

## 10.2

### EVALUATION STUDY OF BUILDING-RESOLVED URBAN DISPERSION MODELS

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## 1. INTRODUCTION

For effective emergency response and recovery planning, it is critically important that building-resolved urban dispersion models be evaluated using field data. Several full-physics computational fluid dynamics (CFD) models and semi-empirical building-resolved (SEB) models are being advanced and applied to simulating flow and dispersion in urban areas. To obtain an estimate of the current state-of-readiness of these classes of models, the Department of Homeland Security (DHS) funded a study to compare five CFD models and one SEB model with tracer data from the extensive Midtown Manhattan field study (MID05) conducted during August 2005 as part of the DHS Urban Dispersion Program (UDP; Allwine and Flaherty 2007). Six days of tracer and meteorological experiments were conducted over an approximately 2-km-by-2-km area in Midtown Manhattan just south of Central Park in New York City. A subset of these data was used for model evaluations.

## 2. METHODS

This study was conducted such that an evaluation team, independent of the six modeling teams, provided all the input data (e.g., building data, meteorological data and tracer release rates) and run conditions for each of four experimental periods simulated. CFD model evaluations in the past have primarily been based on modelers using both measured meteorological and tracer data in developing model improvements. Although this is a reasonable approach in a research setting, it does not indicate the model's performance in a planning or post-incident simulation when

measurements are not available. This study, therefore, examined the model performance when modelers were armed with only the basic meteorological measurements needed to prescribe boundary conditions.

Another unique feature of this model simulation study was that it was conducted for an urban geometry that contained deep street canyons. Buildings are typically between 20 and 40 meters apart across the streets and avenues of New York City, and many of the buildings in the Midtown study area are taller than 150 meters. A previous CFD study, also conducted under the UDP, examined the meteorology near the Madison Square Garden (Hanna et al 2006). However, the geometry of this previous study was more open, with several large, short buildings (such as the Madison Square Garden and Farley Post Office, both under 60 meters tall) in the computational domain compared to the dominantly tall building structure of the current study. Figure 1 shows the area of the MID05 field study with a GoogleEarth image and photograph for visualizing the building geometry.

The evaluation team consisted of scientists from Pacific Northwest National Laboratory. Five of the modeling teams, CFD Research Corporation (CFDRC), GexCon, National Oceanic and Atmospheric Administration/Environmental Protection Agency (NOAA/EPA), Lawrence Livermore National Laboratory (LLNL), and Navy Research Laboratory (NRL), utilized CFD models, while the sixth team, Los Alamos National Laboratory (LANL), used an SEB model. The CFD and SEB models evaluated were:

- CFD-Urban (CFDRC, Coirier et al. 2006)
- FLACS (GexCon, Hanna et al 2004)
- FLUENT-EPA (NOAA/EPA, Huber et al 2005)
- FEM3MP (LLNL, Gresho and Chan 1998)
- FAST3D-CT (NRL, Patnaik et al 2005)
- QUIC (LANL, Williams et al 2004)

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Figure 1. MID05 Study Area in Manhattan. The blue box in Panel (a) shows the 2-km-by-2-km MID05 study domain, and Panel (b) shows the domain in an aerial perspective of Midtown Manhattan extending from the Hudson River on the west to the East River on the east. The domain is just south of Central Park. The skyline of the Midtown study area is shown in Panel (c) where the photograph is taken from the Stevens Institute of Technology in New Jersey. Panel (a) shows the photograph direction.

During the MID05 field study, a rectangular array of approximately 64 outdoor sampler locations was utilized to collect 30-minute averaged tracer concentrations over the study domain. One type of sampler was deployed on an 8 x 8 grid to measure six perfluorocarbon tracers. Interior to the full 8 x 8 grid of samplers, a 6 x 6 grid of outdoor sulfur hexafluoride samplers were co-located with the perfluorocarbon samplers.

Tracer concentration data for two of the four modeling periods were provided to the modeling teams for their own evaluation of their respective models to ensure proper setup and operation. These modeling cases were labeled setup cases. Tracer data were not provided for the second two experimental periods to provide for an independent evaluation of the models and were labeled blind model cases. For each of the two setup and blind model cases, the evaluation team selected one with steady winds and one with variable winds to provide a contrast in the difficulty of prescribing boundary conditions.

