AMS 14th Joint Conference on the Applications of Air Pollution Meteorology with the A&WMA, Atlanta, GA, Jan 30 - Feb 2, 2006.

J1.8 APPLICATION OF CFD SIMULATIONS FOR SHORT-RANGE ATMOSPHERIC DISPERSION OVER OPEN FIELDS AND WITHIN ARRAYS OF BUILDINGS

Wei Tang *
National Research Council Research Associate at National Exposure Research Laboratory,
US Environmental Protection Agency, RTP, NC

Alan Huber
Atmospheric Sciences Modeling Division, in partnership with
US EPA National Exposure Research Laboratory, RTP, NC

Brian Bell, and Walter Schwarz
Fluent, Inc., Hanover, NH

1. INTRODUCTION

Computational Fluid Dynamics (CFD) techniques are increasingly being applied to air quality modeling of short-range dispersion, especially the flow and dispersion around buildings and other geometrically complex structures. The proper application and accuracy of such CFD techniques needs to be assessed. Fluent, Inc and the US EPA National Exposure Research Laboratory are working cooperatively to demonstrate CFD simulation as a proven and applied tool in support of environmental assessment studies (Huber et al., 2004). Part of the ongoing work has focused on the development of computer models and the evaluation of the performance of the FLUENT code in simulating: (1) the atmospheric boundary layer, (2) plume dispersion over an open field, and (3) dispersion within arrays of buildings.

FLUENT Version 6.2 was used for this study. The FLUENT code solves conservation equations for mass, momentum and energy. In addition, FLUENT models the mixing and transport of a chemical species by solving conservation equations describing convection and diffusion for the species. For turbulent flows, the Reynolds-averaged approach is employed to solve the Navier-Stokes equations. A number of turbulence models are provided in FLUENT to achieve closure. In this study, we examined results using the standard k-ε turbulence model (Launder and Spalding, 1972). The goal is to develop and demonstrate applications for applying steady-state Reynolds-averaged Navier-Stokes equations (RANS) with k-ε turbulence model since it is practical for routine applications today. If necessary, future developments will continue on to unsteady solutions using higher order turbulence models. A full description of the code defaults and options is provided in the FLUENT User's Guide (Fluent Inc, 2005).

Case studies based on the Project Prairie Grass field program (Barad, 1958) were used to develop and evaluate CFD simulations of plume dispersion over an open field under thermally neutral and unstable conditions. CFD predictions of arc concentrations were compared with measurements and results of the AERMOD dispersion model (Cimorelli, et al., 2005). Analyses for the near thermally neutral cases have been completed and are summarized herein. Analyses for the thermally unstable cases are ongoing therefore only a case study is presented.

Simulations of dispersion around buildings are being evaluated with data from the Mock Urban Setting Test (MUST) field experiment (Biltoft, 2001). Methods for applying CFD simulations for these complex flow situations are being developed. Only the setup for a case is presented herein. Progress is ongoing and updated results will be summarized in the oral presentation.

2. SIMULATION OF PROJECT PRAIRIE GRASS

While the primary interest in application of CFD methods is to simulate flow around buildings, it is important to demonstrate the ability of the CFD code to correctly model a plume in absence of any buildings, where the flow is relatively simple and well-defined. If there are problems within the code, they can be more easily identified and resolved.

* *Corresponding author address*: Wei Tang, NERL/AMD, Mail drop E243-03, US EPA, RTP, NC 27711; email: tang.wei@epa.gov

The Project Prairie Grass field study (Barad, 1958) includes 70 experiments with continuous releases of neutrally buoyant tracer gas over an open agricultural field. The study provides a good test bed for developing the CFD applications and assessing the code's performance. This field study has routinely been used for evaluating atmospheric dispersion models. In part, this database is the basis for development of the widely applied Gaussian straight-line plume models. By comparing results of the CFD simulations with the Prairie Grass data, we can demonstrate how the CFD model compares with other types of dispersion models. The goal here is not to demonstrate that CFD simulation should be routinely used where applications of Gaussian straight-line plume models have been found to work. Instead we are trying to demonstrate comparability as the basis for applying CFD simulations to more complex thermal environments and where there are significant building influences. The CFD simulation needs to be developed for the many applications where the Gaussian straight-line plume models do not perform as well.

2.1 *Model Methodology*

Simulation of the atmospheric boundary layer is critical to modeling plume dispersion. Good simulation of bulk transport requires that the mean flow field be well modeled, while predicting the right level of turbulence is essential to capturing the turbulent dispersion of a pollutant. Using FLUENT, a two-dimensional (2D) domain (x, z ; wind along x, vertical direction z) was used to simulate a well-developed boundary layer. Vertical profiles were generated for pressure, temperature, mean velocity (U), turbulent kinetic energy (TKE), and turbulent dissipation rate (ε). Required inputs include friction velocity, roughness height and mass flow rate.

