Impact of coupling a microscale computational fluid dynamics model with a mesoscale model on urban scale contaminant transport and dispersion

Mukul Tewaria,⁎, Hiroyuki Kusaka, Fei Chen, William J. Coirier, Sura Kim, Andrzej A. Wyszogrodzki, Thomas T. Warner

⁎ National Center for Atmospheric Research, Boulder, Colorado, United States
b University of Tsukuba, Tsukuba, Japan
c CFD Research Corporation, Huntsville, Alabama, United States

ARTICLE INFO

Article history:
Received 31 December 2008
Received in revised form 24 December 2009
Accepted 19 January 2010

Keywords:
WRF model
CFD model
Transport and dispersion

ABSTRACT

Results are presented from a study designed to evaluate the impact upon urban area transport and dispersion (T&D) modeling accuracy by coupling a microscale computational fluid dynamics (CFD) model with a mesoscale numerical weather prediction (NWP) model. The CFD model taking part in the evaluation was the CFD-Urban model while the NWP model was the Weather Research and Forecasting (WRF) model. The following two different approaches of supplying initial and boundary conditions to drive CFD-Urban were evaluated by comparing the resulting tracer gas transport fields to field data: (i) using observation obtained from a single sounding site during the URBAN 2000 field experiment and (ii) using WRF output in quasi-steady mode. The WRF and the CFD-Urban model results were evaluated against data obtained from the Intensive Observation Period (IOP) 10 during the URBAN 2000 field experiment. It was found that the CFD-Urban T&D prediction was significantly improved when using wind fields produced by downscaling WRF output as initial and boundary conditions. One key reason for such success is that the turning of lower boundary layer wind and pressure gradient are well represented in the time-varying three-dimensional WRF fields.

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1. Introduction

The objective of this study is to explore the potential benefit of coupling a microscale transport and dispersion (T&D) model with a mesoscale numerical weather prediction model in improving T&D modeling in complex urban environments. In the past decade, much progress has been made in order to improve the prediction of airflow and its dispersion in urban regions. For instance, Chan and Leach (2007) developed a computational fluid dynamics (CFD) model called Finite Element Model in 3-Dimensions (FEM3MP) to simulate airflow and dispersion of chemical/biological agents released in urban areas, and evaluated the model with observations from the Intensive Operating Period (IOP) 3 and 9 of the JU-2003 field study conducted in Oklahoma City, Oklahoma. Warner et al. (2004) evaluated the T&D using HPAC (Hazard Prediction and Assessment Capability) model against the URBAN 2000 data for simulating a Sulfur hexafluoride (SF₆) release scenario in Salt Lake City, Utah.

On the other hand, mesoscale models were used to study the T&D and urban processes; e.g. Chin et al. (2005). Miao et al. (2009) have used the Weather Research and Forecasting model (WRF) coupled with the Urban Canopy Model (UCM) (hereafter WRF_UCM) to study the urban heat island and its influence on the diurnal evolution of boundary layer structures over the Beijing metropolitan regions. Using the fine-scale WRF_UCM, Miao and Chen (2008) indicated that the WRF model with 500-m grid spacing is able to simulate the formation of horizontal convective cells over the Beijing areas.

⁎ Corresponding author. 3450, Mitchell Ln, Boulder, CO 80301, United States.
E-mail address: mukul@ucar.edu (M. Tewari).

0169-8095/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.atmosres.2010.01.006

0169-8095/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.atmosres.2010.01.006
Despite the aforementioned progress in T&D modeling, a common problem encountered when using a CFD-Urban model or any other microscale model for urban areas is how to properly specify initial and boundary conditions. Traditionally, most of the microscale models are initialized using observations from a single sounding point, which does not represent the variability of weather elements within urban areas. It is critical that T&D models should be initialized with more detailed atmospheric conditions than what is traditionally used. In this study (one of the first efforts of its kind) we run WRF and WRF_UCM models at sub-kilometer resolution so that the temporal and spatial meteorological fields from the mesoscale models could be used to supply initial and boundary conditions to the CFD-Urban model for the complex environment over the Salt Lake City (SLC) region. The accuracy of the CFD-Urban-simulated urban area contaminant T&D was evaluated against field data. Mesoscale models can provide urban-scale CFD-Urban model with more accurate, spatially-varying initial and boundary conditions while the CFD-Urban model can provide detailed representation of urban processes as a feedback to the mesoscale model.

