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Large Eddy Simulation of Turbulent Flow and Dispersion in Urban Areas and Forest Canopies

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LARGE EDDY SIMULATION OF TURBULENT FLOW AND DISPERSION IN URBAN AREAS AND FOREST CANOPIES

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1. INTRODUCTION

Under the sponsorship of the U.S. DOE and DHS, we have developed a CFD model for simulating flow and dispersion of chemical and biological agents released in the urban environment. Our model, FEM3MP (Chan and Stevens, 2000), is based on solving the three-dimensional, time-dependent, incompressible Navier-Stokes equations on massively parallel computer platforms. The model 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 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 data from wind tunnel (Chan and Stevens, 2000; Chan, et al., 2001) and field experiments (Chan, et al., 2002, 2003; Lee, et al., 2002; Humphreys, et al., 2003; and Calhoun, et al., 2004). Discussed below are several examples to illustrate the use of FEM3MP in simulating flow and dispersion in urban areas and forest canopies, with model results compared against available field measurements.

2. FLOW AND DISPERSION IN FOREST CANOPIES

There have been much effort to understand the processes of momentum, heat and mass exchange between forest canopies and the free atmosphere and advances have been achieved through both numerical simulations and field observations. Finnigan (2000) has published a recent review of turbulent flow within plant canopies. While early theories suggested that canopy turbulence involves a superposition of energetic small scale eddies from plant wakes with surface layer turbulence, more recent studies have shown that canopy flows are dominated by transient, large coherent structures on the scale of the entire canopy. This implies that the traditional “steady-state” Reynolds-average approach to model canopy turbulence and diffusion may be inadequate and more advanced modeling approach such as LES is required.

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2.1 Forest Canopy Field Experiments

The cases selected for this study are: trial No. 11 of the experiments conducted in a South Carolina coastal forest during the summer of 1964 (Shinn, 1969) and a recent air tracer experiment performed in a tropical forest in 2001(Shinn, et al., 2002).

The first case involves a 32-m high forest canopy and a mean wind of 4.5 m/s at 59 m. In addition to wind data, estimates were made for the variation of the leaf area density as a function of height. Florescent particles were released from a bomblet in the diffusion experiment.

The second case was conducted in a 12-m tall evergreen forest with a mean wind of 3.1 m/s at 20-m high under near neutral atmospheric stability and persistent wind conditions. The goal of the experiment was to provide a data set for evaluation of models to describe the behavior of a dispersing vapor cloud in a forest and a data set that would supplement experimental data from the literature. The experiment therefore was not extensive but was planned to be relatively efficient and cost-effective. Sulfur hexafluoride (SF_6) was released near ground level at a rate of 4.1 g/s for periods of 10-20 minutes and concentration were obtained within 60 m of the release point at locations inside and just above the forest canopy. Each air sample was collected by spatially averaging through a line sink, approximated by a horizontal, perforated tube of 15-m in length.

2.2 Model-Data Comparisons

The LES approach was employed for simulating both cases. The simulations were performed with the assumption that the simulated flow was neutrally stable and horizontally homogeneous to allow a relatively small domain to be used. Specifically, a domain size of 360m x 120m x 100m was used for the first case and a domain of 360m x 120m x 60m was used for the second case. Graded mesh was used in both cases, with 121 x 41 x 49 grid points for the first case and 121 x 41 x 37 grid points for the second case, respectively.

Boundary conditions for the flow simulations include no slip on the ground surface and no penetration on the top boundary. In addition, periodic boundary conditions were used in both horizontal directions. A constant pressure gradient in the longitudinal direction was used to maintain the total momentum of the flow, since the top boundary has no momentum fluxes and the

bottom boundary is a momentum sink. After several trials, a value of –0.005 Pascal/m was selected for both cases. It appears to yield a good match between the predicted and measured mean velocity, namely, ~4.5 m/s at 59-m high in the first case and ~3.1 m/s at 20-m high in the second case. Canopy effects were modeled as a drag force in the momentum equations, with an isotropic drag coefficient of 0.15 and a leaf area density function based on the field measurements.

For the dispersion results reported herein (for the second case), a simulation was firstly performed for 30 minutes to establish a statistically stable flow field and then SF_6 was released continuously at a rate of 4.1 g/s on the ground. The flow/dispersion simulation was carried out for 15 minutes and mean quantities for the flow, TKE, and concentration fields were obtained by time averaging the results over the last 10 minutes.

