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LARGE EDDY SIMULATION OF AN URBAN 2000 EXPERIMENT WITH VARIOUS TIME-DEPENDENT FORCING

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1. INTRODUCTION

Under the sponsorship of the U.S. DOE and DHS, we have developed a Computational Fluid Dynamics (CFD) model for simulating airflow and dispersion of chemical/biological agents released in the urban environment. Our model, FEM3MP, is based on solving the three-dimensional, time-dependent, incompressible Navier-Stokes equations on massively parallel computer platforms. The numerical algorithm uses the finite element method for accurate representation of complex building shapes and variable terrain, together with a semi-implicit projection method and modern iterative solvers for efficient time integration (Gresho and Chan, 1998). Physical processes treated in our code include turbulence modeling via the RANS (Reynolds Averaged Navier-Stokes) and LES (Large Eddy Simulation) approaches, atmospheric stability, aerosols, UV radiation decay, surface energy budget, and vegetative canopies, etc.

Predictions from our model are continuously being verified and validated against wind tunnel data (Chan and Stevens, 2000; Chan, et al., 2001) and field measurements (Chan, et al., 2002, 2003, 2004; Lee, et al. 2002; Humphreys, et al. 2003; Calhoun, et al. 2004). One of such examples is a recent model evaluation study performed by Chan, et al. (2004), using data from IOP7 Release 1 of the URBAN 2000 field experiments. Their simulation results demonstrate that, in order to successfully simulate urban dispersion scenarios under light and highly variable winds, it is necessary to use appropriate time-dependent forcing on the inflow boundary.

In this study, the effects of various time-dependent forcing or, more precisely, variations in turbulent fluctuations of inflow velocity, on the dispersion results of the same experiment are investigated. To this end, large eddy simulations were performed with various time-dependent boundary conditions constructed from the 1-sec sonic data collected on the rooftop of City Center building without time-averaging, with 2-min time-averaging, and 5-min time-averaging, respectively. In addition, large eddy simulations of the field experiment were also performed with time-dependent forcing constructed from the predictive results of the COAMPS model (Leach, et al., 2002).

In the following, we first describe briefly the field dispersion experiment being simulated, then present some of the results from our model simulations and compare them against measured data, and finally offer a few concluding remarks.

2. URBAN 2000 FIELD EXPERIMENTS

In the summer of 2000, the U.S. DOE sponsored a field experimental program, URBAN 2000, in Salt Lake City 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 to 26, 2000. Three one-hour releases were conducted for 6 of the 10 IOPs. At the time of the experiments, 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. Fig. 1 shows the instrumentation in the vicinity of the release. More details about the experiments are available in Allwine, et al. (2002).

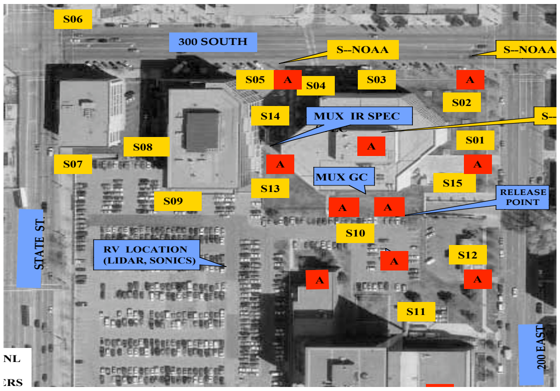

Fig. 1. Instrumentation in the source region of the URBAN 2000 experiments. The release location is on the south side of Heber Wells building in the northeast quadrant of picture. Yellow boxes indicate air sampler locations and red boxes are sonic anemometer locations.