The generated boundary layer profiles were then used as the inlet profiles for the dispersion simulation in a three-dimensional (3D) full domain. Plume dispersion was simulated using the species transport modeling capability in FLUENT. An important model parameter is the turbulent Schmidt number (Sc), since it characterizes the relative diffusion of momentum and pollutant mass due to turbulence:

$$Sc = \frac{\mu_t}{\rho D_t}$$

where μ_t is the turbulent viscosity and D_t is the turbulent diffusivity. Values of Sc from 0.18 to 1.34 have been reported based on field observations under different atmospheric stability and wind conditions (Flesch, 2002). Three values (0.7, 1.0, and 1.3) of Sc were examined here.

In this work, all simulations were run under steady-state conditions assuming constant wind speed and wind direction. These steady solutions were then smoothed over the time weighted distribution of wind direction fluctuation to account for the stochastic variation of wind direction. More details can be found in Tang et al. (2005).

The following sections discuss the results of simulated boundary layer flows and plume dispersion for the Project Prairie Grass conditions.

2.2 *Near Neutral Stability*

2.2.1 Boundary profile

During the Project Prairie Grass, 12 experiments can be classified as near thermally neutral. A summary of the 12 runs can be found in Tang et al. (2005). To demonstrate that a single CFD run can be applied for a given class of thermal stability and thus reduce overall computation time, a generic case was set up with input data determined by averaging meteorological data of the 12 near neutral runs. The mass flow rate was set to a value equivalent to a wind speed of 7.33 m/s at 10 m above the ground (U_{10m}). Average u_* was 0.44 m/s, and average z_0 was 0.012 m, which are similar to values reported by other studies (Briggs, 1982; van Ulden, 1978; Venkatram, 1980).

In Figure 1, the vertical profile of U normalized by U_{10m} is presented for both the CFD simulation and

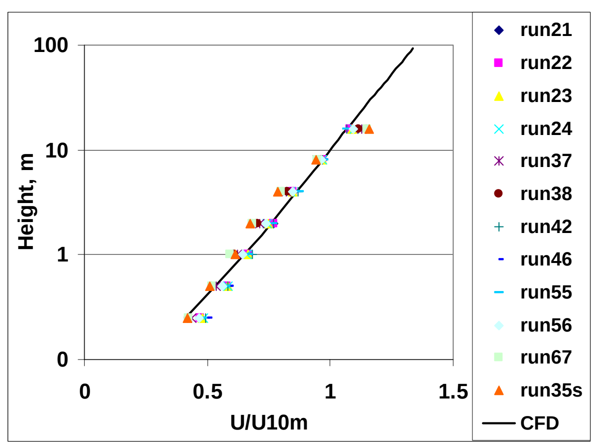


Figure 1. Comparison of modeled and measured vertical wind profiles

the observations during the 12 runs. Regardless of the variability among the 12 runs; the agreement between modeled and measured profiles is reasonably good. The modeled values of U are within ±15% of the measurements. The differences are small and we do not expect significantly improved results by setting a CFD run for each case.

The vertical profile of TKE is presented in Figure 2 for the generic case and compared with estimates based on similarity theory. According to Stull (1988), for a near neutral boundary layer, TKE can be calculated as follows:

$$\frac{\overline{u'^2}}{u_*^2} = A_u\left(1-\frac{z}{z_i}\right)^2$$

$$\frac{\overline{v'^2}}{u_*^2} = A_v\left(1-\frac{z}{z_i}\right)^2$$

$$\frac{\overline{w'^2}}{u_*^2} = \left(1-\frac{z}{z_i}\right)^{1/2}$$

$$TKE = \frac{1}{2}u_*^2\left(A\left(1-\frac{z}{z_i}\right)^2 + \left(1-\frac{z}{z_i}\right)^{1/2}\right)$$

where z_i represents the mixing height which here is taken as the depth of the CFD model boundary layer. A_u and A_v are empirical constants. $A = A_u + A_v$. A range of values were examined for A_u and A_v at 2.5 – 6. Plotted in Figure 2 are profiles for A = 5 and A = 9, where 9 represents the value reported from field studies by Stull (1988). The CFD modeled TKE profile falls between the two curves for the lower part of the boundary layer. The critical zone for this study is within the lower 100 m. For future studies where the critical zone extends

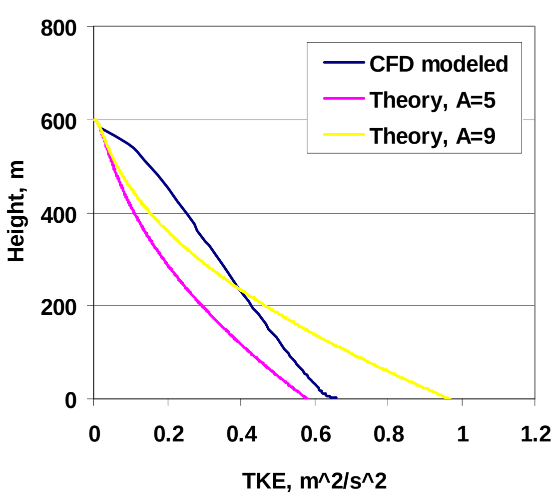


Figure 2. Vertical profile of simulated TKE

deeper into the boundary layer, we can modify our technique to result in a deeper matching zone.