2. Numerical modeling system

2.1. WRF and CFD-Urban models

WRF is a community model, the details of which can be found at http://www.mmm.ucar.edu/wrf/users. In the present work, we use the research-quality version of the WRF model, Advanced Research WRF (ARW core) with nesting capability (WRF V2.0, Skamarock et al., 2005) released in May 2004. Two types of urban parameterization schemes were used in the WRF: 1) a simple urban treatment (Liu et al., 2006), and 2) a coupled Noah/UCM (Kusaka et al., 2001; Kusaka and Kimura, 2004; Chen et al., 2009). CFD-Urban is a suite of Computational Fluid Dynamics modeling software that is being used to simulate the wind, turbulence and dispersion fields in urban areas (Coirier et al., 2005; Coirier and Kim, 2006).

2.2. Coupling WRF with CFD-Urban

2.2.1. Spatial interpolation of WRF data

In order to simplify the interpolation procedures, we average the velocity components to the cell-centers (WRF stored velocity fields at the face-centers and thermodynamic data at the cell-centers). Furthermore, we store the mesh dual (cell-centers) as nodes in the on-disk data representation. The field data is spatially interpolated from hexahedral WRF cells to individual face centroids in the CFD-Urban mesh using a continuous, linear interpolant. The WRF data are used to provide initial and boundary conditions to the CFD-Urban model, which include the velocity components, pressure base state and perturbation potential temperature, turbulence kinetic energy (TKE) and the momentum diffusion coefficient. The TKE dissipation rate for the k-ε model is found from the definition of the diffusion coefficient:

\[ \varepsilon = \rho C_{\varepsilon} \kappa^2 / \mu_t \]  \hspace{1cm} (1)

In this formula, the density (\( \rho \)) is computed from a perfect gas (dry air) equation of state, the turbulence kinetic energy (k) is from the MYJ model and \( \mu_t \) is the momentum diffusion coefficient. The dissipation rates determined from this relation (1) are higher than what is predicted from equilibrium theory, and TKE and dissipation-rates fields from the CFD-Urban solution are typically unrealistic. We defer to future studies to improve this behavior.

2.2.2. Imposing WRF pressure gradient

Pressure forces are supplied onto the boundaries of the CFD-Urban model by finding the difference in the imposed WRF pressure from the local pressure that would be present in an ideal atmosphere. Furthermore, the CFD-Urban model is operated in a constant density mode and does not apply a gravitational source term to the z-momentum equation. If the direct, hydrostatic (i.e. with gravitational source term included) coupling is made, both models must have consistent thermodynamic models (including humidity transport and equations of state), as well as having similar air-to-ground heat transfer models. Small differences in these thermodynamic quantities can produce unrealistic flow behavior in the CFD-Urban model. We found that the best approach was to apply the difference of the local WRF pressure to that of an ideal atmosphere, which the CFD-Urban model uses as the pressure difference from the (constant) CFD-Urban reference pressure. That is, impose on the face-centers of the CFD-Urban mesh:

\[ \Delta P = P_{\text{WRF}} - P_h = P_{\text{WRF}} - P_b \left[ 1 - \frac{1}{\kappa \gamma} \left( \frac{1}{RT_b} \right) (\tau_{z_b})^\kappa \right] \]  \hspace{1cm} (2)

where \( P_b \) represents the base state pressure and \( \kappa = \gamma / (\gamma - 1) \) where \( \gamma = C_p / C_v \)

2.3. Quasi-steady coupling

The quasi-steady mode first computes the steady state, equilibrium flow fields at 15 min intervals, using the WRF data as boundary conditions. The unsteady, contaminant transport evolution equation is then solved using the quasi-steady velocity and turbulence field that is found by linearly interpolating the appropriate steady state velocity and turbulence fields in time. We call this collection of steady-state wind fields a “wind field library” and the blending of these wind fields in time to solve the contaminant transport equation the “unified frozen hydrodynamic solver” as noted in Coirier and Kim (2006).

