

## 7.7 ADDRESSING HUMAN EXPOSURES TO AIR POLLUTANTS AROUND BUILDINGS IN URBAN AREAS WITH COMPUTATIONAL FLUID DYNAMICS (CFD) MODELS

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### 1.0 INTRODUCTION

Computational Fluid Dynamics (CFD) simulations provide a number of unique opportunities for expanding and improving capabilities for modeling exposures to environmental pollutants. The US Environmental Protection Agency's National Exposure Research Laboratory (NERL) has been conducting cooperative research with Fluent, Inc to examine and evaluate the application of CFD models for simulating air pollution along the pathway from source to human exposures. The basic framework of population-based human exposure models separates a person's day into time spent in a series of exposure microenvironments. The environmental concentration in these exposure microenvironments is weighted by the time-spent in each microenvironment to provide a total daily exposure. The detailed spatial resolution of environmental pollution concentrations that is possible from CFD simulations can provide important information that is not available from a single point measurement. There are multiple potential roles for CFD simulations in supporting human exposure studies which will be presented outside of this brief abstract. In this study, we are examining in detail the urban buildings and roadway microenvironments of human exposure to ambient air pollutants. This abstract can present only a summary of some of the issues we are examining and a few examples of progress.

### 2.0 CFD MODEL SETUP

The commercial CFD software FLUENT (<http://www.fluent.com>) along with its model geometry and mesh generating software (GAMBIT) is being used. *Model Geometry and Mesh Set-up in GAMBIT*

There are key elements with many options, which must be set up before GAMBIT calculates a mesh. The model domain boundary conditions (including atmospheric reality) are critical. The inlet and outlet positions relative to the study focus area can be critical. The grid resolution has to take into consideration the ratio between large and small scales of the flow. With a wide range of length scales a structured meshing becomes less flexible, more time consuming and memory intensive. An unstructured approach can reduce meshing time dramatically because a large portion of the process is automated. Unstructured grids provide flexibility in setting up a dense mesh where it is needed and allow for local grid adaptation. Consideration of the temporal scales of interest is also critical.

#### *Model Set-up in FLUENT*

There are key elements with many options, which must be set before FLUENT calculates a solution. The coupled solvers (explicit and implicit) are recommended if a strong inter-dependence exists between density, energy, momentum, and/or species (i.e., finite-rate

reaction modeled flows). The segregated (implicit) solver is preferred in all other cases because of lower memory requirements and more flexibility in solution procedure. For the usual air pollution application the segregated solver is the model of choice. The flow is incompressible and turbulent and the pollutant transport equation can be resolved at the post-processing level because the dispersion does not impact the flow. The turbulence model is chosen according to the complexity of the geometry and the flow. FLUENT offers a variety of models ranging from a one-equation model to a Large Eddy Simulation (LES). Recent Reynolds-Averaged Navier-Stokes (RANS) models seem to significantly improve accuracy of the numerical solution of turbulent flows around buildings but have not been completely satisfactory. LES remains the desired model of choice and will play an increasingly important role in the future as computational capacities continue to increase.

### 3.0 EXAMPLES

The FLUENT software is run using 2 processors on a SGI Onyx2 workstation which is 100% available to this project and using 16-32 processors on the EPA National Environmental Supercomputing Center (NESC) CRAY T3E as it is available. The project is evaluating fundamental features of the software by comparing model simulation results with data from wind tunnel studies. The set up of a range of atmospheric boundary layer characteristics is being studied. Evaluation with wind tunnel measurement data is a critical step. We are particularly interested in examining the improvements resulting from more refined simulations and at what costs. Our goal is to be able to apply CFD simulations for an urban area such as Manhattan. A model for Manhattan has been set up (Figure 1) and we are comparing the CFD simulations of CO concentrations from roadway emissions to four monitoring stations. A single simulation has so far been limited to selecting a region of 2.5 million cells (~ 25% of the domain). Figure 2 shows the diurnal cycle of CO which is dominated by automobile traffic. Morning and afternoon peak concentrations occur during peak traffic periods which is absent during weekend mornings. Meteorological conditions effect daily variability. The highest and lowest concentrations arise between two sites that are closest. This example demonstrated why a single point value is not very reliable for representing a large area of potential exposure. We are working to explain these concentrations. Figure 3 presents an example vertical plane of the wind vectors. Notice the strong upward winds on the lee side of the Empire State Building and the multiple scales of interaction between the buildings and street canyons which contain the pollutant sources. The simulated wind patterns are being compared with measurements in NYC Central Park and surrounding sites. Our progress is encouraging to us. Much more detail and conclusions will follow. Evaluation with other wind tunnel and field data is ongoing and more is needed [collaborators are welcomed].

