19th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
3-6 June 2019, Bruges, Belgium

AN EVALUATION OF THE JOINT OUTDOOR-INDOOR URBAN LARGE EDDY SIMULATION (JOULES) ATMOSPHERIC TRANSPORT AND DISPERSION (AT&D) MODELING SYSTEM

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Abstract: Predicting human exposure to airborne contaminants in urban environments requires numerical models that can resolve both urban atmospheric transport and dispersion (AT&D) and exchanges between indoor and outdoor spaces. Buildings and other structures affect winds, turbulence, and corresponding dispersion patterns of the airborne contaminants. While a range of modeling capabilities exist to address airborne material transport in urban areas, few possess the capability to efficiently and accurately simulate AT&D scenarios within operational timeframes. Recent advances in graphics processing units (GPU) have allowed a building-aware Large Eddy Simulation (LES) atmospheric modeling system to be implemented on a GPU-based computing platform. This GPU-LES system has gone through extensive verification and validation in open-terrain settings under various atmospheric stability environments. Here, we show a preliminary evaluation of an extension of the GPU-LES system to include a "building-aware" urban scenario by simulating a trial from the Mock Urban System Test (MUST) field experiment. This evaluation required 1-m horizonal and vertical grid spacing to resolve the winds and turbulence around and between the 12 x 10 array of rectangular shipping containers. For the trial presented here, the simulated vertical profiles of potential temperature and wind direction generally matched the analogous observed vertical profiles. Comparisons of measured airborne tracer observations show that downwind crosswind peak concentrations and crosswind integrated concentrations fall within the range of variability in MUST observations form this trial. Future work will include adding time-and-space varying realizations of AT&D, analyzing more MUST trials, and further extension of the GPU-LES system to include AT&D simulations of laboratory and real-world urban settings.

Keywords: *Urban Dispersion Modeling, Indoor Dispersion Modeling, Large Eddy Simulation (LES), Graphics Processing Unit (GPU) Computing, Indoor-Outdoor Contaminant Transport and Dispersion, Model Validation, Stable Planetary Boundary Layer*

INTRODUCTION

The Hazard Prediction and Analysis System (HPAC) and the Joint Effects Model (JEM) are emergency response modeling tools used by analysts in the United States (US) to characterize the impact of airborne contaminants in both urban and non-urban environments. Because of the need for rapid solutions, both the non-urban and urban models in these systems use parameterizations to resolve the planetary boundary layer (PBL) turbulence and the influence that buildings have on contaminant dispersion. These parameterizations typically involve statistical characterizations of meteorological parameters associated with the interaction of the environment with building obstacles. While the statistical representations of the contaminant dispersion can address some needs, there are a variety of analysis applications where dynamically produced, short time-averaged, single realization, dispersion solutions are critical for accurately determining the impact of the release (Bieringer et al., 2014). Over the past two years, the Defense Threat Reduction Agency – Joint Science and Technology Office for Chemical and Biological Defense (DTRA-JSTO-CBD) has supported the development and evaluation of a coupled outdoor-indoor urban airborne contaminant modeling capability. This system, called the Joint Outdoor-indoor Urban Large Eddy Simulation (JOULES) system, couples a building-aware Large Eddy Simulation (LES) atmospheric model with an integrated outdoor atmospheric transport and dispersion (AT&D) model and models that simulate the transport of contaminants across the building envelope.

Here, we describe a key enabling technology within JOULES, a LES model that has been implemented on a graphics processing unit (GPU) computing platform. The GPU-LES model has undergone a variety of evaluations to assess its accuracy. The model's origins traces back several decades to the Dutch Atmospheric LES (DALES) which is one of the most extensively tested LES codes used for use in PBL applications (Heus et al. 2010). Schalkwijk et al. 2012, 2015, and 2016 describe the viability of this LES model after implementation on a GPU and discuss the results from an extensive evaluation of the ability of this LES to accurately reconstruct conditions in the PBL. Bieringer et al. (2017, 2019) extended these evaluations and showed that this GPU-LES model can accurately simulate atmospheric dispersion in open-terrain environments across a range of static stability conditions. Here, we describe a further extension of this model evaluation effort to include a "building-aware" urban scenario.