In the following, sample results, with Figs. 1 and 2 from the first case and Figs. 3 through 5 from the second case, are presented and compared with available data. Fig. 1(a) is a snapshot of the velocity and TKE fields on a vertical plane and 1(b) are the corresponding mean flow and TKE fields. Although the mean flow is basically one-dimensional, significant turbulent fluctuations are present as indicated in Fig. 1(a). The patchiness of the TKE field is a manifestation of the coherent structures often observed in canopy flows. As expected, the model predicts in 1(b) a very weak wind inside the forest canopy and a much stronger mean wind above the canopy. Since turbulent shear near the canopy top is the major source of turbulence production, the TKE field peaks immediately above the canopy and decreases only slightly till about two times the canopy height.

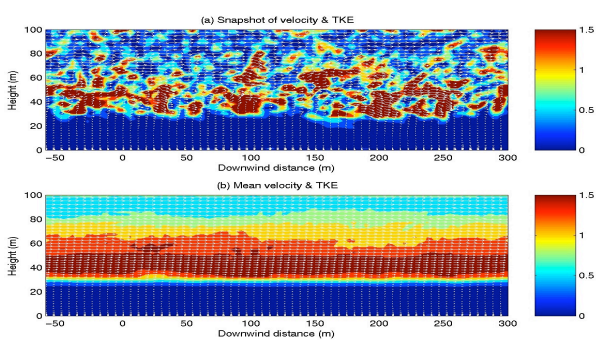

Fig. 1. Predicted velocity and TKE fields on a vertical plane for case 1: (a) Snapshot of velocity and TKE, and (b) Time-averaged velocity and TKE.

Fig. 2(a) shows the longitudinal velocity profiles for various times at a fixed downwind location, while Fig. 2(b) compares the predicted mean velocity profile with the measured data (in *). In general, the agreement between model predictions and measured data, including an upward displacement of the boundary layer by ~70% of the canopy height, is very good. The predicted turbulence intensity and mean TKE profiles in 2(c) and 2(d) are also in good agreement with the measured data. The largest discrepancy in turbulence intensity at z=9.2 m is prabably due to instrument malfunction, which measured a wind speed only ~40% of the values recorded by nearby stations.

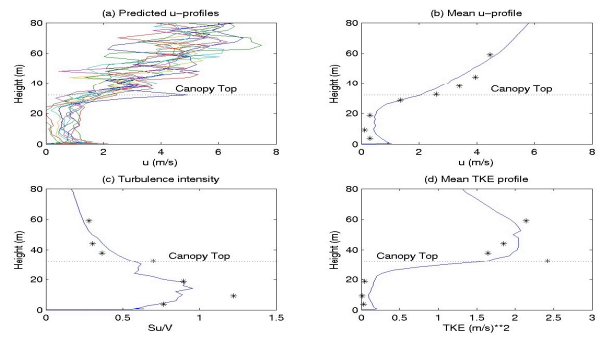

Fig. 2. Predicted versus measured velocity and TKE profiles for case 1: (a) Predicted u-velocity profiles, (b) Mean u-velocity profile, (c) Turbulence intensity profile, and (d) Mean TKE profile. Solid lines are model predictions and asterisks are measured data.

In Fig. 3, snapshots of the predicted velocity and concentration fields on the vertical center plane and z=1.2 m horizontal plane are shown for t=13 minutes after release of the tracer. These plots show that, due to calm winds and low vertical mixing inside the canopy, the bulk of the released tracer tends to stay inside the canopy. Additionally, the vortex structures above the tree canopy have produced the so-called upstream sweep and downstream ejection of the tracer, thus resulting in a rather complex plume in both vertical and horizontal directions.

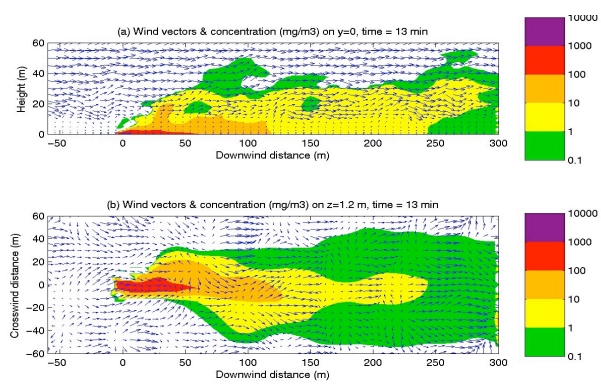

Fig. 3. Snapshots of predicted wind vectors and concentration contours (in mg/m^3) on two planes at time=13 minutes after start of source release for case 2: (a) Vertical center plane, and (b) z=1.2 m horizontal plane.

