One-Way Coupling of the WRF–QUIC Urban Dispersion Modeling System

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(Manuscript received 7 January 2015, in final form 30 May 2015)

ABSTRACT

Simulations of local weather and air quality in urban areas must account for processes spanning from meso- to microscales, including turbulence and transport within the urban canopy layer. Here, the authors investigate the performance of the building-resolving Quick Urban Industrial Complex (QUIC) Dispersion Modeling System driven with mean wind profiles from the mesoscale Weather Research and Forecasting (WRF) Model. Dispersion simulations are performed for intensive observation periods 2 and 8 of the Joint Urban 2003 field experiment conducted in Oklahoma City, Oklahoma, using an ensemble of expert-derived wind profiles from observational data as well as profiles derived from WRF runs. The results suggest that WRF can be used successfully as a source of inflow boundary conditions for urban simulations, without the collection and processing of intensive field observations needed to produce expert-derived wind profiles. Detailed statistical analysis of tracer concentration fields suggests that, for the purpose of the urban dispersion, WRF simulations provide wind forcing as good as individual or ensemble expert-derived profiles. Despite problems capturing the strength and the elevation of the Great Plains low-level jet, the WRF-simulated near-surface wind speed and direction were close to observations, thus assuring realistic forcing for urban dispersion estimates. Tests performed with multilayer and bulk urban parameterizations embedded in WRF did not provide any conclusive evidence of the superiority of one scheme over the other, although the dispersion simulations driven by the latter showed slightly better results.

1. Introduction

Urban areas account for roughly 50% of the global population and are projected to account for 70% by 2050 (UN 2008). The increase in urban population and associated growth in energy demand and fossil fuel usage leads to air quality problems affecting an increasingly larger population (Grimm et al. 2008). As the population distribution shifts toward urban areas, the need to understand the processes governing urban air quality, urban weather, and microclimate grows in importance. Further, urban security and adaptive response are a challenge that must be addressed by cities vulnerable to accidental or intentional biological, chemical, or radiological releases (Bugliarello 2005; NRC 2003).

Local weather and air quality in urban areas are a result of micrometeorological processes interacting with
the large-scale meteorological conditions. Therefore, simulations of local urban environments require an integration of mesoscale processes with finer-scale processes characteristic of the urban canopy layer (UCL). Many different models (parameterizations) have been developed that provide urban fluxes of pollutants, heat, and momentum for mesoscale models (Brown and Williams 1998; Dupont et al. 2004; Grimmond and Oke 2002; Ikeda and Kusaka 2010; Kondo et al. 2005; Lee and Park 2008; Martilli et al. 2002; Masson 2000). These urban models have various levels of complexity and parameterize the effects of buildings, roads, and green infrastructure (e.g., trees, grass, or ponds) on the radiation budget, as well as on heat, momentum, and moisture transport in the UCL. These parameterizations enable mesoscale models to respond to the presence of the urban forcing without a need to explicitly resolve urban processes. These urban parameterizations, however, do not resolve the UCL flow and cannot be used for buildingscale micrometeorological behavior and dispersion.

A different approach that enables detailed representation of the urban energy budget, flow, and dispersion is to drive large-eddy simulations (LES) or Reynolds-averaged Navier–Stokes (RANS) simulations with a mesoscale model (e.g., Baik et al. 2009; Conry et al. 2015; Kanda et al. 2013; Kwak et al. 2015; Liu et al. 2012; Lundquist et al. 2012; Miao et al. 2014; Park et al. 2012). This coupling allows for a realistic representation of the mesoscale forcing simultaneously with urban-scale processes. The coupled mesoscale–RANS dispersion system of Kwak et al. (2015) even includes atmospheric chemistry. In general, these coupled models have shown for dispersion problems that localized concentration variability is often missed when buildings are unresolved. Unfortunately, there are challenges with these types of approaches. For example, driving an LES model with mesoscale forcing is difficult, as switching from one-dimensional diffusion in a mesoscale model to three-dimensional mixing requires very large fetches, or advanced methods accelerating turbulence generation in nested LES domains (Muñoz-Esparza et al. 2014; Früh et al. 2011). Further, as a consequence of the very high resolution of the LES or RANS models, these coupled systems are computationally intensive, which severely limits their applicability for urban weather and dispersion forecasting purposes. In fact, Miao et al. (2014) noted that “efforts should be made to develop simplified CFD [computational fluid dynamics] models for emergency response programs.”