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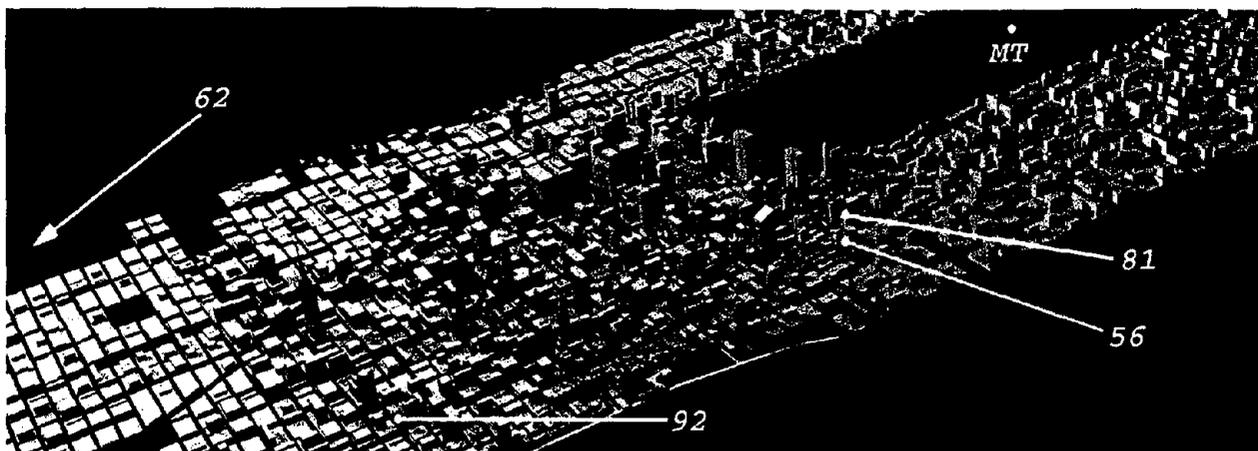


Figure 1. Manhattan CFD model domain with CO sites (81,56,92,62) and meteorological tower (MT) location.

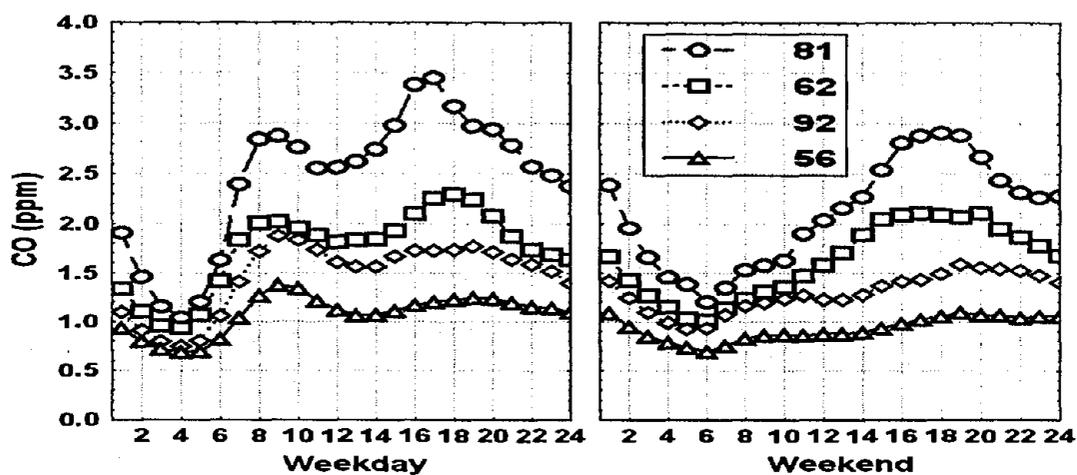


Figure 2. Annual-averaged (1996-98) diurnal cycle of Carbon Monoxide at four sites.