2.2.2 Plume concentrations

Ratios of observed centerline concentrations (C_o) to model predictions (C_p) are plotted in Figure 3 for 8 out of the 12 neutral runs. The other 4 runs are not included because wide variation of wind direction was observed and their arc concentrations appear to have more than one peak value. As shown in Figure 3, all ratios are within the two horizontal thin lines, demonstrating that the model predictions of centerline concentrations were well within a factor of two of the observations. The 3 colored lines represent average values of C_o/ C_p for the 8 runs using different Schmidt numbers. It appears that on average, predictions using a Sc of 1.0 agree best with the observations. The scattered points, representing ratios for each run, are based on simulations with Sc = 1.0. Ratios for each run with Sc = 0.7 and 1.3, not shown here, would appear similarly scattered about their plotted averages. As demonstrated here, it is difficult to assign a single Sc number to characterize dispersion in various atmospheric boundary conditions. Flesch et al. (2002) reported similar observations from a tracer experiment. Nevertheless, we found that simulations with Sc in the range of 1.0 to 1.3 performed best in matching the measurements of the Project Prairie Grass.

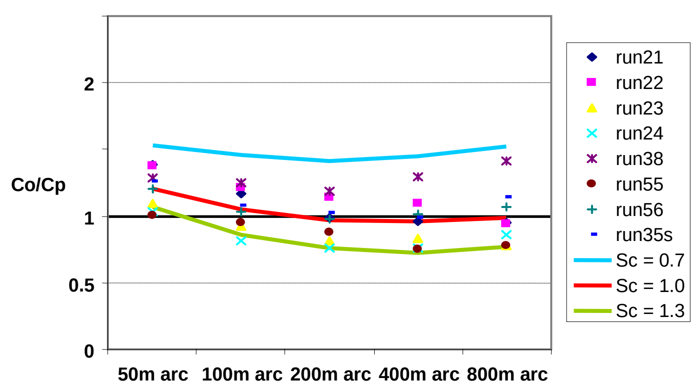


Figure 3: Ratio of measured and modeled centerline concentration at 5 arcs

In addition to centerline concentrations, comparisons were conducted for the crosswind concentration profiles at all arcs and the available vertical concentration profiles at the 100 m arc.

Figure 4 presents example comparisons of the crosswind profiles of normalized concentrations at the 5 sampling arcs for run 55. Also presented here are the model results of AERMOD, which were acquired from the model evaluation databases developed by the US EPA (2005). The CFD-based simulation of plume spread and centerline concentrations was found to match the measurements at all 5 arcs. Similar results have been observed for the other 8 near neutral runs with relatively constant wind direction. In general, simulations with Sc = 1.0 have the best agreement