In this paper, we examine a slightly different approach in which a mesoscale weather model is coupled to a “simplified CFD” fast-response urban flow and dispersion model. With this system, high-resolution wind and dispersion fields can be obtained at a fraction of the computational cost associated with LES and RANS computations. This effort is part of the Green Environmental Urban Simulations for Sustainability (GEnUSiS) project, which has an overall aim to develop the tools and science needed to design more sustainable cities (Bailey et al. 2014; Addepalli et al. 2013). Our one-way coupled system consists of the Weather Research and Forecasting (WRF) Model (Skamarock et al. 2005) and the Quick Urban and Industrial Complex (QUIC) Dispersion Modeling System (Brown et al. 2013; Gowdharan et al. 2011; Pardyjak et al. 2009; Singh et al. 2009). The aim is to understand how well a coupled WRF–QUIC system can predict dispersion in real cities in comparison with simulations driven by expert-derived wind profiles from field-experiment data. Here, we focus on the mean wind coupling between WRF and QUIC, with future work exploring potential turbulence coupling and two-way couplings between WRF and QUIC.

We present the WRF and QUIC models and their setup in section 2. Section 3 discusses coupling between the models and presents validation of the WRF-simulated profiles against observations and expert profiles. Section 4 discusses and validates dispersion simulations driven by WRF (executed with bulk and multilayer urban schemes), the expert-derived wind profiles, and an ensemble of expert-derived wind profiles, using Joint Urban 2003 (JU2003) tracer measurements. Conclusions are summarized in section 5.

2. Description and setup of the coupled models

a. The Weather Research and Forecasting Model

WRF is a community modeling system designed for both operational weather forecasting and atmospheric research (Skamarock et al. 2005). It has been extensively evaluated and contains advanced physics options that allow for simulations, using either real-data or idealized configurations, covering a wide range of meteorological phenomena. Since WRF may be run in research or forecast mode, it can provide a smooth transition from research to operational applications. WRF also contains tools required for model setup, initialization, and validation including an analysis and observational data preprocessing module, a data assimilation system, and postprocessing and verification tools. This completeness of WRF makes it well suited for simulation and forecasting tasks that require atmospheric analyses based on meteorological measurements as well as topography and land-use data. The nesting capabilities of WRF allow for a telescoping series of increasingly finer-resolution domains to be used, providing a multiscale simulation. WRF
uses vertically stretched, terrain-following, pressure-based coordinates. Both one-way and two-way nesting are supported, with an option for moving nests. These nesting capabilities allow coarse resolution in the outer WRF domain to provide a large- or synoptic-scale weather simulation, while the innermost domain runs at higher resolutions to simulate the finescale details required for driving smaller-scale models.

To capture the synoptic and mesoscale low-level flow characteristics over Oklahoma City, Oklahoma, a four-domain nested WRF setup was used with horizontal grid resolutions of 36 km (160 × 120 grid points), 12 km (211 × 181), 4 km (283 × 241), and 1.33 km (361 × 301). The geographic location of the domains is shown in Fig. 1.