In Fig. 4, the mean velocity and concentration fields, averaged over time=5 to 15 minutes, are shown on the vertical center plane and z=1.2 m horizontal plane, respectively. This figure indicates a region of concentration greater than 10 mg/m^3 extending to about 10 m vertically, ~40 m laterally, and ~110 m in the downwind direction. The region with concentration greater than 100 mg/m^3 is much smaller, reaching only a few meters high and ~50 m in the downwind direction. As hinted by Fig. 4(b), a somewhat longer averaging time is probably needed in order to obtain a plume more symmetric about its centerline.

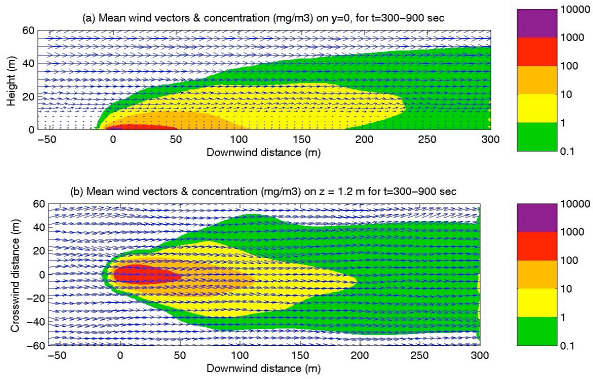

Fig. 4. Predicted mean wind vectors and concentration contours (in mg/m^3) on two planes for case 2: (a) Vertical center plane, and (b) z=1.2 m horizontal plane.

The predicted mean concentrations and measured data at various locations are compared in Fig. 5. In general, the agreement is very good for downwind locations at x=7.2, 20, and 38 m. The drop-off rates of concentration at z=1.2 m are ~1/X $^{0.49}$ from the model and ~1/X $^{0.57}$ from the data. At x=54 m, however, the agreement is poor. It is believed that this discrepancy was due to the line-sink sampler being located on the shoulder rather than on the centerline of the plume.

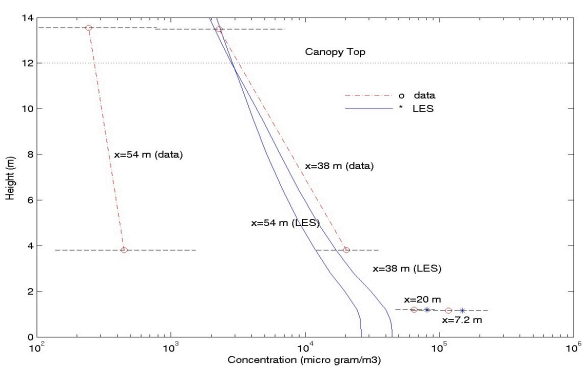

Fig. 5. Comparison of predicted versus measured mean concentrations (microgram/m^3) at various heights and downwind locations for case 2.

3. FLOW AND DISPERSION IN URBAN AREAS

Urban dispersion is an extremely complex problem, involving many physical processes and a wide range of length and time scales. The length scales typically span from building, urban, to regional and the time scales involve could range from minutes to days. Currently no single model is capable of treating all relevant physics and is able to simulate such a wide range of length and time scales. One possible approach is to construct a nested modeling system within a regional model to accommodate all spatial and temporal scales. An alternative approach is to build a system consisting of models of various scales with appropriate coupling among such models.

In the following, we present and discuss some results from a model validation study of FEM3MP in simulating a nighttime dispersion experiment conducted in Salt Lake City under light and highly variable winds.

3.1 The Urban 2000 Field Experiments

In the summer of 2000, DOE sponsored a field experimental program, Urban 2000, 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 one-hour 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. More details about the experiments are available in Allwine, et al. (2002).

3.2 Model-Data Comparisons

Release No. 1 of IOP 7 was selected for the present study. Shown in Fig. 6 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 to the southeast of Heber Wells building (the odd-shaped building near the center of Fig. 7) 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 winds were light and highly variable during the release.

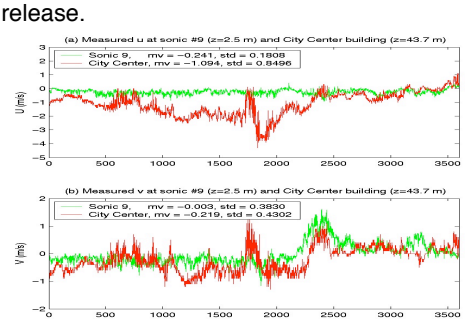

Fig. 6. Horizontal velocity components recorded by Sonic No.9 and sonic anemometer on the rooftop of City Center building during Release 1 of IOP 7.

