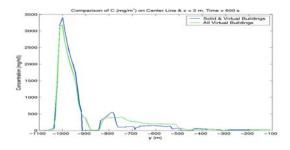


Fig. 4. Predicted centerline concentrations from a hybrid mesh of solid and virtual buildings (blue line) and an all virtual-building mesh (green line).

3. TIME-DEPENDENT FORCING

In the summer of 2000, DOE sponsored a field experimental program, Urban 2000 (Allwine, et al., 2002), to address the urban dispersion problem, with a focus on the near-to-intermediate regions of releases. Meteorological and dispersion data were collected for 10 intensive observation periods (IOPs) during the early morning hours from October 2-26, 2000. Three onehour releases were conducted for 6 of the 10 IOPs. At the time of the experiments, the surface winds were generally quite light (often 1 m/s or lower) and variable in direction, with only IOP 10 exhibiting somewhat consistent southeasterly direction. Thus, for most of the IOPs, a time-dependent boundary condition approach to represent the unsteady, large scale forcing on model simulations is considered to be more appropriate.

Release No. 1 of IOP 7 was selected for such an investigation. Shown in Fig. 5 are the 1-sec data of velocity components recorded during the release by two sonic anemometers: sonic No. 9 located at z=2.5 m and about 60 m in the southeast of the Heber Wells building (the odd-shaped building near the center of Fig. 6) and another on the rooftop (z=43.7 m) at the NE corner of the City Center building (the dark-rooftop building directly south of Heber Wells). These measurements clearly show the wind was light and highly variable during the release.

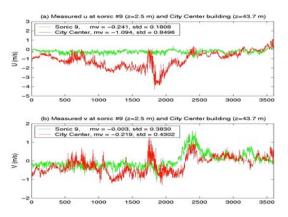
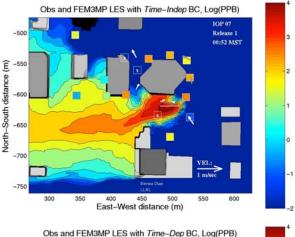


Fig. 5. Horizontal velocity components (1-sec data) recorded by Sonic No. 9 and the sonic anemometer on the rooftop of City Center building during Release 1 of IOP 7.

Three LES simulations, using different boundary conditions, were performed for the release. In the first simulation, a steady inlet velocity of 0.386 m/s and 93.1 degrees in direction (obtained by averaging the sonic 9 data) was used. The other two simulations used respectively the 1-sec wind data measured by sonic 9 and that on the rooftop of the City Center building as boundary conditions. In each case, a flow field was first simulated for 30 min prior to the start of the dispersion simulation. Each of the dispersion simulation was performed for 60 min, with a ground level, line source of SF_{6} released at a rate of 1 g/s from the south of Heber Wells building. For brevity, only the major results are summarized here, but more details are available in Chan (2004).

Fig. 6 shows a comparison of the timeaveraged (for t = 50-55 min) concentration patterns on z=1 m plane from two of the simulations. Also superimposed in the figure are the data obtained by the gas samplers, which are plotted as small squares with colors indicating their respective concentration levels. Obviously, the predicted plume shape and concentration patterns are quite different. The simulation with steady inlet velocity has produced a plume mostly being transported to the west-southwest region. On the other hand, the simulation using the sonic data of City Center building has produced a plumed being dispersed in all directions with a significant part of the plume drifted to the North, which is highly consistent with the measured concentrations.



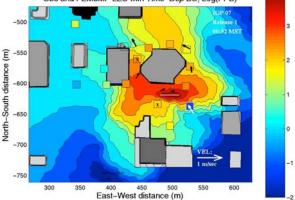


Fig. 6. Predicted time-averaged (for t=50-55 min) concentration patterns on z=1 m plane from simulations using steady inlet velocity (top panel) and time-dependent boundary conditions with sonic data of the City Center building (bottom panel).

In Fig. 7, the predicted, time-averaged concentrations at the gas sampler locations in the vicinity of the Heber Wells building are compared with the observed data. As seen in the figure, results from the simulation using steady inlet velocity (blue line) are very poor, because the simulated plume misses most of the sampler locations (see the top panel of Fig. 6). Significant improvements were obtained from the simulation using the sonic 9 data (green line), with most of the predicted concentrations agreeing with the observed data within a factor of 5 or so. The simulation using the sonic data of City Center building has further improved the agreement between model predictions (red line) and measured data to be within a factor of 2 for most of the sampler locations.