Dispersion simulations were performed with WRF for intensive observational periods (IOPs) 2 (release 1) and 8 (release 2) of the JU2003 field experiment conducted in Oklahoma City (Allwine and Flaherty 2006). Initial and boundary conditions for these simulations were generated from the North American Regional Reanalysis provided by the NOAA/OAR/ESRL Physical Science Division (http://www.esrl.noaa.gov/psd/; Mesinger et al. 2006). The static land-use and topography fields were initialized using MODIS data. WRF was configured with 70 vertical levels starting from 6 m AGL and going up to 16 km, with 11 equidistant layers within first 200 m above the ground and run with Monin–Obukhov surface-layer physics, the Noah land surface model, and the Bougeault and Lacarrere (BouLac; Bougeault and Lacarrere 1989) planetary boundary layer (PBL) scheme. Two WRF cases were considered, one with the bulk urban parameterization (Liu et al. 2006) and one with the multilayer urban canopy model (Chen et al. 2011). When the bulk parameterization is used, urban patches are treated in the land surface model in a similar way as vegetated ones. The urban effects are represented only by changed vegetation and soil properties (e.g., the roughness length is set to 0.5 m, while the vegetation fraction is set to 5%, leaf area index is set to 1.0, surface albedo is set to 0.15, and wilting point is 0.4).

The multilayer scheme, on the other hand, parameterizes the 3D effects of buildings in a form of sources and sinks of moisture, heat, and momentum vertically distributed throughout the urban canopy layer. It accounts
for the effects of walls, streets, and rooftops on momentum, turbulent kinetic energy, and potential temperature. It also captures radiative effects of streets and walls on the model radiation budget to provide a comprehensive representation of the impact of the urban canopy layer on the boundary layer. The simulation details are presented in Table 1.

Two 24-h periods were simulated: from 0000 UTC 2 July through 0000 UTC 3 July 2003 for IOP2 and from 0000 UTC 25 July through 0000 UTC 26 July 2003 for IOP8. The WRF output for the most inner domain was saved at 15-min intervals.

b. Fast-response urban dispersion model—QUIC

QUIC was originally developed as a building-resolving fast-response urban dispersion model (Brown et al. 2013). The wind model, QUIC-URB (Singh et al. 2008), is a building-resolving diagnostic wind model that relies on empirical parameterizations to produce realistic average urban wind fields. QUIC-Plume is an urbanized Lagrangian dispersion model (Williams et al. 2004) that has various algorithms designed to handle important plume transport characteristics in cities. In comparison studies, QUIC has been shown to compare well with traditional CFD models in predicting wind and concentration fields (Flaherty et al. 2007; Gowardhan et al. 2011; Neophytou et al. 2011). Graphical processing unit (GPU)-accelerated versions of QUIC-Plume exist (Singh et al. 2011); however, in this work, the standard Fortran executable was used. More recently, as part of the GenUSiS project, the QUIC Dispersion Modeling System has been expanded to include modules to compute radiative heat transport with vegetation as well as advective heat and moisture transport in cities (Bailey et al. 2014; Briggs et al. 2014). This more generalized solver, designed to help understand and solve complex urban sustainability problems, was not utilized in this study.

All simulations were run with QUIC version 6.01, which was configured with a single domain, covering an area of $1180 \times 1210$ m (in the east–west and north–south directions, respectively) with a 5-m horizontal resolution grid. The vertical direction used 64 levels with a resolution of 3 m. The coverage of the QUIC domain is presented in Fig. 1 (insert) and Fig. 2. All simulations were run assuming a neutral atmosphere within the urban domain. A total of 5 000 400 neutrally buoyant passive particles were released for each simulation. The particle concentrations were computed on a grid with the same resolution as the

![Fig. 2. The 3D view of the plan view shown in Fig. 1 of the Oklahoma City central business district. Note that the tallest building within the domain has a height of 152 m and that the release point is shown by the arrow.](image-url)
velocities (5 m × 5 m × 3 m). The source was assumed to be a sphere with a diameter of 1 m. Consistent with tracer releases during the JU2003 field campaign, during the IOP2 simulation a total of 9.025 kg of material was continuously released over a 30-min period, whereas for the IOP8 simulation 5.488 kg was released. The simulation parameters are identical to those specified in Brown et al. (2013) and additional details may be found therein.