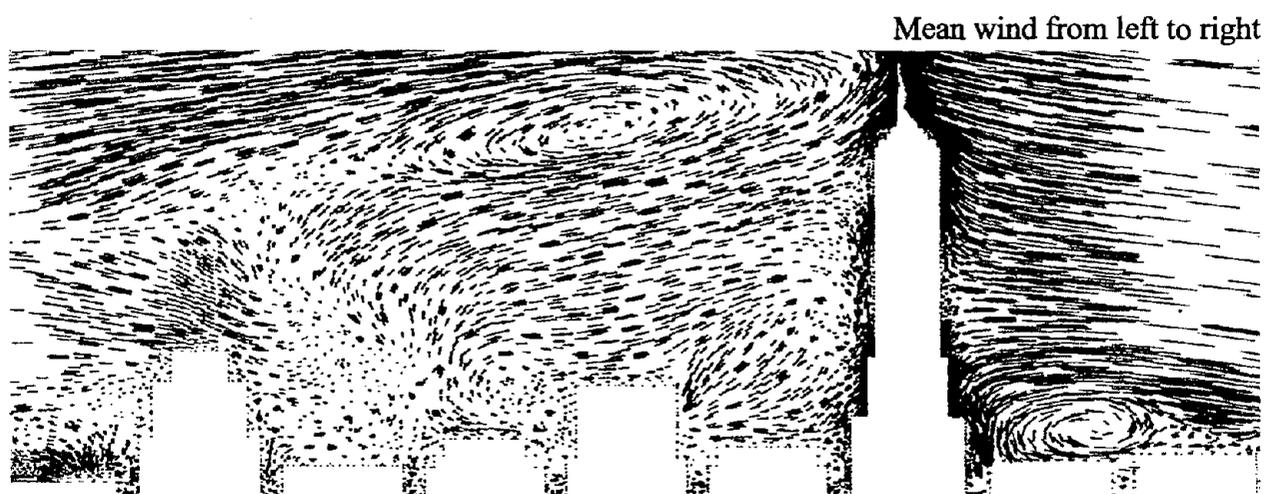


Figure 3. Example vertical plane of wind field (vector direction and speed) for a CFD simulation from the Manhattan domain (largest building is the Empire State Building).

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1. REPORT NO. <b>EPA/600/A-00/07B</b>	2.	3. BF
4. TITLE AND SUBTITLE Addressing Environmental Challenges with Computational Fluid Dynamics	5. REPORT DATE	
	6. PERFORMING ORGANIZATION CODE	
7. AUTHOR(S) <sup>1</sup> Alan H. Huber, <sup>2</sup> Mark Bolstad, <sup>2</sup> Mathew Freeman, <sup>2</sup> Santir Rida, <sup>1</sup> Eric S. Bish, and <sup>1</sup> Karl H. Kuchlert	8. PERFORMING ORGANIZATION REPORT NO.	
9. PERFORMING ORGANIZATION NAME AND ADDRESS <sup>1</sup> Same as Block 12  <sup>2</sup> USEAP Scientific Visualization Center Lockheed-Martin, RTP, NC  <sup>3</sup> Fluent Inc. 10 Cavendish Court Lebanon, NH 03766	10. PROGRAM ELEMENT NO.	
	11. CONTRACT/GRANT NO.	
12. SPONSORING AGENCY NAME AND ADDRESS National Exposure Research Laboratory Office of Research and Development U.S. Environmental Protection Agency Research Triangle Park, NC 27711	13. TYPE OF REPORT AND PERIOD COVERED	
	14. SPONSORING AGENCY CODE EPA/600/9	
15. SUPPLEMENTARY NOTES		
16. ABSTRACT  Computational Fluid Dynamics (CFD) simulations provide a number of unique opportunities for expanding and improving capabilities for modeling exposures to environmental pollutants. The US Environmental Protection Agency's National Exposure Research Laboratory (NERL) has been conducting cooperative research with Fluent, Inc to examine and evaluate the application of CFD models for simulating air pollution along the pathway from source to human exposures. The basic framework of population-based human exposure models separates a person's day into time spent in a series of exposure microenvironments. The environmental concentration in these exposure microenvironments is weighted by the time spent in each microenvironment to provide to a total daily exposure. The detailed spatial resolution of environmental pollution concentrations that is possible from CFD simulations can provide important information that is not available from a single point measurement. There are multiple potential roles for CFD simulations in supporting human exposure studies which will be presented outside of this brief abstract. In this study, we are examining in detail the urban buildings and roadway microenvironments of human exposure to ambient air pollutants. This abstract can present only a summary of some of the issues we are examining and a few examples of progress.		
17. KEY WORDS AND DOCUMENT ANALYSIS		
a. DESCRIPTORS	b. IDENTIFIERS: OPEN ENDED TERMS	c. COSATI
18. DISTRIBUTION STATEMENT <b>RELEASE TO PUBLIC</b>	19. SECURITY CLASS ( <i>This Report</i> ) <b>UNCLASSIFIED</b>	21. NO. OF PAGES <b>2</b>
	20. SECURITY CLASS ( <i>This Page</i> ) <b>UNCLASSIFIED</b>	22. PRICE