3. Numerical experiments

The WRF model was configured with five, two-way interactive, nested grids with a finer grid at 0.5 km as shown in Fig. 1(a). There were 16 levels within the lowest 2 km in the atmosphere to better resolve the boundary layer. The numerical experiments are listed in Table 1. The results from CFD-Urban model run using WRF_UCM data initialization is not shown because they are close to WRF model results. The zoomed-in image of domain-5 with a rectangle showing the CFD-Urban model domain is shown in Fig. 1(b). For WRF/WRF_UCM runs, we use a gridded (30-meter) urban land-use data with detailed classifications for the SLC urban...
zones: low-intensity (land-use category 31 in pink color),
high-intensity residential (land-use category 32 in dark pink
color), and the industrial/commercial zone (land-use category
33 in red color) in combination with USGS 24-category
dataset.

The CFD-Urban-model mesh (Fig. 2) is constructed using a
quadtree-prismatic/octree, Cartesian mesh generator that is
embedded in a solution adaptive flow solver (Coirier and Kim,
2006). The green cross in the figure represents the release
location during IOP 10. The CFD-Urban mesh covers a domain
of 8.4 by 7.4 by 1 km and contains approximately 325,000
cells, with higher lateral resolution in the Central Business
District (CBD) growing to approximately 200 m near the
domain boundaries. The mesh is clustered (stretched) in the
z-direction, normal to the ground plane, with higher
resolution near the ground growing smoothly to approxi-
mately 40 m near the upper boundary. Computational cells
that lie completely within buildings are removed while
buildings that occupy partial cells are modeled using the
drag model. Digital elevation data are used to map the
constant height ground plane mesh to be conformal to the
terrain using a displacement model.

For evaluation of WRF and WRF_UCM model results, we
used Sulfur hexafluoride (SF\textsubscript{6}) data from intensive operations
period (IOP 10) of URBAN 2000.

4. Results and discussion

4.1. Evaluation of WRF and WRF_UCM model results

The main purpose of the present study is to show the
impact of coupling the microscale CFD-Urban model with the
WRF modeling system so the evaluation of the WRF forecast
is done in order to check the quality of the data which is going
to drive the CFD-Urban model. For these evaluations, we
compared near-surface wind and temperature time series
with observations. We selected four sites over the model
domain (shown in Fig. 1) with different land-use types:

<table>
<thead>
<tr>
<th>Numerical experiments</th>
<th>Initialization</th>
</tr>
</thead>
<tbody>
<tr>
<td>WRF: Use Simple Urban in WRF</td>
<td>NCEP Eta data assimilation system (EDAS)</td>
</tr>
<tr>
<td>(24 h run starting 00UTC, 25 Oct 2000)</td>
<td>Same</td>
</tr>
<tr>
<td>WRF_UCM: Use WRF/UCM</td>
<td>Raging Water Sounding data</td>
</tr>
<tr>
<td>(24 h run starting 00UTC, 25 Oct 2000)</td>
<td>Raging Water Sounding data</td>
</tr>
<tr>
<td>Raging Waters Single Sounding</td>
<td>WRF/WRF_UCM data</td>
</tr>
<tr>
<td>Initialization (RW mode)</td>
<td></td>
</tr>
<tr>
<td>WRF-CFD-Urban Coupling</td>
<td></td>
</tr>
<tr>
<td>(Quasi-steady mode)</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 2. Surface mesh of CFD-Urban model. The green cross represents the release location during IOP10 experiment.
Green City Center (GCC; industrial/commercial zone), Hunter High School (M05, a PNNL site at low intensity residential area), UMASS and ATDD (both rural sites at the time of the experiment).