For each IOP, we drove QUIC with a set of expert profiles used in previously published simulations, and with the WRF-simulated profiles. The expert profiles used here are based purely on the analysis of available data (Hanna et al. 2007; Neophytou et al. 2011) or have been adjusted within the uncertainty bounds of the measurements to ensure that QUIC modeled winds best match observations (Brown et al. 2013; Coirier et al. 2007). The dispersion simulations driven with expert profiles are used as a benchmark to evaluate WRF-driven simulations. For IOP2 we used three expert wind profiles indicated as Brown (Brown et al. 2013), Gowardhan (Brown et al. 2009), and Neophytou (Neophytou et al. 2011). For IOP8 (Fig. 8, below), we used the expert wind profiles from Brown (Brown et al. 2013), Gowardhan (Brown et al. 2009), Hanna (Hanna et al. 2007; Britter and Hanna 2003), and I. Sykes (2014, personal communication). Additionally, for both IOPs we computed mean expert profiles representing an ensemble of all profiles. A summary of the expert profile parameters is presented in Table 2.

3. Coupling and validation of the WRF profiles

In the coupled system, WRF is one-way coupled with QUIC. The former provides realistic synoptic and mesoscale forcing, whereas the latter is responsible for detailed simulation of the flow and dispersion in the UCL. QUIC is driven by WRF, but there is no feedback between QUIC and WRF. For coupling, WRF wind speed and direction data are interpolated horizontally to the center of the QUIC inflow boundary (middle red diamond on the southern boundary in the Fig. 1 insert), and vertically to each QUIC level. A logarithmic wind profile with a surface roughness length of 0.8 m (default in the WRF bulk urban scheme for high-density residential areas) is used to interpolate winds to QUIC levels located below the lowest WRF level. Profiles are updated at 15-min intervals.

To assess the capability of the coupled system for urban dispersion, we test this system on two JU2003 IOPs: daytime IOP2 release 1 and nighttime IOP8 release 2. For each IOP, we investigate WRF capabilities in terms of generating realistic large-scale inflow boundary conditions for the urban-scale simulations. We do this directly, by comparing the simulated wind speed profiles with a set of published expert profiles derived from the JU2003 observations, and indirectly, by analysis of the IOP2 and IOP8 dispersion simulations driven by the expert profiles and by WRF.

The QUIC model computes its own vertical wind speed profile within the UCL by representing the effects of building on the urban canopy flow. Therefore, it is not clear to what degree urban processes should be represented in WRF providing inflow boundary conditions for coupled WRF–QUIC simulations. To investigate this aspect, for each IOP, we performed two WRF simulations—one with a simple bulk urban parameterization (indicated in the text as u0) and one with the multilayer urban canopy scheme (indicated as u2).

**WRF-simulated wind profiles**

To assess WRF’s capability as a source of meteorological forcing for the high-resolution QUIC model, we compared WRF’s forecast wind speed profiles with observational data collected during the JU2003 field experiments. As is typically the case in cities, significant spatial variability existed among the wind speed profiles from different instruments. For the purpose of validation of the WRF-simulated profiles, wind speed data were horizontally averaged to create an integrated wind profile. In our analysis we used the Pacific Northwest National Laboratory (PNL) sodar, Argonne National Laboratory (ANL) sodar (Botanic Garden), ANL sodar (Christian Church), and Lawrence Livermore National Laboratory (LLNL) crane sonics. Locations of these instruments can be found in appendix A of Allwine and Flaherty (2006).