BACKGROUND

JOULES Description

Until recently, the high computational burden required to form ensembles of single-realization, time-varying dispersion solutions using a LES atmospheric model coupled with an AT&D model has limited its use to a few proof-of-concept studies. One of the principle goals of the development and testing of JOULES is to leverage emerging technological advances in GPU computing to make LES modeling feasible for use in urban AT&D applications. A key enabling technology within JOULES is a GPU-LES atmospheric model called the GPU Resident Atmospheric Simulation Program (GRASP). The LES on which GRASP is based was originally developed to provide high resolution simulations of clouds, winds, and turbulence and designed to be run on central processing unit (CPU) computing platforms. Scientists at Delft University of Technology (TU Delft) and Whiffle B.V. have since adapted this model to run on GPU-based architectures (Schalkwijk et al. 2012, 2015, and 2016). This advancement significantly reduces the time and computational resources needed to produce AT&D simulations at building-aware scales enabling the development of ensembles of single-realization dispersion solutions.

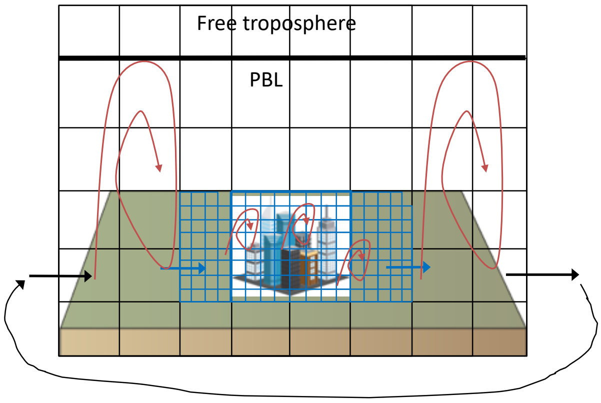

Figure 1. A notional depiction of the nested grid approach used in JOULES.

Accurately simulating the time-varying, near surface winds and turbulence flows in a building-aware urban environment requires: 1) the eddies to be accurately represented within the full depth of the PBL; 2) the model's horizontal and vertical grid spacing to be sufficiently small so that the buildings and the winds and turbulence between them can be explicitly resolved; and 3) the model to be numerically stable in environments with a steep or vertical lower boundary (e.g. a building's facade). JOULES has been adapted to address all three of these issues. The first two challenges were addressed through the implementation of a one-way grid nesting capability. The grid nesting allows for simulations to be configured such that the outer nest can use a coarser-spaced horizontal and vertical grid spacing that allows for domains that are sufficiently large in the vertical and horizontal to properly spin up the turbulent eddies through the full depth of the PBL. The inner nest(s) allows for both the eddies and turbulence to be downscaled to the finer scale with a horizontal and vertical spacing sufficient to resolve the obstacles and the flow around/between them. The outer nest uses a cyclic lateral boundary condition to spin up the turbulence, and the inner domains are one-way nests that do not influence the parent nest (Figure 1). This nesting approach was necessary to address the first two requirements listed above and to meet the memory constraints of the GPU hardware. The third challenge was addressed through an implementation of an Immersed Boundary Method (IBM) surface layer parameterization. This approach has been demonstrated to keep the atmospheric model numerically stable at the walls of the buildings (Lundquist et al. 2012; Tomas et al. 2017).

Urban "Building-Aware" JOULES Model Evaluation

Our team is currently in the process of extending the evaluation of the GPU-LES modeling system to building-aware urban meteorological and AT&D simulations through comparisons with data from field trials and laboratory studies. These data range from experiments that measure flow and dispersion over regular arrays of rectangular obstacles to real-world, city terrain landscapes.

The initial assessment, presented here, examines the ability and accuracy of the GPU-LES system to simulate the AT&D in a regular array of rectangular obstacles. The Mock Urban Setting Test (MUST) was chosen as field trial for use in this evaluation due to a combination of factors including the use of a simple obstacle array, the availability of detailed meteorological data, and dispersion measurements made with fast-response propylene sensors. This experiment focused on near-range dispersion with concentration measurements being made within a 12-by-10 array of shipping containers with dimensions of 12.2 m (length) x 2.43 m (width) x 2.54 m (height) with a spacing of 7.9 m in width and 12.9 m in the length direction. Figure 2 provides an illustration of the obstacle array, the locations of the propylene sensors, the location of the tracer release and surface wind vectors from the LES. Most of the experimental trials were conducted at night in weakly to extremely stable conditions. Further details on the obstacle array, instrumentation deployed, and experimental trials conducted are available in Biltoft (2001).