The simulated dispersion experiment, release 1 of IOP 7, was conducted under light and highly variable winds and with a line source of SF_6 released at ground level from the south side of Heber Wells building for 60 minutes. Shown in Fig. 2(d) are the 1-sec sonic data

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*Corresponding author address: Stevens T. Chan, Lawrence Livermore National Laboratory, P.O. Box 808, L-103, Livermore, CA 94551, e-mail: schan@llnl.gov recorded during the release on the rooftop (z=43.7 m) at the NE corner of City Center building (which is south of Heber Wells and on the southern edge of Fig. 1). These measurements show that winds were indeed light and highly variable during the release. The wind direction was initially northeasterly and then changed rather abruptly to southeasterly during the last 25 minutes of release. Fig. 2(a)-(c) are time-averaged results obtained with various averaging times and will be referred to in the next section.

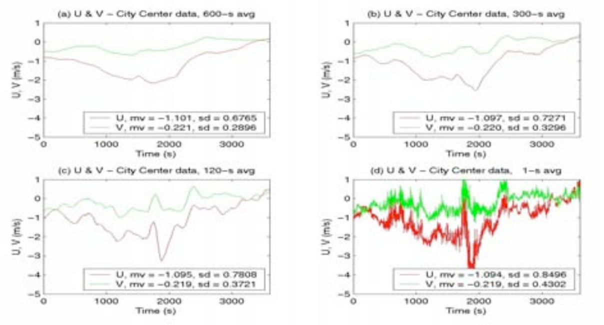

Fig. 2. Time-series of horizontal velocity components obtained by using various averaging times for the sonic data: (a) 10-min average, (b) 5-min average, (c) 2-min average, and (d) the actual 1-sec sonic data.

3. MODEL-DATA COMPARISONS

In this section, predicted concentration patterns in the vicinity of the release location from four numerical experiments using various time-dependent forcing are summarized and compared with available data. Three of the numerical experiments involve using time-averaged or the 1-sec sonic data and the remaining case involves the use of predictive results from the COAMPS model. In each case, a flow field was first simulated for 30 minutes prior to the start of the dispersion simulation. Each of the dispersion simulations was performed for 60 minutes, with a ground level, line source of SF_6 released at a rate of 1 g/s from the south side of Heber Wells building. For brevity, only major results are presented and compared herein.

3.1 Time-dependent Forcing with Sonic Data

Three large eddy simulations, using different time-dependent forcing by using the velocity components depicted in Fig. 2(b)-(d), were performed. Specifically, the three sets of data were used to construct the respective time-dependent boundary conditions, with logarithmic variations in the vertical direction, for each of the simulations.

Fig. 3 shows a comparison of the time-averaged (for t = 50-55 minute after start of the release) concentration patterns on z=1 m plane from the first two simulations. Also superimposed in the figure are observed data from the gas samplers, which are plotted as small squares with the same color scheme. Obviously the plume shapes and concentration patterns predicted by the two simulations are quite different. The simulation using 5-min time-averaged data as forcing has produced a smaller plume confined mostly to the east and south sides of Heber Wells building. On the other hand, the simulation using 2-min time-averaged data as forcing has produced a larger plume extending much further to the north of Heber Wells building, apparently due to enhanced turbulent mixing in the area from the inflow. As a result, the predicted concentration patterns are also in better agreement with observed data.

