EVALUATION OF URBAN ATMOSPHERIC TRANSPORT AND DISPERSION MODELS USING DATA FROM THE JOINT URBAN 2003 FIELD EXPERIMENT

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Abstract: We have evaluated the performance of several urban atmospheric transport and dispersion models by comparing model predictions to tracer gas concentrations measured during the Joint Urban 2003 field experiment in Oklahoma City, USA. These models include the Urban Canopy, Urban Dispersion Model (UDM), and Micro-SWIFT/SPRAY (MSS) modes within the HPAC modelling suite, QUIC-URB/QUIC-PLUME models, and the MESO/RUSTIC models. We discuss some of the results of these comparisons, including relative model performance according to bias and scatter metrics, differences in model behavior for predictions of daytime versus nighttime releases, and operational considerations such as runtime differences.

Key words: *Atmospheric transport and dispersion, point-to-point protocol, model evaluations, urban models, HPAC, MESO/RUSTIC, QUIC-URB/QUIC-PLUME, Joint Urban 2003.*

1. INTRODUCTION

The potential effects of the atmospheric release of hazardous materials continue to be of concern, particularly in urban areas. Estimates of the effects of hazardous releases within an urban environment on the underlying population are required to aid planning, emergency response, and recovery efforts. These estimates require accurate knowledge of the concentrations of dispersed material in time and space. For several years we have been engaged in an ongoing independent evaluation of several models that were developed to predict the atmospheric transport and dispersion (T&D) of hazardous materials in urban areas. The work reported here expands on our previous evaluation of the U.S. Defense Threat Reduction Agency's (DTRA) Hazard Prediction and Assessment Capability (HPAC) (Warner et al., 2007, Warner et al., 2008, Urban et al. 2007) to include the QUIC-URB/QUIC-PLUME models developed by Los Alamos National Laboratory and the MESO/RUSTIC models developed by ITT Corporation. By comparing model predictions to measurements of tracer gas releases in the Joint Urban 2003 (JU03) field experiment, we were able to compare the performance of three urban T&D models within HPAC to that of the QUIC and MESO/RUSTIC models. This work summarizes some of the major conclusions developed from our multi-year study of urban T&D models.

2. BRIEF DESCRIPTION OF JOINT URBAN 2003

Under the joint sponsorship of the U. S. Department of Defense (Defense Threat Reduction Agency – DTRA) and the U. S. Department of Homeland Security, a series of tracer gas releases were carried out in Oklahoma City (OKC) starting on 28 June and ending on 31 July 2003 (Allwine et al., 2004). This field experiment, referred to as "Joint Urban 2003", included ten intensive operating periods (IOPs), in which the tracer gas sulfur hexafluoride (SF_6) was released in downtown Oklahoma City. In total, twenty-nine 30-minute continuous SF_6 releases were conducted with 2 hours of sampler monitoring following the start of each release. The results presented here compare predictions of tracer concentrations generated after one hour of continuous transport and dispersion with the measurements from samplers located at 3 meters above ground level (AGL) in the Central Business District (CBD). Additional information about the JU03 experiment as applied to our studies can be found in Warner et al., 2007.

3. BRIEF DESCRIPTION OF URBAN HPAC

DTRA's HPAC (v4.04 SP3) is composed of a suite of software modules that can generate source terms for hazardous releases, retrieve and prepare meteorological information for use in a prediction, model the transport and dispersion of the hazardous release over time, and plot and report the results of these calculations (DTRA, 2001). For hazardous material transport and dispersion, HPAC uses the SCIPUFF model and an associated mean wind field model (Sykes et al., 1996). SCIPUFF is a Lagrangian model for atmospheric dispersion that uses the Gaussian puff numerical method and bases its turbulent diffusion parameterization on second-order closure theories. If HPAC is given observations or predictions generated by a mesoscale meteorological model, it can create mass-consistent wind fields that can be used to transport the hazardous material. Within HPAC two weather modules can be used to prepare these mass-consistent wind fields – SWIFT (ARIA Technologies, 2001) and MC-SCIPUFF. In this study, the creation of HPAC predictions was completed using SWIFT when possible.