To successfully simulate the flow and dispersion under such conditions is quite a challenge because of the low and highly variable winds. Three large eddy 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 time-dependent boundary conditions constructed respectively from the 1-sec sonic data measured by sonic 9 and that on the rooftop of the City Center building. In each case, a flow field was simulated for 30 min prior to the start of the dispersion simulation. Each dispersion simulation was performed for 60 min, with a ground level, line source of SF_6 released at a rate of 1 g/s on the south of Heber Wells building.

Shown in Fig. 7 are the predicted, time-averaged (for t = 50-55 min) concentration patterns on z=1 m plane from the simulation using time-independent inflow boundary conditions. Also superimposed in the figure are field data collected by gas samplers, which are plotted as small squares with the same color scheme. Obviously, the predicted plume shape and concentration patterns are quite different from those indicated by the field data. The predicted plume is mostly being dispersed to the west–southwest region, which is contrary to a plume surrounding the building as suggested by the measured data.

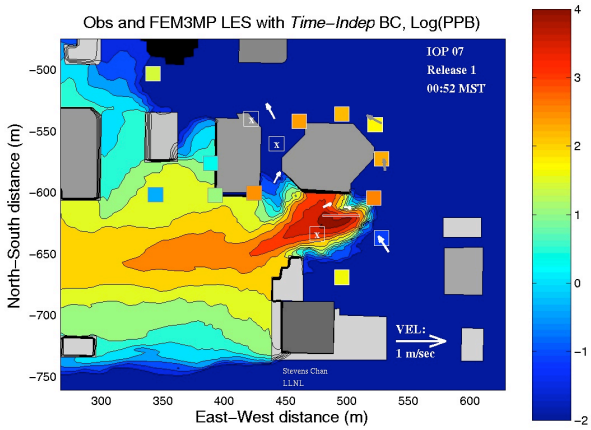

Fig. 7. Predicted time-averaged (for t=50-55 min) concentration patterns on z=1 m plane from simulation using time-independent boundary conditions based on time-averaged sonic 9 data.

In Fig. 8, concentration patterns from the simulation using time-dependent boundary conditions based on the actual 1-sec sonic No. 9 data are depicted and compared with the measured data. As a result of using the actual time-dependent forcing, instead of time-independent forcing used previously, the predicted plume is seen to spread also to the east and north, thus producing a plume shape in better agreement with what is suggested by the measured data.

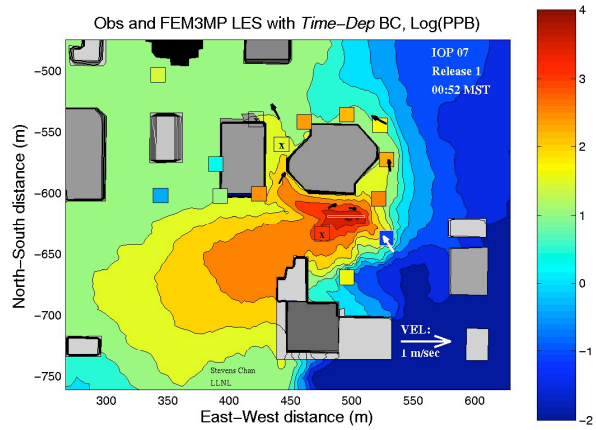

Fig. 8. Predicted time-averaged (for t=50-55 min) concentration patterns on z=1 m plane from simulation using time-dependent boundary conditions constructed from 1-sec sonic 9 data.

In Fig. 9, results from the simulation using time-dependent forcing based on the 1-sec sonic data collected on the rooftop of the City Center building are plotted and compared with field measurements. As is seen, this simulation has produced a plume being dispersed in all directions with a significant part of the plume drifted to the north and between buildings. The predicted plume shape and concentrations are the most consistent with what is indicated by the measured data. These results imply that the City Center sonic data are fairly representative of the upwind conditions during the dispersion experiment.

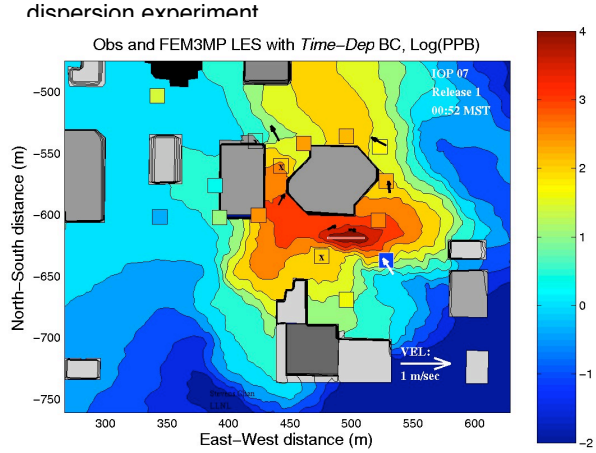

Fig. 9. Predicted time-averaged (for t=50-55 min) concentration patterns on z=1 m plane from simulation using time-dependent boundary conditions constructed from 1-sec sonic data collected on the rooftop of City Center building.