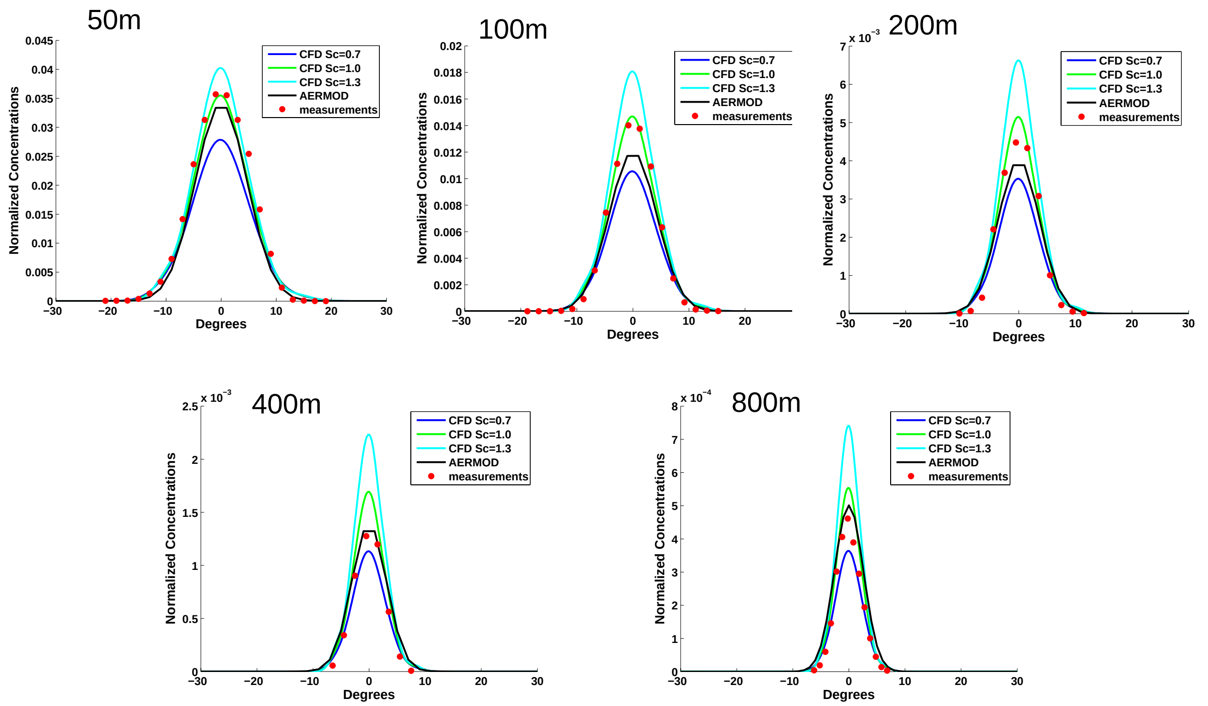


Figure 4. Comparison of crosswind profile of arc concentrations for Run 55

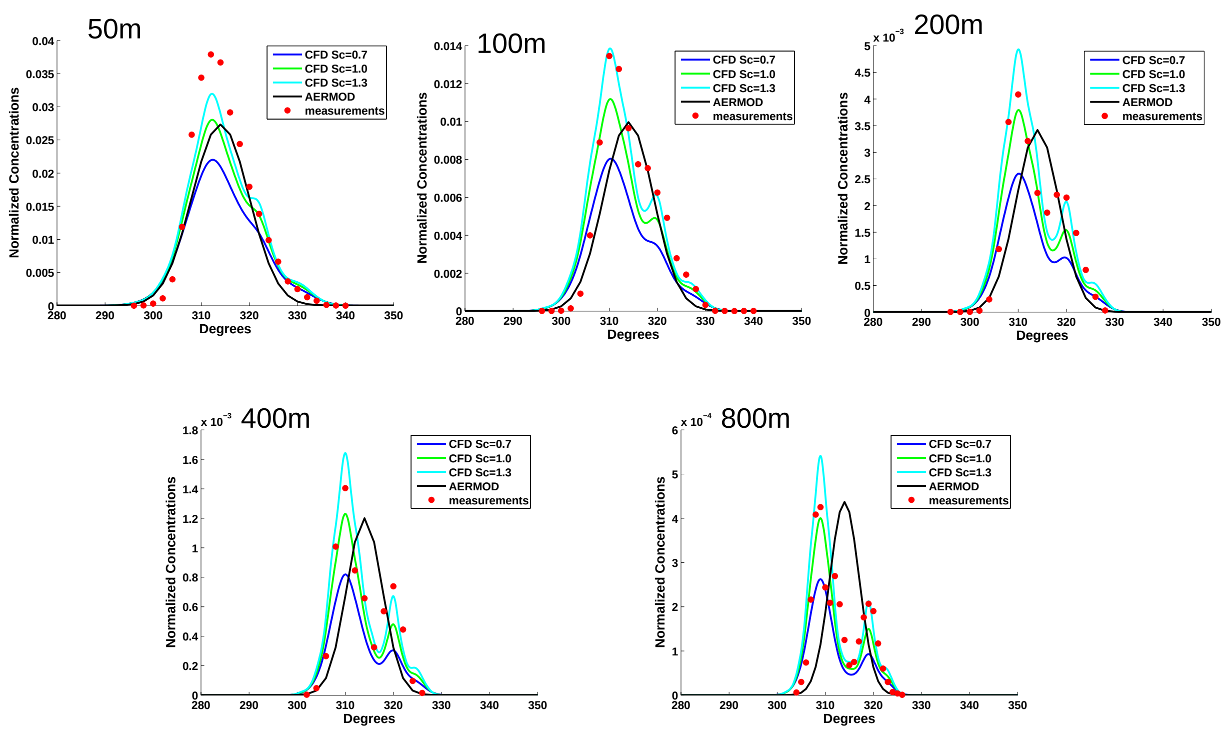


Figure 5. Comparison of crosswind profile of arc concentrations for Run 46

with the measurements, while at the 50m arc, simulations with Sc = 1.3 perform best for 5 out of the 8 runs. As expected, for simple dispersion in an open field, predictions by AERMOD are well within the range of the measurements. Similar comparisons are present in Figure 5 for run 46, which has wide variation of wind direction resulting in two peak values across the arc of concentrations. The CFD-based simulation is shown to capture both peaks caused by the wind direction variation.