For this study, we generated predictions using three urban T&D modes that are available within HPAC. The baseline urban capability is referred to as Urban Canopy ("UC") mode, which employs a modification of the vertical wind and turbulence profiles appropriate for an urban canopy. The Urban Dispersion Model (UDM) (denoted "DM") computes the transport and dispersion of an instantaneous discharge of pollutant based on ensemble mean Gaussian puff dispersion methodology, but allows surface obstacles to modify the dispersion patterns according to an empirical parameterization based on extensive wind tunnel experiments (Hall et al., 2002). Micro SWIFT/SPRAY (MSS) (denoted "MS"), which consists of the sub-models Micro-SWIFT and Micro-SPRAY (Moussafir et al., 2004). Micro-SWIFT, like the SWIFT module mentioned above, creates mass consistent gridded wind fields, but also creates zones of modified wind flow around urban obstacles. Micro-SPRAY is a Lagrangian particle dispersion model (derived from SPRAY) that can account for urban obstacles. The version of HPAC which we evaluated also included a capability called the Urban Windfield Module (UWM), which uses computational fluid dynamics (CFD) techniques to predict the steady-state wind field inside the urban boundary layer (Lim et al., 2003). It was intended to represent an improvement over simply using SWIFT for urban applications. We did include predictions generated using the UWM mode in this study because we previously found that it its use does not significantly and consistently improve HPAC predictions, but greatly increases HPAC runtimes.

4. BRIEF DESCRIPTION OF QUIC-URB/QUIC-PLUME

QUIC (Quick Urban and Industrial Complex) consists of two independently-running models (Pardyjak and Brown, 2001, Williams et al., 2001). QUIC-URB, an urban airflow model, feeds three dimensional wind velocity information to QUIC-PLUME, an urban Lagrangian particle dispersion model. QUIC-URB uses a modified Röckle diagnostic/empirical approach to produce mass-consistent wind fields in urban environments. QUIC-PLUME generates three-dimensional concentration time histories of transported material, accounting for urban obstacles. QUIC results are denoted here using the abbreviation "QU."

5. BRIEF DESCRIPTION OF MESO/RUSTIC

MESO/RUSTIC consists of two independently-running models (Burrows et al., 2007, Diehl et al., 2007, Hendricks et al., 2007). RUSTIC (Realistic Urban Spread and Transport of Intrusive Contaminants), an urban airflow model, feeds steady-state three dimensional wind velocity and turbulence information to MESO, an urbanized Lagrangian particle dispersion model. RUSTIC solves a simplified version of the compressible Reynolds-averaged Navier-Stokes (RANS) computational fluid dynamics equations in order to run faster than conventional RANS CFD models, and includes also includes an empirically parameterized k-ω model of isotropic turbulence with an added buoyancy production term, which allows the incorporation of atmospheric stability effects. MESO generates three-dimensional concentration time histories of transported material, accounting for urban obstacles. MESO/RUSTIC results are denoted here using the abbreviation "MR."

6. OVERVIEW OF PROTOCOL FOR COMPARISONS BETWEEN MODELS

The different models under consideration incorporate different assumptions and degrees of physical modelling. Since the values of certain input and operational parameters could have different consequences for different models, rather than try to achieve perfect parity in these parameters between models, we instead ran each model in the manner recommended by its developers. For example, not all models used the same size or grid resolution for the computational domain, and the several different particle dispersion models used different numbers of tracer particles. We did, however, condition the models using the same meteorological inputs, which ultimately drive the transport and dispersion.

Due to some practical concerns involved with the operation of QUIC-URB/QUIC-PLUME and MESO/RUSTIC, we scaled down the scope of this study compared to the scope of our previous study of Urban HPAC. Due to the limited Oklahoma City building database that accompanied the QUIC models, we limited our study to a comparison of model predictions covering only a subset of the near-surface level samplers in the OKC CBD, as opposed to the full set of CBD samplers and sampler arcs that extended several kilometres downwind from the tracer release sites. Because of the relatively slow runtimes associated with generating steady-state wind field solutions using RUSTIC, we considered only two meteorological input options corresponding to measurements from meteorological instruments located upwind of the tracer gas releases. Furthermore, we were able to generate RUSTIC predictions for only the first hour following the start of each tracer gas releases (instead of two hours), so we only compared predictions from all the models generated during the first hour of simulated T&D, which may be appropriate given the restricted sampler domain.