The setup and blind cases also differed in the types and time-averaging of meteorological data that were supplied. Thirty-minute rooftop meteorological station data, rooftop sodar data,

and ground-based radar wind profiler data were provided for each of the modeling cases. This is essentially the set of data that would be available for an emergency response in the New York City area. For the setup cases, however, 5-, 10-, 15-, and 60-minute rooftop and street-level meteorological station data were also made available. These data represent the full suite of meteorological information available from the field experiment, and were provided to give the modeling groups the tools to conduct a thorough assessment of the model boundary conditions during the setup phase of this study.

### 3. RESULTS

The tracer concentrations resulting from the model simulations were provided to the evaluation team in a standard format for consistency in inter-comparing model results. The two main data formats that were requested of the model groups were (1) concentration values at the 30-minute average measurement positions and (2) concentration and wind values on a rectangular three-dimensional grid with 10-m horizontal grid resolution.

A paired-in-time-and-space comparison between the CFD and SEB model output and the field measurements was conducted using the BOOT code (Chang and Hanna 2005), which computes standard statistical measures of model performance. In addition, the fraction of false positive and negative model predictions was computed. BOOT statistics (such as the bias and fractional bias) revealed that the models tended to overestimate the near-surface plume concentrations. This overall overestimation was driven primarily by an overestimate in the peak concentration (near the source). This was true of both the setup and blind cases.

False positive and false negative fractions were also computed using a routine separate from BOOT. The threshold value used to determine whether there was a significant plume signal was related to the measurement limit of detection. The typical fraction of false positive and negative values over the 2-hour simulation period of each model simulation case was each about 0.30. False negative values tended to be higher and false positive values tended to be lower for setup case 1 and blind case 1 (compared with setup case 2 and blind case 2, respectively). In terms of emergency response, false negative values will have a more detrimental effect than false positive

values, so a conservative band around the modeled area of impact should be included for emergency response.

Comparisons of the measured and modeled concentration contour plots were also conducted. The main differences between the models and the observations were in the plume centerline axis orientation, peak concentration values, plume spread, and in the timing of the plume dissipation. Differences in plume axis orientation appear to result from preferential channeling simulated by the models, whereas the observations tended to transport the material more nearly along the mean wind direction. In many cases, the plume spread predicted by the model was larger than the observed plume spread. It is not clear what mechanism drove these differences.

An example of the variety of modeled plumes compared with the measured plume pattern for one 30-minute period concurrent with a tracer release is presented in Figure 2. Wind speeds during this case were moderate to light, while wind direction was steady from the south. The portion of the plume enclosed within the light blue contour line is considered significantly different from a zero concentration. For simplicity, the base map only includes the streets and avenues, and does not include the buildings themselves.

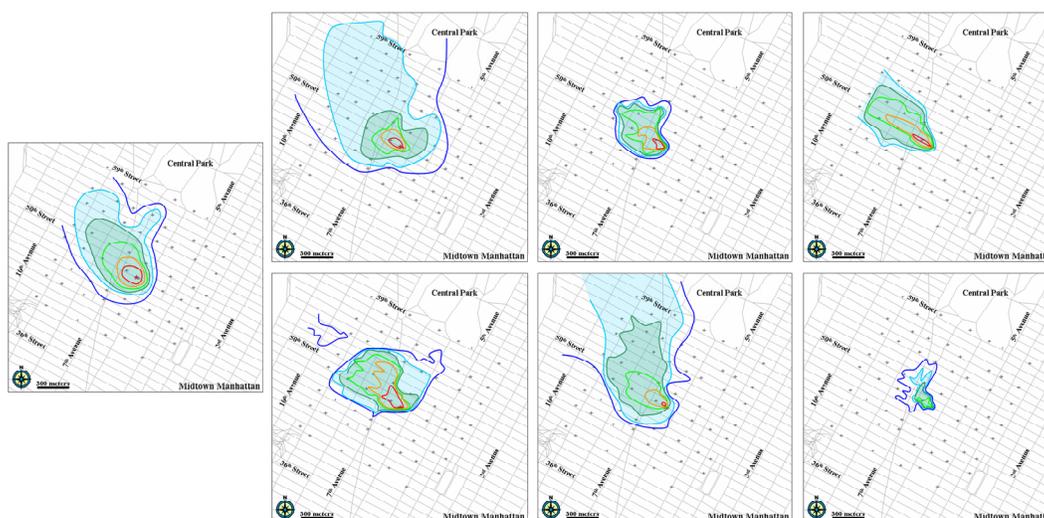


Figure 2. Comparison between the observed concentration pattern (left panel) and the six modeled concentration patterns for a single 30-minute period during the tracer release.