Similarly, the WRF data have been interpolated to the locations of these sensors and averaged to obtain an integrated WRF profile. To assess variability in

<table>
<thead>
<tr>
<th>Expert</th>
<th>Friction velocity $u^*$ (m s$^{-1}$)</th>
<th>Roughness length $z_0$ (m)</th>
<th>Wind direction ($^\circ$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>IOP2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Brown</td>
<td>0.363</td>
<td>0.1</td>
<td>215</td>
</tr>
<tr>
<td>Gowardhan</td>
<td>0.371</td>
<td>0.2</td>
<td>215</td>
</tr>
<tr>
<td>Neophytou</td>
<td>0.463</td>
<td>0.6</td>
<td>215</td>
</tr>
</tbody>
</table>

| IOP8      |                                     |                            |                          |
| Brown     | 0.795                               | 1.0                        | 160                      |
| Gowardhan | 0.520                               | 0.2                        | 165                      |
| Hanna     | 0.560                               | 1.2                        | 151                      |
| Sykes     | 0.605                               | 3.0                        | 166                      |
measured wind speed and direction across different sensors and locations, standard deviations have been computed from observational data at each measurement height. (The mean observational profiles, standard deviation, and the WRF-simulated wind speed and direction profiles for IOP2 and IOP8 are presented in Figs. 4 and 7, respectively, which are described in detail later.)

1) WIND PROFILES FOR IOP2 (DAYTIME)

As shown in Fig. 3, the vertical atmospheric structure 2.5 h after the beginning of daytime IOP2 release 1 [1830 UTC (1330 LST)] shows a well-developed mixed layer extending to 2000 m AGL surmounted by a weak inversion. At this time, as expected, the boundary layer is significantly deeper than the 400 m observed in early morning soundings by Wang et al. (2007). Remnants of the decaying Great Plains low-level jet (LLJ) can be observed with wind speed profiles that include maxima at 500 and 1200 m AGL (Wang et al. 2006). The thermal structure of the atmosphere was captured correctly by WRF, but the model struggled to produce a realistic representation of the complex vertical wind structure. In general, WRF underestimated the wind speed maxima at 500 and 1200 m AGL (see Fig. 3).

The measured and simulated wind speed profiles for the first 120 m (depth of the QUIC domain) are presented in Fig. 4. Despite problems capturing the vertical flow structure, the WRF-simulated low-level wind speed profiles averaged across the locations of sodars and crane sonics between 1600 and 1700 UTC (1100 and 1200 LST) matches the averaged observations surprisingly well with root-mean-square errors (RMSE) of 0.54 and 0.56 m s⁻¹ for the u0 and u2 runs, respectively. Within the layer between 30 and 80 m, the modeled winds were generally within the range of observed values indicated in Fig. 4 (the horizontal bars represent the standard deviation computed from the various sensors). The prescribed surface roughness length in the bulk urban representation (set to 0.8 m) appears to impose higher drag compared to the multilayer urban model. As a consequence, the bulk urban scheme yields slightly lower wind speeds and better captures the profile from 40 to 80 m AGL. However, the multilayer urban parameterization produces higher wind speeds above 80 m, which match the observations better at higher elevations. The comparison with the wind profiler data below 30 m shows that, regardless of the level of sophistication of the urban parameterization, WRF failed to fully capture the flow deceleration within the UCL and overestimated wind speeds near the surface, where the impact of the buildings is expected to be the most pronounced. The wind directions simulated with these two configurations are very similar, and generally within the standard deviation computed from observations. The RMSE between averaged observations and WRF simulations computed for the wind direction between 1600 and 1700 UTC was 11.94° for the u0 run and 13.98° for the u2 case.