We selected two trials from this experiment for use in the evaluation and will present results from one of these trials here. The selection of the trials was based on a combination of the availability of vertical profile measurements of winds and temperatures, a release location either upwind or near the upwind edge of the obstacle array, and a near surface wind direction suitable to transport the propylene tracer over the four rows of down-wind sensors. Due to the scale of this experiment, it was necessary to utilize a horizontal and vertical grid spacing of 1 m in the inner nest of the

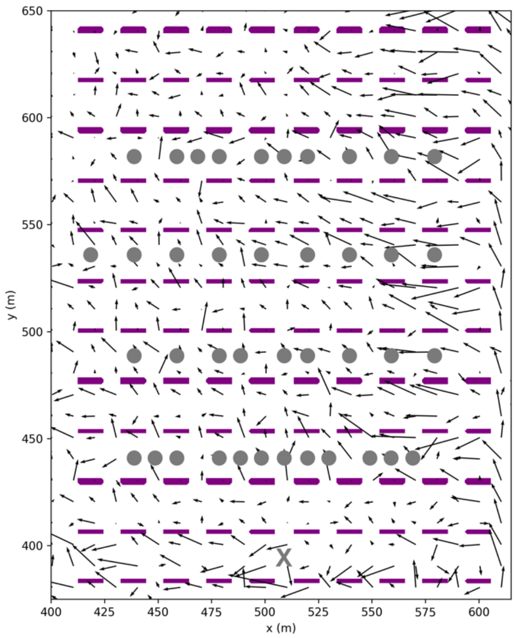

Figure 3. A depiction of the simulated MUST obstacle array (purple rectangles), propylene sensor locations (grey filled circles), release location (grey X), and near surface wind vectors.

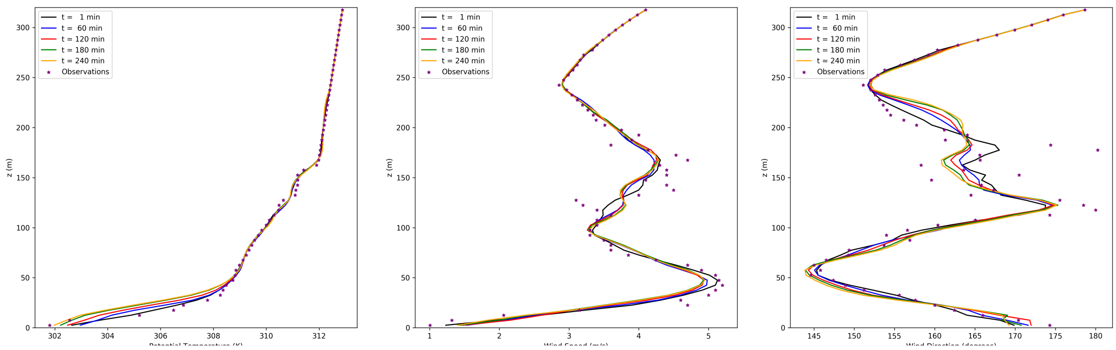

Figure 2. Vertical profiles of potential temperature, wind speed, and wind direction. The markers denote observations from the MUST trials and the lines correspond with GPU-LES model output at 60, 120, 180, and 240 minutes after the model start time.

LES model. This enabled the model to both resolve the obstacles and near-surface flow field as well as the very shallow boundary layer present during the trials. The field trial presented here began at 2304 local standard time (LST) on 24 September 2001. The averaged surface winds were 1.01 ms^{-1}, the surface friction velocity was 0.26 ms^{-1}, the surface potential temperature was 301.8 K, and the Obukhov length was 91 m. To recreate these conditions, the GPU-LES was initialized with a surface potential temperature of 302 K, a surface roughness of 0.5 cm, and a surface heat flux of -4 Wm^{-2} for an open-terrain region approximately 250 m southwest of the obstacle array. The GPU-LES model was also initialized with the measured vertical profile of the winds and temperature and allowed to spin up the winds and turbulence over a period of 3 hours. This was a complex scenario with a very shallow (~50-m depth) stable PBL. There was also considerable shear with height in the wind speeds and direction within these layers. Figure 3 illustrates the characteristics of the atmospheric conditions in this trial and that after a 3 to 4-hour spin-up period, the GPU-LES was able to largely able to replicate the major atmospheric features present in the vertical profiles of winds and temperature.

After a 3-hour model spin-up period, a 19-minute continuous unit release was specified at the lowest model level at a location just inside the array of obstacles, as depicted by the 'X' in Figure 2. A second unit tracer release was specified outside of the obstacle array and used as a reference. Data from the GPU-LES were saved at a 1-minute time interval. This allowed for a comparison of the dispersion pattern resulting from the release within the obstacle array with a release outside of the array. Figure 4 provides an illustration of the near surface concentration pattern from the in-array and outside-array releases and the near surface wind vectors from the GPU-LES simulation.