As Figure 2 shows, the contour lines are shown crossing through areas where buildings exist. The surface analyses of the measured concentrations were based on an interpolation of 200-m resolution field measurements (represented

as small grey plus-signs in Figure 2). The effects of the buildings were not explicitly taken into consideration for the observed concentration contours, but these contours represent the bulk character of the plume. The contour plots of the

modeled concentration, on the other hand, were based on 10-m resolution gridded output. Therefore, these contours incorporate the building effects in the representation of the plume footprint. Figure 2 serves to provide a broad contrast in the measured and modeled plumes, and to emphasize the differences that can exist between the modeled plume contours.

Note that the particular time period shown in Figure 2 is not representative of the statistics described above. The relative character of the modeled plumes with respect to the measured plume changes with subsequent time steps. When the modeled plume footprint is smaller than the measured footprint (as is seen for some of the plots in Figure 2), the false negative values tend to be high.

#### 4. CONCLUSIONS

As part of the study of building-resolved urban dispersion models, current gaps and opportunities for future research and development were identified. An abbreviated version of the list developed during the course of this study is presented here.

First and foremost, additional field, wind tunnel, and numerical studies are needed to develop new and improved modeling approaches to address some of the model weaknesses. CFD and SEB modeling must be strengthened to operate in planning and emergency response modes. A fundamental component of building-resolved modeling is the specification of the urban geometry. Up-to-date building databases should be created and provided in several formats that can easily be ingested by models. Additional analyses should be conducted to formalize guidance for prescribing boundary conditions when only a relatively sparse set of meteorological measurements are available.

The study results are currently being documented in a final report, which is projected for completion by October 2007. Due to the sensitive nature of the tracer measurement results, the report will be designated as Official Use Only.

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#### REFERENCES

- Allwine, KJ, and JE Flaherty. 2007. Urban Dispersion Program Overview and MID05 Field Study Summary. PNNL-16696. Pacific Northwest National Laboratory, Richland, WA. [Available online at [http://www.pnl.gov/main/publications/external/technical\\_reports/PNNL-16696.pdf](http://www.pnl.gov/main/publications/external/technical_reports/PNNL-16696.pdf)]
- Chang, JC and SR Hanna. 2005. Technical descriptions and user's guide for the BOOT statistical model evaluation software package, Version 2.0. [Available online at <http://www.harmo.org/kit/>]
- Coirier, WJ, Kim, SK. 2006. CFD modeling for urban area contaminant transport and dispersion: Model description and data requirements. *6th Symposium on the Urban Environment*. Atlanta, GA. Amer. Meteor. Soc.
- Gresho, P, and S Chan. 1998. Projection 2 goes turbulent – and fully implicit. *Int. J. Comp. Fluid Dyn.* **9**. 249-272.
- Hanna, SR, MJ Brown, FE Camelli, ST Chan, WJ Coirier, OR Hansen, AH Huber, S Kim, and RM Reynolds. 2006. Detailed simulations of atmospheric flow and dispersion in downtown Manhattan: An application of five computational fluid dynamics models. *Bull. Amer. Meteor. Soc.* **87** (12). 1713-1726.
- Hanna, SR, OR Hansen, and S Dharmavaram. 2004. FLACS air quality CFD model performance evaluation with Kit Fox, MUST, Prairie Grass, and EMU observations. *Atmos. Environ.* **38**. 4675-4687.

Huber, A, M Freeman, R Spencer, B Bell, K Kuehlert, and W Schwarz. 2005. Applications of CFD simulations of pollutant transport and dispersion within ambient urban building environments: Including homeland security. *AWMA 98<sup>th</sup> Annual Conf.* Minneapolis, MN. AWMA. CD-ROM, Paper #1241.

Patnaik, G, JP Boris, FF Grinstein, and J. Iselin. 2005. Large scale urban simulations with FCT in *High-Resolution Schemes for Convection-Dominated Flows: 30 Years of FCT*. D. Kuzmin, R. Lohner, and S Turek, eds., Springer. pp. 105-130.

Williams, MD, MJ Brown, B Singh, and D Boswell. 2004. QUIC-PLUME Theory Guide. Los Alamos National Laboratory. LA-UR-04-0561. 22 pp.