In Fig. 10, the predicted, averaged concentrations at the gas sampler locations in the vicinity of Heber Wells building are compared quantitatively with the measured data (circles in magenta). Again, results from the simulation using time-independent inlet velocity (blue line) are very poor, since the simulated plume misses most of the sampler locations (see Fig. 7). Significant improvements are obtained from the simulation using the actual 1-sec 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 City Center sonic data has further improved the agreement between model predictions (red line) and measured data to within a factor of 2 for most of the sampler locations.

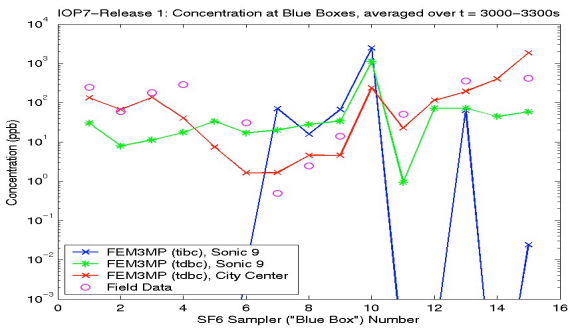

Fig. 10. Comparison of time-averaged (for t=50-55 min) concentrations measured at gas sampler locations (circles in magenta) and predicted by simulations using time-independent boundary conditions (blue line), time-dependent boundary conditions based on sonic No.9 data (green line), and time-dependent boundary conditions based on City Center sonic data (red line).

The above results demonstrate clearly the importance of imposing appropriate time-dependent forcing in dispersion simulations involving light and highly variable winds. Our results also show that model predictions can be greatly improved, even only data from a single sensor are available. For more accurate model predictions, however, more data in space and time to adequately represent the large scale forcing are needed. Such data have to be provided by field measurements and/or accurate larger scale models.

4. FUTURE PLANS

We will continue to conduct model verification and validation studies, using field data from Urban 2000 and Joint Urban 2003 experiments. Particular focus will be placed on different atmospheric stability and on inflow boundary conditions and their effects on the accuracy of model predictions.

While high-resolution CFD models are very useful for emergency planning, vulnerability analyses, post-event assessments, and development of mitigation strategies, such models generally require large computer resources and long turnaround times and are thus unsuitable for emergency response situations. To meet such needs, we are developing a simplified CFD approach for integration into the 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, while the remaining buildings are represented as drag elements (or virtual buildings) with much coarser grid resolution. Early test results (Chan, et al., 2004) indicated the approach is potentially very cost-effective and is being further evaluated via a quantitative comparison with data collected during the Joint Urban 2003 field experiment.

Besides the afore-mentioned efforts, we are incorporating FEM3MP into an adaptive dispersion model (ADM) framework to further improve its adaptability, flexibility and efficiency. We are coupling our flow solver with adaptive mesh refinement and developing rapid geometry-to-mesh techniques and approaches to support geometrically complex structures as well as urban simulations. This effort utilizes the SAMRAI (Structured Adaptive Mesh Refinement Application Interface) and the Rapsodi grid generation tools available within LLNL (Hornung, et al., 2002; Petersson 2002). The ADM approach will enable us to simulate flow and dispersion in larger urban areas and, at the same time, focus high grid resolution on the urban area of interest.

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: 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. Symposium on Environmental 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, AMS Annual Meeting, Seattle, WA, January 11-15, 2004.

Finnigan, J., 2000, Turbulence in Plant Canopies, Annual Rev. Fluid Mech., 32:519-571.

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

Hornung, R. and S. Kohn, 2002: Managing Application Complexity in the SAMRAI Object-Oriented Framework. Concurrency and Computation: Practice and Experience, 14, 347-368.

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.

Petersson, N. 2002: A Software Demonstration of “rap”: Preparing CAD Geometries for Overlapping Grid Generation, Proceedings of the 8th International Conference on Numerical Grid Generation in Computational Field Simulations, UCRL-JC-147260.

Shinn, J.H., 1969, Analysis of Wind Data From a South Carolina Coastal Forest, U.S. Army Electronics Command, Research and Development Tech. Report ECOM-6036.

Shinn, J., R. Pletcher, and S. Chan, 2002: A Simplified Dispersion Experiment in a 12-M Forest, AMS 25th Conference on Agricultural and Forest Meteorology, Norfolk, VA, May 2002, 22-23.

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