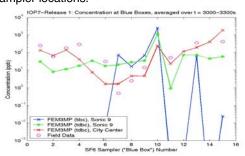


Fig. 7. Comparison of time-averaged (for t=50-55 min) concentrations measured at gas sampler locations (in magenta) and predicted by simulations using steady inlet velocity (blue line), time-dependent boundary conditions with sonic No.9 data (green line), and time-dependent boundary conditions with sonic data of the City Center building (red line).

4. SUMMARY AND CONCLUSIONS

In this paper, we have presented and demonstrated the effectiveness of a simplified CFD approach for modeling urban dispersion. The combined use of solid and virtual buildings in the same CFD code offers the flexibility of using high grid resolution near targeted buildings and much coarser grid resolution for non-targeted buildings without seriously compromising the overall solution accuracy. Early testing of the approach shows that results similar to those from the more accurate, all solid-building approach can be obtained with an order-of-magnitude savings in computational cost.

The time-dependent boundary condition capability (for representing unsteady, large scale forcing) in FEM3MP has been evaluated using data from one of the Urban 2000 dispersion experiments. Our results demonstrate clearly the importance of imposing appropriate time-dependent forcing in dispersion simulations involving light and highly variable wind conditions. Our results also show that model predictions can be improved greatly, even only data from a single sensor are used. For more accurate model predictions, however, more data in space and time to represent adequately the large scale forcing are needed. Such data have to be provided by field measurements and/or accurate larger scale models.

We will continue to work on the time-dependent boundary condition problem and develop schemes to couple with larger scale models. We will also further extend and evaluate the simplified CFD approach, with the objective of producing a sufficiently fast CFD model for integration into NARAC's operational modeling system.

5. REFERENCES

- Allwine, K., J. Shinn, G. Streit, K. Clawson, and M. Brown, 2002: Overview of Urban 2000, Bulletin of the American Meteorological Society 83 (4), 521-536.
- Calhoun, R., F. Gouveia, J. Shinn, S. Chan, D. Stevens, R. Lee, and J. Leone, 2002: Flow Around a Complex Building: Experimental and RANS/ Gaussian Model Comparisons, to appear in JAM.
- Chan, S. and D. Stevens, 2000: An Evaluation of Two Advanced Turbulence Models for Simulating the Flow and Dispersion Around Buildings, The Millennium NATO/CCMS Int. Tech. Meeting on Air Pollution Modeling and its Application, Boulder, CO, May 2000, 355-362.
- Chan, S., D. Stevens, and W. Smith, 2001: Validation of Two CFD Urban Dispersion Models Using High Resolution Wind Tunnel Data, 3rd Int. Sym. on Environ, Hydraulics, ASU, Tempe, AZ, Dec. 2001, 107.

- Chan, S., R. Lee, and J. Shinn, 2002: Large Eddy Simulation of Turbulent Flow and Diffusion Above and Within Forest Canopies, AMS 12th Joint Conf. on the Application of Air Pollution Meteorology with the Air and Waste Management Association, Norfolk, VA, May 2002, 101-102.
- Chan, S., M. Leach, and W. Dannevik, 2003: CFD Simulation of a Prairie Grass Field Dispersion Experiment, 7th Annual GMU Transport and Dispersion Modeling Workshop, Fairfax, VA, June 2003.
- Chan, S., 2004: Incorporation of Large Scale Forcing into a Building Scale CFD Model, Workshop on Merging Mesoscale and CFD Modeling Capabilities, AMS Annual Meeting, Seattle, WA, January 2004.
- Humphreys, T., S. Chan, and R. Lee, 2003: Validation of CFD Near Building Dispersion with Urban 2000 Data for Steady and Time-dependent Boundary Conditions, 7th Annual GMU Transport and Dispersion Modeling Workshop, Fairfax, VA, June 2003.
- Lee, R., T. Humphreys, and S. Chan, 2002: High Resolution Modeling of Atmospheric Releases Around Buildings, AMS 12th Joint Conf. on the Application of Air Pollution Meteorology with the Air and Waste Management Association, Norfolk, VA, May 2002, j5-6.

ACKNOWLEDGEMENTS

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.