RESULTS

In the MUST field trial, propylene measurements were made with 40 fast-response sensors deployed in four rows, as shown in Figure 2. The configuration of the sensors enables us to examine a variety of properties of dispersion within the array where the enhanced turbulence associated with the obstacles increases the lateral and vertical dispersion of the propylene. Measured crosswind peak concentration (CWPC) and crosswind integrated concentration (CWIC) were examined and are presented here. The measured peak concentrations were determined by taking the peak value from the 50-Hz propylene measurements within a 1-minute interval across each row of sensors over 19 minutes. These peak-concentration values were then compared to the CWPC from the GPU-LES model. The left plot of Figure 5 shows that the decrease in peak concentration values versus downwind distance from the observed release is comparable to that derived from the GPU-LES model results. The blue markers depict the observations from the MUST field trial and the grey lines depict the result from a single dispersion realization from the GPU-LES. The black line is the average of the LES realizations. CWPC values from the simulation were also comparable to the observations near the release location, however were lower at ranges from 50 to 175 m downwind of the release suggesting the LES is not able to resolve these peak values as well further downwind. A similar analysis was conducted for CWIC. The plot on the right of Figure 5 also shows a similar result where the measured CWIC values at the four downwind distances show a similar value to that seen in the ensemble of model simulations for this calculation. The CWIC minima starting at ~12 m from the source and spaced every ~25 m are associated with the obstacle array.

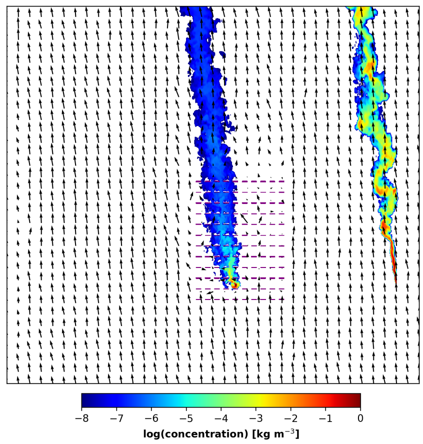

Figure 5. A depiction of two "single-realization" dispersion patterns and wind vectors from the GPU-LES simulations of the MUST field trial.

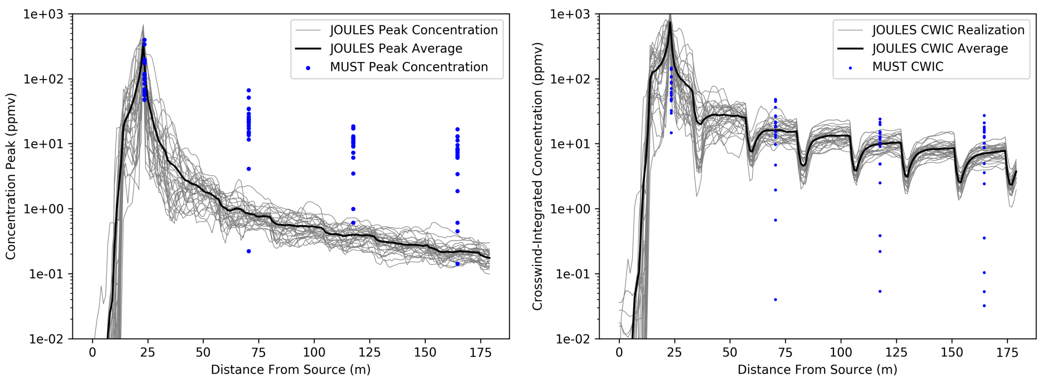

Figure 4. Downwind crosswind peak concentrations (left) and downwind crosswind integrated concentrations (right) from MUST observations (blue dots) and the GPU-LES simulation (grey lines). The solid black line is the average of the LES simulation results.