Observed time series of 2-m temperature, surface wind speed, and wind direction at four sites are used to evaluate WRF simulations for the 0.5 km resolution domain (Figs. 3, 4 and 5). A nighttime temperature difference of about 2 °C at 06 Z observed between the rural (ATDD) and urban/residential (M05) station demonstrates the urban heat island. The warming is a result of the weaker nighttime cooling and release of heat stored during daytime within the urban canopy as compared to the rural areas. Both UMASS and GCC sites located near the center of the Salt Lake Valley depict similar patterns of the nighttime temperature changes: the initial decrease in the evening, local minimum in the middle of the night and further increase to the evening values. These changes may be a result of the observed drainage flow in the valley caused by the variation of the surface energy budget on the mountain slope. At three of the four locations (i.e., at UMASS, ATDD and Hunter High School), the WRF and WRF_UCM 2-m temperatures are close to each other, and the mean values are generally within 1° of the observations. At the GCC site WRF_UCM, in general, gives better temperature prediction than WRF. The WRF results show 3 °C positive bias while the WRF_UCM is closer to observations with about 1 °C difference. During the nighttime conditions WRF_UCM results show a negative bias of the 1 °C amplitude. Such disagreement between the observations, WRF_UCM and WRF results may be explained by the complexity of the local flow at the GCC location. The GCC site is highly affected by a close presence of significant building structures while the WRF results represent the average characteristics within the whole 500-m size grid box. The wind observations in Fig. 4

**Fig. 3.** 2m temperature (°C) from 00Z to 15Z on 25 October 2000 at Green City Center, UMASS, ATDD and Hunter High School (M05). Dark grey lines with triangles represent the WRF model results, grey lines with closed circle represent the WRF_UCM results, and black lines represent the observations.
show complex structures of highly turbulent flow in the street canyon in the vicinity of large buildings: City Center and Heber-Wells. Because of the discrepancy between land-use characteristics used in WRF urban parameterizations and the complexity of the local flow at the GCC site, a significant difference between WRF results and observations for this particular site can be expected.

During the nighttime of the IOP 10, the wind conditions within the Salt Lake Valley were determined by the interaction between the southerly synoptic wind flow and the valley mountain canyon drainage flow. The modeled 10-m wind speeds presented in Fig. 4 show positive bias during most of the evaluation period. These are generally within 2 m s\(^{-1}\) compared to observations. Except for the Hunter High School site, the WRF and WRF_UCM results are close to each other. The mean model wind direction in Fig. 5 stays in good agreement with observations at three sites, with bias not exceeding 10–20 \(^{\circ}\) for most of the time. The comparison with the GCC site is difficult due to large oscillations in the observational data. These oscillations are presumably affected by the large surrounding urban structures (City Centers and Heber-Wells buildings), which cannot be resolved on the WRF model grid.

The discrepancies between the observed and modeled near-surface wind field may be attributed to the improper representation of the building drag and surface roughness slowing down the drainage flow (Chin et al., 2005). Due to the complex environment of the Salt Lake City region, it is difficult to discriminate the urban effects from the unresolved topographical flow features on the 0.5-km model grid. A more detailed analysis for finding the sources of the positive bias in the model 10-m wind speed is challenging and beyond the scope of this paper; hence, it is deferred here.
4.2. Evaluation of CFD-Urban model results

The CFD-Urban T&D modelling accuracy is assessed by comparing predicted to measured concentration values at sensor locations using standard statistical measures. The study here focuses upon using two measures: geometric mean bias \((MG)\) and the fraction of predictions within a factor of 2 \((FAC2)\).

\[
MG = \exp\left(\ln C_o - \ln C_p\right)
\]

\[
FAC2 = \text{fraction of data that satisfy } 0.5 \leq \frac{C_p}{C_o} \leq 2.0
\]

In the equations above, the averaging operator is taken over samplers located in four groupings \((\text{arcs})\): near the source, R2, R3 and R4, corresponding to the CBD, 2-km, 4-km and 6-km arcs in the field test \((\text{Fig. 1, Warner et al., 2004})\). The white rectangles in \text{Fig. 7} correspond to these sampler arcs R2, R3 and R4.