7. METEOROLOGICAL INPUT OPTIONS THAT WERE EXAMINED

A large variety of meteorological measurements were collected during JU203, and we created model predictions using measurements from two instruments located upwind of the tracer gas release sites. Two representative meteorological ("MET") input options were examined for this comparative study. The "PNS" MET input corresponded to using the SODAR observations that were available from the Pacific Northwest National Laboratory (PNNL) meteorological instruments ~1.6 km upwind from the releases; this input was intended to be representative of an upwind vertical wind profile that could be used as input into HPAC. The "PO7" MET option corresponded to a set of observations from a single location 40 meters AGL on the roof of the Oklahoma City Post Office building (just upwind of downtown); this input was intended to be representative of a single downtown observation that could be used as input for the Urban HPAC predictions. The wind measurements were averaged on a 15-minute time scale, corresponding to four wind updates per one hour of simulated transport and dispersion. The operation of RUSTIC required that the model be run once per steady-state wind field generated, so this corresponded to four RUSTIC runs per simulated release. Although SWIFT is the recommended/default meteorological pre-processor for HPAC, some runs for some MET input options aborted due to a SWIFT error; when this occurred, we used MC-SCIPUFF as the meteorological pre-processor for all the simulated releases for that MET option. The PNS MET input option corresponded to running HPAC using MC-SCIPUFF, whereas the PO7 MET input option corresponded to running HPAC using SWIFT.

In addition to the wind inputs described above, MESO/RUSTIC also uses measured values of the upwind and city-center sensible heat flux as strongly recommended inputs. Since HPAC is also capable of accepting these values as inputs, we conducted a study excursion that examined the effects on Urban HPAC prediction quality of using the sensible heat flux as an input.

8. PROTOCOL FOR PAIRED IN SPACE AND TIME COMPARISONS

For this analysis we compared predictions and observations paired in space and time, referred to “point-to-point” comparisons. For each release, predictions and observations were compared using the four 30-minute average concentrations obtained during the one-hour observation period following each release. We computed thirteen statistical measures for each comparison, including the fractional bias (FB) and scatter metrics such as the normalized mean square error (NMSE), and normalized absolute difference (NAD). We also used a user-oriented measure of effectiveness (MOE) (Warner et al., 2004b) that measures both scatter and bias and allows for assessments of the ability of the model to predict either the “hazardous” region (i.e., the region above a concentration threshold of interest) or total average concentrations.

9. BRIEF SUMMARY OF RESULTS

Figures 1 and 2 show comparisons of all the urban T&D models under consideration according to user-oriented MOE plots based on the point-to-point comparison of model predictions of 30-minute average concentrations with sampler observations in the OKC CBD during the JU03 experiment. These results illustrate some of the trends discussed below.

Day vs. Night Releases and Predictions

In our previous study (Warner et al., 2007, Warner et al., 2008, Urban et al. 2007), we found that there was a substantial difference in the performance of Urban HPAC predictions of the daytime releases versus the releases at night. For all MET input options, the daytime releases tended to be under-predicted and the releases at night tended to be over-predicted for the UC and DM modes, but the MS mode tended to have a slight over-prediction bias for both daytime and nighttime releases. By scatter metrics, Urban HPAC predictions using SWIFT-associated MET inputs (i.e., PO7) resulted in substantially more scatter at night than during the day, with the exception of MS. For the MC-SCIPUFF-associated MET input options (i.e., PNS), the scatter results were much more similar for the day and night Urban HPAC predictions. The prediction quality of QU and MR, like that of MS, was found to differ little between predictions of daytime and nighttime releases.

Relative Model Performance for Nighttime Releases

We previously found that the MS and DM HPAC modes offer improvement over the UC mode for MET input options that invoke SWIFT (i.e., PO7). This result can be considered especially important because the use of SWIFT corresponds to a recommended and default mode of Urban HPAC. For the releases at night that used MC-SCIPUFF-associated MET input options (i.e., PNS) results were mixed with no Urban HPAC mode consistently offering improvement. MR performs no worse than any Urban HPAC mode for either MET input option, whereas QUIC performs adequately for predictions of nighttime releases generated using the PO7 MET input option, but quite poorly for predictions generated using the PNS MET input option. The PNS MET option was derived from SODAR data are investigating the effect of inconsistent low-altitude winds in urban and suburban SODAR data from the JU03 data set.