For the purpose of defining inflow boundary conditions for urban dispersion simulations, wind profiles must be specified because of difficulties in finding representative single point/instrument measurements for the whole model domain. Hence, power-law or logarithmic “expert profiles” are used, which represent the best inflow wind conditions for the dispersion models. We use dispersion simulations driven with expert profiles as a benchmark to evaluate WRF-driven simulations using data collected during JU2003. As illustrated in Fig. 5, all expert profiles seem to converge at ~70 m AGL. WRF-simulated winds (especially for the u2 run) are very close to the mean expert profile near the surface but at higher levels are up to 1.2 m s⁻¹ slower than the mean expert profile. This is surprising, because when compared directly with the observations, the opposite seems to be true. WRF overestimates the wind speed within the urban canopy layer but compares well at higher elevations (see Fig. 4). It should be noted that the expert profiles are a result of subjective analyses of the data and represent the best estimate of the inflow conditions, rather than exactly matching the measured data themselves. The fact that the WRF simulations match expert profiles in the urban canopy layer seems to be more important in terms of driving the QUIC dispersion model than a direct match with...
the observations, which are strongly affected by urban infrastructure unresolved by WRF.

2) WIND PROFILES FOR IOP8 (NIGHTTIME)

Even though there are multiple radio soundings available for IOP8, none of them provided valid wind speed measurements over Oklahoma City for IOP8. For that reason, we decided to take advantage of the sounding taken in Norman, Oklahoma (~30 km south of Oklahoma City), 6 h after the beginning of the IOP8 tracer release 2. The observed wind speed and potential temperature profiles at this time are presented in Fig. 6. This early morning observational period was characterized by stable atmospheric stratification and the presence of a nocturnal LLJ centered ~500 m AGL. Similar to IOP2, WRF captured the thermal structure well but had problems rendering the strength and elevation of the LLJ. The magnitude of the simulated jet maximum was ~15 m s⁻¹, while the observations at the Norman station suggest a maximum wind speed ~20 m s⁻¹. The simulated jet maximum was also ~500 m higher than observed.

The underestimation of the strength of the LLJ may explain the underestimation of the near-surface wind speed between 80 and 120 m visible in Fig. 7. For IOP8, the agreement between the simulated and observed wind speed up to 12 m is worse than for IOP2 with RMSE of 2.68 m s⁻¹ for the u0 case and 2.34 m s⁻¹ for the u2 case. The wind direction prediction, however, was slightly better for IOP8 than for IOP2 (RMSE of 8.9° for the u0 and 8.0° for u2). The multilayer urban canopy model (UCM) run (u2) seems to provide more realistic results in terms of both wind speed and direction. The greater drag at the surface generated by the multilayer UCM helps to slow down the near-surface flow to better match observations. The change in the wind direction within the UCL captured in the u2 run also matches the observations better than the simple u0 case, yielding virtually constant wind direction within the first 120 m.

Despite the discrepancies between the simulations and observations, both WRF profiles are within the range of the expert profiles above 60 m. Below this level, however, the u2 profile matches the expert profiles much better than the u0 case, which overestimates the wind speed by up to 1 m s⁻¹. Despite the poor representation of the magnitude and elevation of the LLJ, the agreement between the simulated and the synthetic profiles is surprisingly good in the lowest 120 m, where the WRF u2 wind speeds are very close to Gowardhan and Brown (see Fig. 8). It seems that in this particular case the underestimation of the strength of the LLJ compensates for WRF’s inability
to represent flow deceleration within the UCL and produces surface winds similar in strength to the ones suggested by the experts.

4. Urban dispersion results for the coupled WRF–QUIC system

As discussed in the previous section, an assessment of WRF as a source of input wind profiles for urban modeling based solely on the comparison with the observations and expert profiles is ambiguous. The simulated wind profiles for the daytime IOP2 matched well with wind profilers but were significantly lower in the upper part of the QUIC domain than the expert ones. For the nighttime IOP8, on the other hand, the wind speed was generally overestimated at the surface as compared with the wind profilers but matched well the expert profiles. Additionally, WRF had problems capturing the LLJ, which is known to significantly enhance mixing in the nocturnal boundary layer (Hu et al. 2013). Therefore, to unequivocally assess how well the WRF–QUIC system performs, we conducted two full sets of dispersion simulations (for IOP2 and IOP8) using the QUIC model driven by all of the available expert profiles, the mean (ensemble) expert profile and WRF with (WRF u0) and without (WRF u2) the multilayer urban parameterization. The dispersion results were compared with each other and analyzed qualitatively by comparison with the observed concentrations. Additionally, standard statistical measures were computed for each run to allow for a quantitative analysis.