Figure 6 presents the vertical profiles at two locations on the 100m arc for run 55. The vertical profiles were well predicted by the model. Similar results have been observed for other near neutral runs.

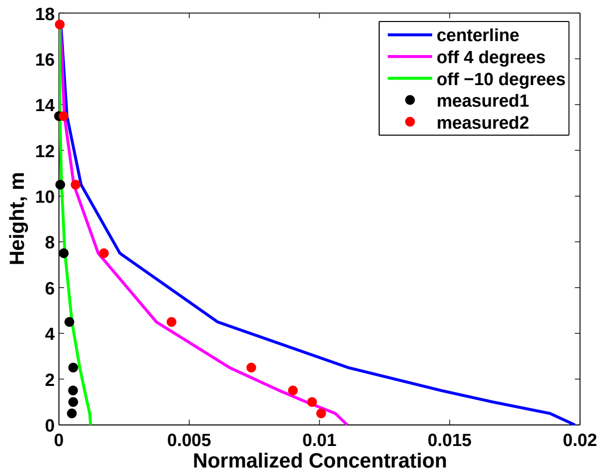


Figure 6: Comparison of vertical profile at 100m arc (Sc = 1.0) for Run 55. Measured 1 is at 10 degrees to the left of the centerline; measured 2 is 4 degrees to the right of the centerline.

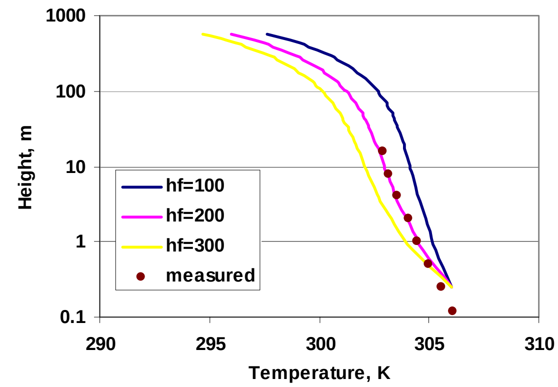
2.3 *Unstable Conditions*

Similar methodology as described in Section 2.1 is being applied to case studies of experimental runs under unstable conditions during Project Prairie Grass. Some modifications were made to account for the enhanced turbulence and to simulate its effect on dispersion. Extensive model evaluation is ongoing. Some preliminary results are presented here, and more updated results will be reported during the oral presentation.

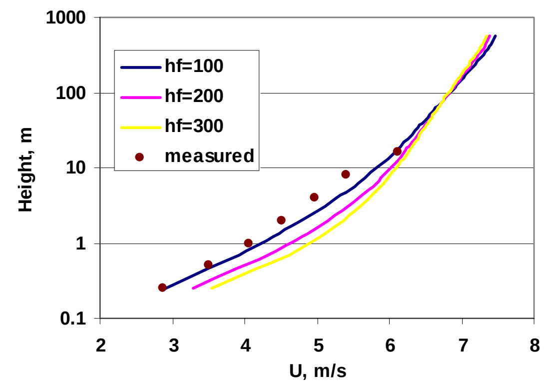
2.3.1 Boundary profile

For simulations of thermally unstable boundary layers, the FLUENT code was modified so that TKE generation caused by buoyancy is calculated based on potential temperature gradient. Net heat flux (hf) was added on the ground, and ground temperature was set to the measured value. One case study based on run 8 was set up with $u_* =$ 0.34 m/s, z_0 = 0.008 m, L = -18 m, and U_{10m} = 5.49 m/s. By adjusting the amount of heat flux, we can generate a temperature gradient to match the measured data as shown in Figure 7a.

(a) Vertical profiles of temperature



(b) Vertical profiles of mean velocity



(c) Vertical profiles of TKE

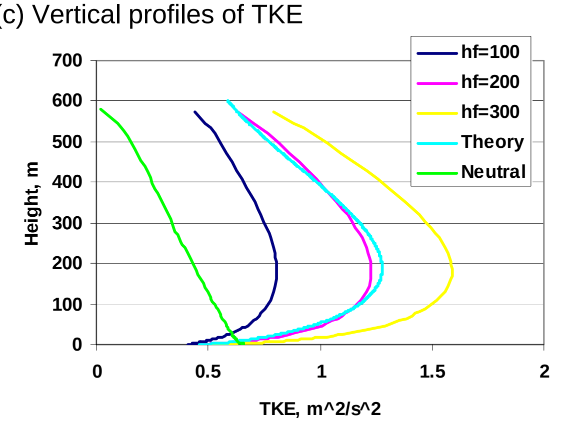


Figure 7: Vertical characterizations of simulated unstable boundary layer with different heat flux (hf)

The simulated profiles of mean velocity are shown in Figure 7b, and compared with the measurements. The best comparison is hf = 200 W/m^2 for temperature, and hf = 100 W/m^2 for mean velocity. Some fine adjustments on heat flux and mass flow rate are needed to match both measured temperature and mean velocity with the same surface boundary conditions.