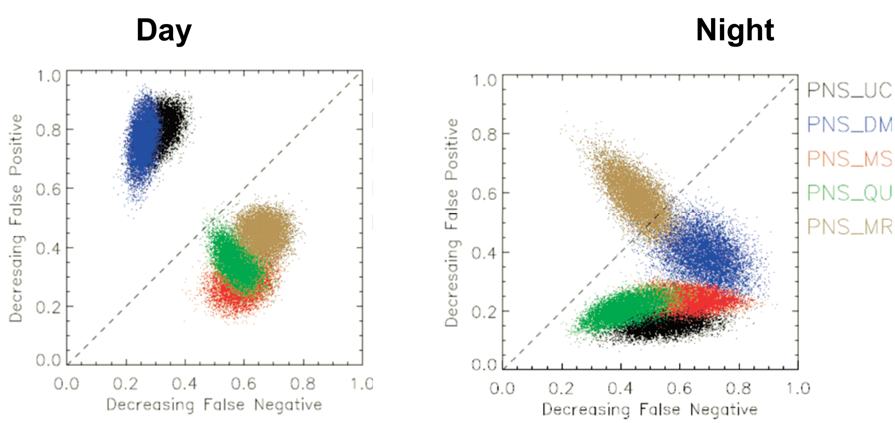

Figure 1. Comparisons of Bootstrap-Resampled User-Oriented Measure of Effectiveness (MOE) Values for Urban T&D Model Predictions of the 17 Daytime (Left) and 12 Nighttime (Right) Releases of JU03 Within the CBD Using the PNS MET Input Option. The models represented are HPAC/Urban Canopy (UC), HPAC/UDM (DM), HPAC/MSS (MS), QUIC-URB/QUIC-PLUME (QU), and MESO/RUSTIC (MR). [MOE values nearer to the “perfect” value of (1,1) represent improved predictions; values “above” the diagonal line correspond to under-predictions, whereas values “below” the diagonal line correspond to over-predictions.]

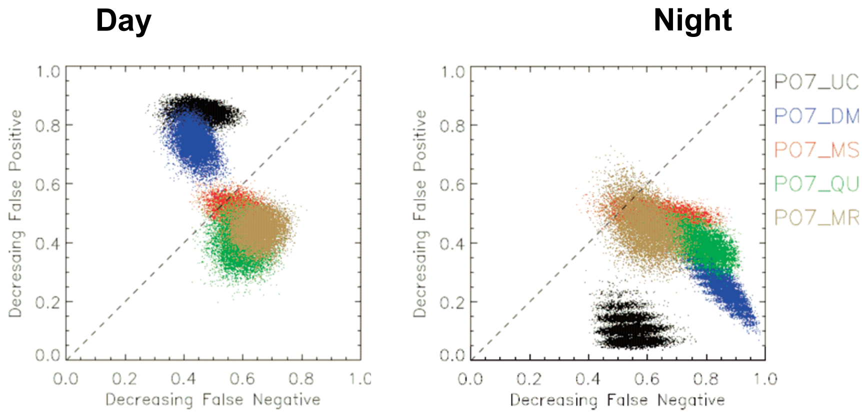

Figure 2. Comparisons of Bootstrap-Resampled User-Oriented Measure of Effectiveness (MOE) Values for Urban T&D Model Predictions of the 17 Daytime (Left) and 12 Nighttime (Right) Releases of JU03 Within the CBD Using the PO7 MET Input Option. The models represented are HPAC/Urban Canopy (UC), HPAC/UDM (DM), HPAC/MSS (MS), QUIC-URB/QUIC-PLUME (QU), and MESO/RUSTIC (MR). [MOE values nearer to the "perfect" value of (1,1) represent improved predictions; values "above" the diagonal line correspond to under-predictions, whereas values "below" the diagonal line correspond to over-predictions.]

Relative Model Performance for Daytime Releases

We previously found no trend in Urban HPAC mode performance for daytime releases that was consistent across MET input options. We found similar results for QU and MR, except MR appeared to have a performance advantage over MS and perhaps QU for predictions of daytime releases generated using the PNS MET input option (but not the PO7 MET input option). MS, QU, and MR tend to be closer to zero prediction bias than UC or DM, which tend to under-predict.

Runtime Considerations

In addition to model accuracy, operational concerns such as model runtimes should be considered. We found that UC and UDM run on the order of minutes per simulated release in the OKC CBD, MSS and QUIC run in tens of minutes, and MESO/RUSTIC runs in tens of hours or more (due to the RUSTIC runtime and the need to run RUSTIC four times per release).

10. CONCLUSIONS

Several robust conclusions can be drawn from our evaluation of Urban HPAC in the JU03 experiment. The UC and DM Urban HPAC modes tend to over-predict concentrations for daytime releases under-predict concentrations for nighttime releases. MS, QU, and MR tend to have little difference in prediction bias between predictions of daytime and nighttime releases, with perhaps a slight overall over-prediction bias for each model. All models tend to offer improvement over the UC mode for nighttime predictions generated using the PO7 (SWIFT-related) MET input option. Results were mixed for the daytime releases and for the PNS (MC-SCIPUFF-related_ MET input option at night, although MR tended to be a relatively good performer for daytime predictions generated using PNS MET and QU tended to be a relatively poor performer for nighttime predictions generated using PNS MET. In terms of runtimes, UC and DM predictions can be generated in an order of magnitude less time than MS and QU predictions, whereas MR predictions can be generated in one to two orders of magnitude more time than MS and QU predictions.

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