CONCLUSIONS

In this manuscript, we described a system, called JOULES, that enables detailed simulations of ensembles of single-realization airborne material transport in urban and interior locations. Prior work has demonstrated that this model can accurately reconstruct microscale atmospheric conditions and dispersion in open terrain environments. Here we describe preliminary results from an effort to demonstrate the tools ability to accurately reconstruct meteorological conditions and atmospheric dispersion in urban locations. Data from the MUST field trial were used for this initial assessment. Results were presented illustrating that the GPU-LES can reconstruct a complex nocturnal, stable scenario with a very shallow boundary layer with directional shear. The directional shear was greater than 50 degrees in the lowest 100 m and the GPU-LES was able to replicate a weak low-level jet signature that was observed at the top of the PBL. Preliminary dispersion results suggest that the enhanced turbulence associated with the obstacle array is resolved by the GPU-LES, enhancing dispersion of the airborne material. The simulated CWIC values are comparable to those observed in the field trial. Comparisons with MUST dispersion measurements show reasonable agreement in the decrease in crosswind peak and integrated concentrations as a function of downwind distance from the release location. Future work will explore the accuracy of the GPU-LES using water tank data from a novel new magnetic resonance imager (MRI) data set (Shim et al. 2019) and data from urban field trials such as Joint Urban 2003 (Allwine et al. 2004; Allwine and Flaherty 2006).

REFERENCES

Allwine K.J., M. Leach, L. Stockham, J. Shinn, R. Hosker, J. Bowers, J. Pace, 2004: Overview of joint urban 2003—an atmospheric dispersion study in Oklahoma City, symposium on planning, nowcasting and forecasting in the urban zone. American Meteorological Society, January 11–15, 2004, Seattle, Washington. Available at *http://www.ametsoc.org*.

Allwine K.J., J.E. Flaherty, 2006: Joint urban 2003: study overview and instrument locations, PNNL-15967. Pacific Northwest National Laboratory, Richland, WA.

Bieringer, P.E., A.J. Annunzio, N. Platt, G. Bieberbach, J. Hannan, 2014: Contrasting the use of single-realization versus ensemble-average atmospheric dispersion solutions for chemical and biological defense analyses. *J. Appl. Meteor. Climatol*., 53, 1399–1415.

Bieringer, P.E., A.J. Piña, M.D. Sohn, H.J.J. Jonker, G. Bieberbach, Jr., D.M. Lorenzetti, R.N. Fry, Jr., 2017: Large Eddy Simulation (LES) Based System for Producing Coupled Urban and Indoor Airborne Contaminant Transport and Dispersion Solutions. *18th International Conference on Harmonisation within Atmospheric Dispersion Modeling for Regulatory Purposes.,* 9-12, October 2017, Bologna, Italy.

Bieringer, P.E., A.J. Piña, H.J.J. Jonker, M.D. Sohn, D.M. Lorenzetti, R.N. Fry Jr.: A Graphics Processing Unit (GPU) Large Eddy Simulation (LES) Based System for Producing Airborne Contaminant Transport and Dispersion Solutions. *In review, Boundary Layer Meteorology.*

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, 58 pp.

Heus T, van Heerwaarden C, Jonker H, Pier Siebesma A, Axelsen S, van den Dries K, Geoffroy O, Moene A, Pino D, de Roode S, de Arellano J (2010) Formulation of the Dutch Atmospheric Large-Eddy Simulation (DALES) and overview of its applications. Geosci Model Dev 3(2):415–444.

Lundquist, K.A., F.K. Chow, and J.K. Lundquist, 2012: An immersed boundary method enabling large-eddy simulations of flow over complex terrain in the wrf model. *Mon. Wea. Rev.*, **140**, 3936–3955.

Tomas, J.M., H.E. Eisma, M.J.B.M. Pourquie, G.E. Eisinga, H.J.J. Jonker, J. Westerweel, 2017: Pollutant Dispersion in Boundary Layers Exposed to Rural-to-Urban Transitions: Varying the Spanwise Length Scale of the Roughness, *Bound-Lay. Meteorol.,* **163,** 225–251.

Schalkwijk J., Griffith E.J., Post F.H., Jonker H.J.J., 2012: High-performance simulations of turbulent clouds on a desktop PC: exploiting the GPU. *Bull Am Meteorol. Soc.* **93**, 307–314.

Schalkwijk J., Jonker H.J.J., Siebesma A.P., Bosveld F.C., 2015: A year-long large-eddy simulation of the weather over Cabauw: an overview. *Mon Weather Rev.* **143**, 828–844.

Schalkwijk J., Jonker H.J.J., Siebesma A.P., 2016: An Investigation of the Eddy-Covariance Flux Imbalance in a Year-Long Large-Eddy Simulation of the Weather at Cabauw., *Bound-Lay. Meteorol.* **160,** 17–39.

Shim, G., D. Prasad, C.J. Elkins, J.K. Eaton, and M.J. Benson, 2019: 3D MRI Measurements of the Effects of Wind Direction on Flow Characteristics and Contaminant Dispersion in a Model Urban Canopy. *In Press: Environmental Fluid Dynamics.*