Figure 7c presents the simulated profiles of TKE when different amounts of heat flux are applied at the ground. Also plotted is an estimated profile based on similarity theory (Stull, 1988). The equations used are:

$$\frac{\overline{u'^2}}{u_*^2} = B_u$$

$$\frac{\overline{v'^2}}{u_*^2} = B_v$$

$$\frac{\overline{w'^2}}{w_*^2} = 1.8\left(\frac{z}{z_i}\right)^{2/3}\left(1-0.8\frac{z}{z_i}\right)^2$$

$$TKE = \frac{1}{2}\left(Bu_*^2 + 1.8w_*^2\left(\frac{z}{z_i}\right)^{2/3}\left(1-0.8\frac{z}{z_i}\right)^2\right)$$

where empirical constants B_u = 4, B_v = 4, B = B_u+B_v = 8.

The CFD results are consistent with the profile based on similarity theory, in terms of the height at which TKE value peaks. The profile for hf = 200 W/m^2 matches best with the theory. There is significant enhancement of turbulence in the thermal boundary layer when compared with the TKE profile under near neutral conditions.

2.3.2 Plume concentrations

Figure 8 presents example comparisons of the crosswind profiles of normalized concentrations at the 5 sampling arcs for run 8 with different heat flux added on the ground. Estimates by AERMOD (US EPA, 2005) are also plotted. The CFD results are consistent with AERMOD results, especially when hf = 200 W/m^2. The degree of agreement varies at the 5 arcs. More case studies are being carried out to improve the model performance. Schmidt number used for this example is 0.7. Other values need to be examined.

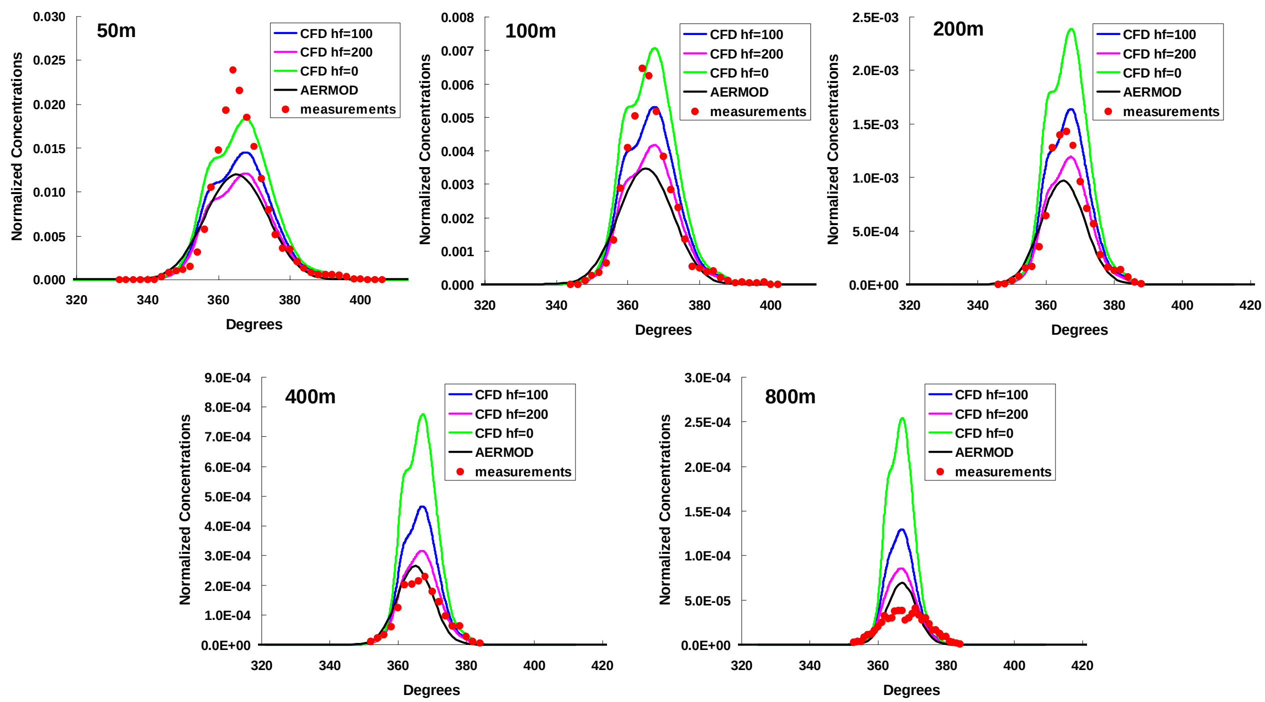
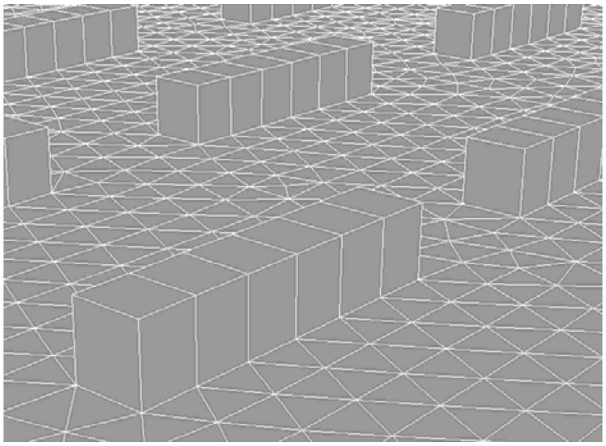
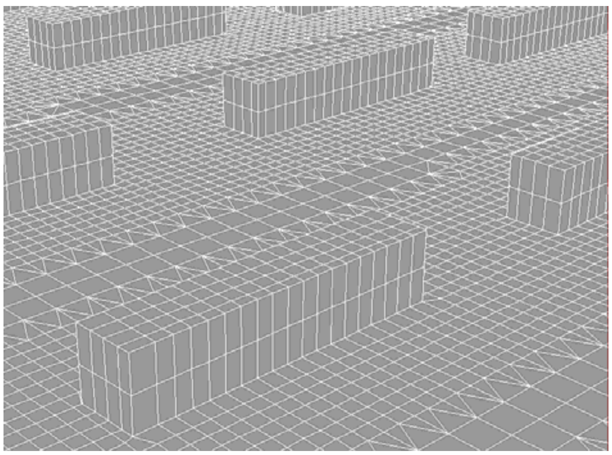