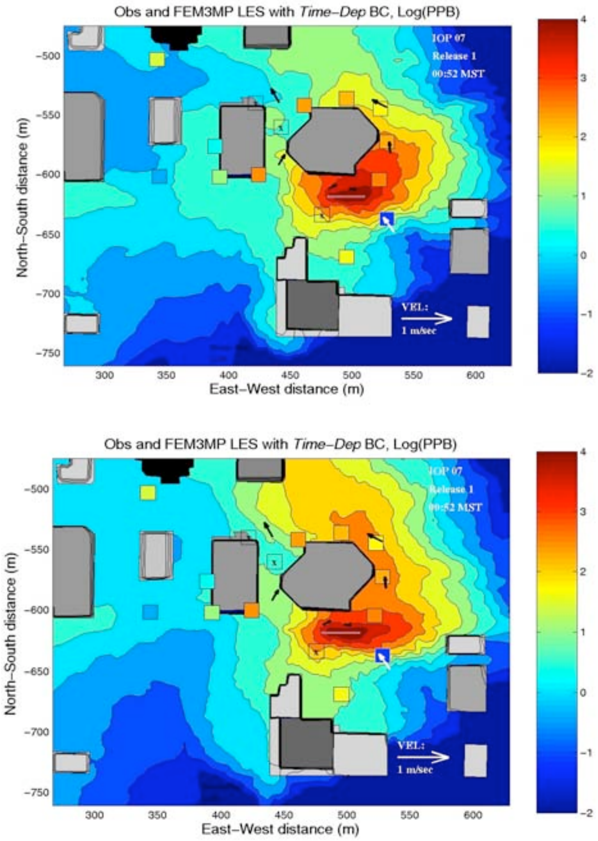

Fig. 3. Predicted time-averaged (for t=50-55 min) concentration patterns on z=1 m plane from the simulation using 5-min averaged sonic data (top panel) and the simulation using 2-min averaged sonic data (bottom panel) as time-dependent forcing. Colored small squares are observed concentration.

In Fig. 4, the predicted time-averaged (t = 50-55 min) concentration patterns on z=1 plane from the simulation using the 1-sec sonic data as forcing are compared with the observed data. As a result of even more turbulence coming in from upwind, this simulation has produced a plume being dispersed in all directions with a significant part of the plume drifted to the west and in the nearby street canyon. The predicted plume is the largest and the predicted concentration patterns are the most consistent with observed data among all three simulations.

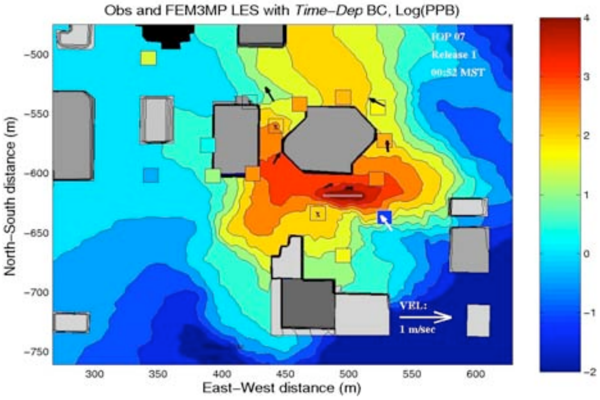

Fig. 4. Predicted time-averaged (for t=50-55 min) concentration patterns on z=1 m plane from simulation using the actual 1-sec sonic data as time-dependent forcing. Colored small squares are observed concentration.

With the assumption of the 10-min averaged results in Fig. 2(a) being the mean velocity components, the turbulence kinetic energy (TKE) of the inflow are evaluated and plotted in Fig. 5. The mean values of TKE in Fig. 5(b)-(d) are 0.019, 0.068, and 0.146, respectively. Rough estimates of the mean values of TKE near Heber Wells building (by averaging the results over a 300 m x 300 m area and time=50-55 min) from the three simulations are 0.155, 0.201, and 0.252, respectively. Thus the range of mean TKE induced by buildings in the source region is about 0.11 to 0.14, which is comparable to the mean value of TKE in the 1-sec sonic data. This fact explains partly why the gross features of the predicted plumes are very similar, although the TKE values of the inflow are considerably different. However, variations in turbulent fluctuations of the inflow do play an important role in the details and accuracy of the predicted results as shown earlier.

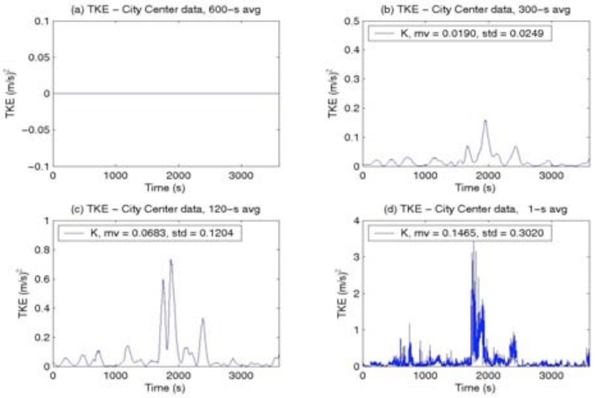

Fig. 5. Time-series of TKE corresponding to the velocity components depicted in figure 2. The 10-min averaged results of Fig. 2(a) are considered as the mean velocity components.