The two numerical experiments \((\text{RW mode and quasi-steady mode})\) described in \text{Table 1} were evaluated. The measured \("\text{observed}"\) quantities are taken from the URBAN 2000 IOP10 data, and are represented as \(C_o\), while the computed \("\text{predicted}"\) values are \(C_p\). The averages are taken over each arc. For our statistical comparisons, we use 4 \("\text{arcs}\)\), shown in \text{Hanna et al. (2003)}. As is noted by many earlier investigators, an \="\text{acceptable}\"\) model will have:

- \(0.7 < MG < 1.3\)
- \(FAC2 > 0.5\)

For those samplers that indicate a concentration of less than 10 ppt, and if the predicted concentration value at this same sampler is less than 10 ppt, we reset the predicted value to 5 ppt, in order to introduce a \="\text{floor}\"\) or minimum value within a factor of 2 of the sensitivity of the sampler. There are significant deficiencies when using the RW mode, namely...
atmospheric soundings were taken at one measurement location, whose representativeness is inadequate for the domain size considered here. There is no appropriate pressure data to apply at the CFD-Urban boundaries, which would miss important large-scale pressure gradients; turbulence data are either missing or in non-equilibrium with the wind speed profiles. To overcome the lack of consistent turbulence model data we use a Monin–Obukhov Similarity (MOS) profile with: \( u^* = 0.35 \text{ m/s} \), \( z_o = 0.55 \text{ m} \), and a MOS length scale of 80 m, which is found from the supplied wind profile data. For the wind direction, we directly use the measured data. The FAC2 and MG calculations for the above two experiments are presented in Table 2. It is evident from the table that using WRF three-dimensional fields (even at the 12-h forecast time) instead of single-point observed initial conditions leads to significant improvement. Except for locations R2 and R3, the WRF-CFD-Urban produced FAC2 are larger than the threshold value of 0.5 while the values of FAC2 from CFD-Urban using single sounding are less than 0.5 at all locations. Similar results are found for MG comparisons. When averaging these statistics over all locations, the superior performance of WRF-CFD-Urban is clear.

Table 2
Statistics showing the comparison of 2 different scenarios of CFD-Urban model initialization.

<table>
<thead>
<tr>
<th>Statistic experiment</th>
<th>Location</th>
<th>Near source</th>
<th>R2</th>
<th>R3</th>
<th>R4</th>
<th>All</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAC2: RW Single Sounding Initialization (RW mode)</td>
<td>FAC2: WRF-CFD-Urban Coupling (Quasi-steady mode)</td>
<td>0.12</td>
<td>0.17</td>
<td>0.36</td>
<td>0.38</td>
<td>0.18</td>
</tr>
<tr>
<td>MG: RW Single Sounding Initialization (RW mode)</td>
<td>MG: WRF-CFD-Urban Coupling (Quasi-steady mode)</td>
<td>0.57</td>
<td>0.42</td>
<td>0.36</td>
<td>0.5</td>
<td>0.51</td>
</tr>
<tr>
<td>MG: RW Single Sounding Initialization (RW mode)</td>
<td>25.42</td>
<td>14.11</td>
<td>4.58</td>
<td>5.06</td>
<td>15.83</td>
<td></td>
</tr>
<tr>
<td>MG: WRF-CFD-Urban Coupling (Quasi-steady mode)</td>
<td>0.74</td>
<td>1.59</td>
<td>1.96</td>
<td>2.05</td>
<td>1.04</td>
<td></td>
</tr>
</tbody>
</table>

In addition to MG and FAC2, predicted maximum concentrations are compared to measurements for all sensor locations in the scatter plots in Fig. 6. The underestimation of concentration from CFD-Urban in the RW mode, to a large degree, is improved in the prediction of the coupled WRF-CFD-Urban, which is consistent with statistics shown in Table 2. The dispersion of plume transport from the two sets of the experiment 60 min after the 3rd release of SF6 is shown in Fig. 7. The important vertical and lateral velocity variations imposed by WRF upon the CFD-Urban calculations and the lateral pressure gradient imposed by WRF was a significant forcing term that drove the plume transport in the direction similar to the observations (Fig. 7b), and the CFD-Urban using WRF conditions produced concentration which are better compared with observations than those obtained from using a single sounding.