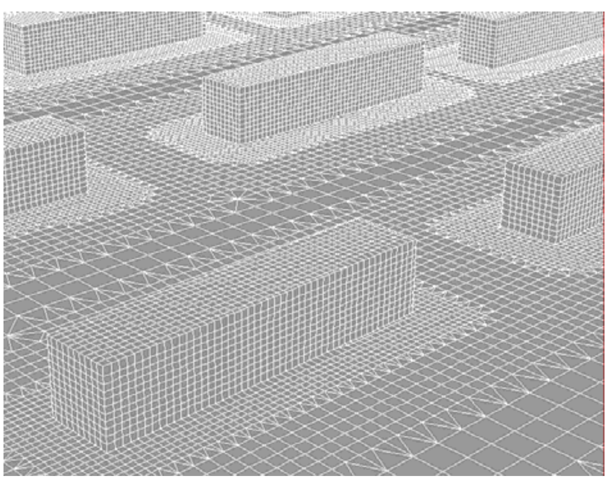
Figure 8. Comparison of crosswind profile of arc concentrations for Run 8



(a) 364K Mesh



(b) 1.3M Mesh



(c) 6M MESH

Figure 9: Three different meshes for simulation of MUST

3. SIMULATION OF MUST FIELD EXPERIMENT

Simulations of dispersion around buildings are being evaluated with data from the MUST field experiment (Biltoft, 2001, Yee and Biltoft, 2004). This near full-scale experiment was designed to support urban dispersion model development and validation. The 68 tracer gas releases were conducted in an array of 10 by 12 shipping containers at the U.S. Army Dugway Proving Ground in Utah. The MUST experiment provides extensive spatial and temporal measurements of dispersion data and meteorological data.

The same two-step approach as used in case studies of Project Prairie Grass are being applied to the MUST experiment. Boundary profiles are generated using a 2D domain and are used as the inlet boundary profiles for simulations of dispersion within arrays of obstacles. A domain of 300 m by 300 m by 50 m was created. The obstacle array, with overall width and length of 193 m and 171 m, is centered on the ground of the domain. Three different volume meshes are being tested to examine mesh dependency, as shown in Figure 9. Steady-state solution of the flow field is first obtained using standard k-ε turbulence model. The transient solver is then used to simulate the release of the tracer gas and the development of the plume. The simulations are ongoing and results will be summarized during the conference presentation.

4. CONCLUSIONS

CFD modeling has emerged as a promising technology for simulating wind flow and pollutant dispersion, especially in urban microenvironments. In order to have confidence in such models, thorough evaluation and consideration of dispersion mechanisms are required.