3.2 Time-dependent Forcing with COAMPS Results

When relevant field data are not readily available for constructing appropriate large scale forcing on the boundary for a local scale model such as FEM3MP, an alternative is to use the predictive results of a larger scale model. We have investigated such an approach using the results of COAMPS. Generally, nested COAMPS runs are made and relevant results from the finest nest are extracted to construct the time-dependent forcing required in FEM3MP simulations.

In the present case, COAMPS was run with five nests of 0.5, 1.5, 4.5, 13.5, 40.5 km grid resolutions, each consisting of 61x61x36 grid points, for a period of time. Then the mean velocity and TKE profiles at three locations (in the finest nest) being closest to the east, north, and south edges of the FEM3MP computational domain were extracted from the COAMPS results. Finally random perturbations, based on the predicted mean TKE values, were added to the mean velocity components to yield the time-dependent boundary conditions necessary for subsequent FEM3MP simulations.

As an example, Fig. 6 shows the resulting time-dependent horizontal velocity components and the corresponding TKE at the height of 4 m on the east inlet plane. The incoming mean wind is nearly easterly for the first 20 minutes and then gradually changes to northeasterly for the remaining time of the release.

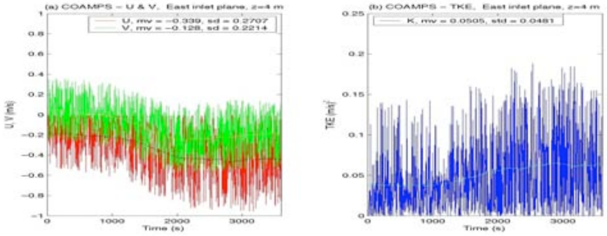

Fig. 6. Time-series of horizontal velocity (left panel) and TKE (right panel) at z=4 m constructed from the mean values of velocity and TKE of the COAMPS run. Velocity components similar to those in the left panel were used as time-dependent forcing on the inlet planes in subsequent FEM3MP simulations.

With the above time-dependent forcing, large eddy simulations for flow and dispersion were performed subsequently. Fig. 7 shows the predicted time-averaged (for t=50-55 min) concentration patterns on z=1 m plane and a comparison with the observed data. Due to a southeasterly wind initially veering to a northeasterly wind later (which is opposite to the direction indicated by the sonic data), the simulation has produced a plume extending mostly to the west, with part of the plume being channeled through street canyons in the north. Although the predicted concentration patterns have reproduced some of the observed data, there are some misses on the east of Heber Wells building and significant over-predictions near the west edge of the plume.

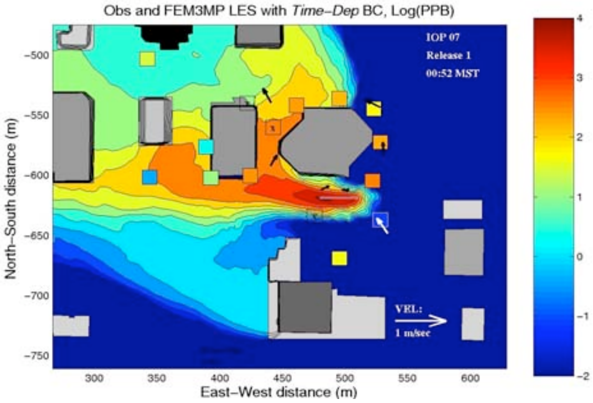

Fig. 7. Predicted time-averaged (for t=50-55 min) concentration patterns on z=1 m plane from the simulation using COAMPS results as time-dependent forcing. Colored small squares are observed concentration.