In summary, the success of WRF-CFD-Urban to produce T&D prediction is due to the fact that the quasi-steady state runs (made at 15-min time intervals of the IOP10) give consistently good flow fields that have trends and behavior matching the WRF fields. The turning of lower boundary layer wind to NNW from N is well represented in WRF (shown in Fig. 7b), and the imposed WRF pressure gradient is felt by the CFD-Urban calculations. These improved steady-state flow fields result in significantly improved plume transport behavior and statistics.

5. Conclusions

A very high-resolution numerical modeling study was conducted over the complex terrain and complex urban areas in Salt Lake City. Using sub-kilometer-scale mesoscale WRF model-simulated meteorological fields as input for initial and boundary conditions required by CFD-Urban leads to significant improvement in replicating observed dispersion during the URBAN 2000 IOP10. WRF was run using two urban treatments: a simple modification of the Noah LSM and the more sophisticated WRF_UCM, but there was little difference in the result for this particular application. Therefore, for the

![Fig. 6. Predicted vs. Measure Concentration Values for (a) Raging Waters, (b) Quasi-Steady Model.](image-url)
initialization of CFD-Urban, we have only shown the results from WRF model. Although the results from the WRF_UCM model are not shown in the context of initialization of CFD-Urban a mesoscale model evaluation at the four sites was shown as it would provide insight for future work. At one of the four sites for which mesoscale model evaluation was done, WRF_UCM produces higher wind bias compared to WRF. It would be interesting to further investigate WRF_UCM by varying different UCM parameters specified through the urban parameter table. Our study found that the urban T&D modeling accuracy is quantifiably improved when the CFD-Urban model is coupled to the WRF model in a quasi-steady fashion. This mode of operation downscales velocity, turbulence and thermodynamic fields from the NWP model at set time intervals, where at these time intervals, the CFD-Urban model is run in a steady-state mode, using the downscaled data as initial and boundary conditions. The wind fields produced by this periodic downscaling are used in an Eulerian T&D model embedded in CFD-Urban. The key reason for this significant improvement in WRF-CFD-Urban coupling is that the turning of lower boundary layer wind and pressure gradient are well represented in the time-varying three-dimensional WRF fields but absent in the traditional approach of using single-point sounding to drive CFD-Urban. A further improvement in the T&D modeling accuracy may be achieved by upsampling the flow structures from building resolved scales (e.g. turbulence, drag forces, thermal effects) to the mesoscale model grid and increasing accuracy of urban canopy layer parameterizations within WRF which provides initial and boundary conditions to the CFD-Urban model. We expect to include the upsampling data transfer mode in the near future.

Acknowledgements

The authors gratefully acknowledge the support for this work from a Small Business Innovation Research Phase I project, funded through the Defense Threat Reduction Agency/TDOC, Technical Monitor CDR Stephanie Hamilton/USN. Part of this work is also supported by the NCAR FY07 Director Opportunity Fund. The valuable comments of Dr. Margaret A LeMone, Dr. C.M. Kishtawal and the reviewers helped in improving the manuscript.

References


Fig. 7. SF6 gas dispersion concentration 60 min after the third release for CFD-Urban model using (a) single sounding from the Raging Waters, (b) quasi-Steady Model. The contours are the concentration of SF6 (in PPT) and the dots represent the observed concentrations in the same scale as the color bar. White rectangles are added at the 2 km, 4 km and 6 km sampler arcs in order to highlight the model comparison with observations at these locations.