Model dispersion in absence of obstacles is a critical first step before application to more complex situations with flow and dispersion around buildings and other geometrically complex structures. Case studies based on the Project Prairie Grass field program were used to develop and evaluate CFD simulations of plume dispersion over an open field. Analysis for the near thermally neutral cases has been completed. The simulated results demonstrated good agreement with tracer gas release data, in terms of both the whole plume distribution and the centerline concentration. Work has been extended to thermally unstable wind transport and there is ongoing work that must be completed. Updated results will be provided during the conference oral presentation.

Simulations of dispersion around buildings are being evaluated with data from the MUST field experiment which involves obstacle arrays. Simulations of pollution dispersion within obstacle arrays over periods of varying wind speed and direction are more challenging than for the same over open fields. Best methods for applying CFD simulations for these complex flow situations are being developed. Updated results will be provided during the conference presentation.

This paper demonstrates that CFD methods can well simulate the atmosphere-like boundary layer and plume dispersion over an open field. While atmospheric turbulence is known to be non-isotropic, applications of *k-ε* turbulence model appears to be sufficient for simulating plume dispersion. We anticipate Gaussian plume models are adequate for many applications without complicated building influences. The goal of our ongoing research is to demonstrate applications to more complex situations where the Gaussian plume models likely fail. Broader use of CFD modeling should be expected once applications can be demonstrated using established standard practices. For an experienced CFD modeler setup of the boundary layer simulation should take less than a day followed by 2 to 7 days to set up and run the specific case study for a small area surrounding an industrial facility depending on the number of buildings involved. More experience is needed to establish good estimates. This research is leading to the development of general guidelines to support future broad application of CFD code for simulating short-range atmospheric dispersion of pollution where refined solutions are needed.

Disclaimer – The research presented here was performed in part under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement number DW13921548. Although it has been reviewed by EPA and NOAA and approved for publication, it does not necessarily reflect their policies or views.

REFERENCES:

Barad, M.L. (Editor), 1958. *Project Prairie Grass. A field program in diffusion*. Geophysical Research Paper, No. 59, Vols. I and II, Report AFCRC-TR-58-235, Air Force Cambridge Research Center, Bedford, MA.

Biltoft, C.A., 2001. *Customer Report for Mock Urban Setting Test*, DPG Document No. WDTC-FR-01-121, West Desert Test Center, U.S. Army Dugway Proving Ground, Dugway, Utah.

Briggs, G.A., 1982. Similarity forms for ground-source surface-layer diffusion. *Boundary-Layer Meteorology*, 23, 489-502.

Cimorelli, A. J.; Perry, S. G.; Venkatram, A.; Weil, J. C.; Paine, R. J.; Wilson, R. B.; Lee, R. F.; and Peters, W. D. 2005: AERMOD: A dispersion model for industrial source applications. Part 1: General model formulation and boundary layer characterization. *J. Appl. Meteorol.*, 44, 682-692.

Flesch, T.K.; Prueger, J.H.; Hatfield, J.L. 2002. Turbulent Schmidt number from a tracer experiment. *Agricultural and Forest Meteorology*. 111:299-307.

Fluent Inc, 2005. *FLUENT 6.2 User's Guide*. Fluent Inc, Lebanon, NH.

Huber, A.H.; Tang, W.; Flowe, A.; Bell, B.; Kuehlert, K.; and Schwarz, W., 2004. Development and applications of CFD simulations in support of air quality studies involving buildings. 13th Joint Conference on the Applications of Air Pollution Meteorology with the Air & Waste Management Association, (CD-ROM) Vancouver, British Columbia, Canada, August 23-27, 2004.

Launder, B.E. and Spalding, D.B. 1972. Lectures in Mathematical Models of Turbulence. Academic Press, London, England.

Stull, R.B., 1988. An Introduction to Boundary Layer Meteorology. 1st edition. Kluwer Academic Publishers. Dordrecht.

Tang, W.; Huber, A.H.; Bell, B.; Kuehlert, K.; and Schwarz, W. Example application of CFD simulations for short-range atmospheric dispersion over the open fields of project prairie grass. The Air & Waste Management Association 98th Annual Conference and Exhibition, (CD-ROM) Minneapolis, Minnesota, June 21-24, 2005.

US EPA, 2005, website accessed, http://www.epa.gov/scram001/dispersion_prefrec.htm#aermod van Ulden, A.P., 1978, Simple estimates for vertical diffusion from sources near the ground, *Atmospheric Environment.* 12:2125–2129.

Venkatram, A., 1980, Estimating the Monin-Obukhov length in the stable boundary layer for dispersion calculations. *Boundary-Layer Meteorology*, 19, 481-485

Yee, E. and Biltoft, C.A., 2004. Concentration fluctuation measurements in a plume dispersing through a regular array of obstacles. *Boundary-Layer Meteorology*, 111, 363-415.