In Fig. 8, predicted, time-averaged concentrations at gas sampler locations in the vicinity of Heber Wells building from all four simulations are compared with observed data. As seen in the figure, predicted results from the simulation using COAMPS results (cyan dash-dotted line) are rather poor, with quite a few misses and over-predictions. Results from the simulation using 5-min averaged sonic data (blue line) are considerably better. Significant improvements were obtained from the simulation using the 2-min averaged sonic 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 1-sec sonic data as forcing has further improved the agreement between model predictions (red line) and observed data to within a factor of 2 for most of the sampler locations. The normalized mean square errors from the four simulations are 3.55, 3.69, 2.69, and 1.40, respectively.

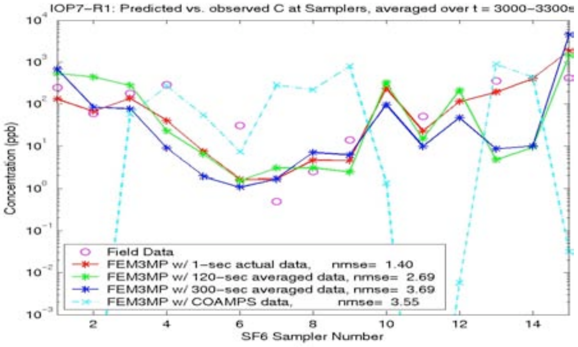

Fig. 8. Comparison of time-averaged (for t=50-55 min) concentrations predicted by simulations using COAMPS results (cyan dash-dotted line), 5-min averaged sonic data (blue line), 2-min averaged sonic data (green line), and the 1-sec sonic data (red line) against observed data (open circles in magenta).

4. SUMMARY AND CONCLUSIONS

The time-dependent forcing capability in FEM3MP has been evaluated using observed data from one of the URBAN 2000 dispersion experiments. Our results demonstrate clearly the importance of imposing appropriate time-dependent forcing, including turbulent fluctuations of the inflow, in simulating urban dispersion scenarios involving light and highly variable winds.

Among the four numerical experiments, predicted concentrations from the simulation using COAMPS predicted results as time-dependent forcing are the least accurate, partly due to coarse grid resolution (500 m for the finest nest) and perhaps partly due to inadequate parameterization of urban canopy effects. Predicted concentrations from the two simulations using time-averaged sonic data as time-dependent forcing are in much better agreement with the observed data, mainly attributing to a more realistic representation of the inflow velocity and upwind turbulence. However it is observed that the accuracy of model prediction degrades considerably as more turbulent fluctuations are removed from the inflow. As expected, concentrations predicted by the simulation using the 1-sec sonic data are the most consistent with observed data, because it uses the most realistic upwind conditions.

Our simulations also indicate that reasonably accurate model predictions can be realized, even if relevant measured data are available from a single sensor only. For more accurate model predictions, however, more data in space and time to represent adequately large scale forcing are needed. Such data have to be provided by field measurements and/or accurate larger scale models with sufficiently fine grid resolution and adequate parameterization of urban canopy effects.

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, 2004: Flow Around a Complex Building: Comparisons between Experiments and a Reynolds-Averaged Navier-Stokes Approach, Vol. 43, JAM, 696-710.

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., T. Humphreys, and R. Lee, 2004: A Simplified CFD Approach for Modeling Urban Dispersion, 2004 AMS Annual Meeting, Seattle, WA, Jan. 11-15, 2004.

Gresho, P. and S. Chan, 1998: Projection 2 Goes Turbulent – and Fully Implicit, Int. J. of Comp. Fluid Dynamics, 9, 249-272.

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.

Leach, M., S. Chin, J. Leone, Jr., G. Sugiyama, and H. Walker, 2002: Urban Effects in Numerical Models and Evaluation with Field Experiments Data, Part III: Comparisons to Tracer Data, 4th Symposium on the Urban Environment, Norfolk, VA, May 20-24, 2002.

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.

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