a. Performance measures

The predicted concentrations $C_p$ were quantitatively validated against observations $C_o$ in terms of the number of matched zeros, fractional bias (FB), normalized mean-square error (NMSE), geometric mean (MG), geometric variance (VG), and percent within a factor of 2 (FAC2) and 5 (FAC5), following Hanna and Chang (2012) and Brown et al. (2013):

$$FB = \frac{2(C_o - C_p)}{C_o + C_p}.$$  

$$NMSE = \frac{(C_o - C_p)^2}{C_o \times C_p},$$

$$MG = \exp[\ln(C_o) - \ln(C_p)],$$

$$MG = \exp\{[\ln(C_o) - \ln(C_p)]^2\}.$$  

The normalized absolute difference (NAD) was computed using the following formula:

$$NAD = \frac{|(C_o) - (C_p)|}{C_o + C_p}.$$
All statistics were computed only if both $C_P$ and $C_O$ were greater than the minimum level of quantification (MLOQ) estimated as $10^{-2}$ g m$^{-3}$ following Brown et al. (2013). The only difference between the methodologies used here and in Brown et al. (2013) is that we used this same conditioning for all statistical measures, while Brown et al. (2013) computed FAC2 and FAC5 if either $C_P$ or $C_O$ was above MLOQ.

To assess how well the simulations matched the observed plume shape, the measure of model effectiveness (MOE) was computed following Brown et al. (2013). Points within the plume points were defined as those with concentrations above the threshold value $C_t$. The value of $C_t$ was set to $10^{-2}$ g m$^{-3}$ as in Brown et al. (2013). The MOE values for the four cases presented in Figs. 9 and 10 are shown in Fig. 11. The MOE values for the remaining cases are in Table 3.

The MOE components were computed using the following equations from Warner et al. (2004):

$$MOE_{FP} = 1 - \frac{N_{FP}}{N_P} \quad \text{and} \quad (6)$$

$$MOE_{FN} = 1 - \frac{N_{FN}}{N_O}, \quad (7)$$

where $N_{FN}$ is the number of false negative detections, that is, the number of sensors for which predicted concentration $C_P < C_t$ and observed concentration $C_O > C_t$ (points outside of the modeled plume, which in fact are within the observed plume). $N_{FP}$ is the number of false positive detections, that is, the number of sensors for which predicted concentration $C_P > C_t$ and observed concentration $C_O < C_t$ (plume points according to the model, which in fact are outside of the observed plume). $N_P$ is the number of sensors with predicted concentrations above the $C_t$ threshold (number of sensors within the predicted plume), and $N_O$ is the number of sensors with observed concentrations above the $C_t$ threshold (number of sensors within the observed plume). Hence, the MOEs are unity for perfect overlap and decrease with increasing false positives and false negative predictions.

The 95% confidence levels ($\Delta_{95\%} MOE$, shown as error bars in Figs. 11 and 14, below) have been computed using the jackknife technique, following Benedict and Gould (1996), using the following equations:

$$\Delta_{95\%} MOE = 1.96[\text{var}(MOE_{\text{jack}})]^{1/2}, \quad (8)$$

$$\text{var}(MOE_{\text{jack}}) = \frac{N - 1}{N} \sum_{i=1}^{N} (MOE_{\text{jack},i} - \overline{MOE}_{\text{jack}})^2, \quad (9)$$

$$\overline{MOE}_{\text{jack}} = \frac{1}{N} \sum_{i=1}^{N} MOE_{\text{jack},i}, \quad (10)$$
MOE

\[ \text{MOE}_{\text{jack},i} \] is the MOE computed from a jackknife resample obtained removing \( i \)th pair of the observations–simulations, and \( N \) is the total number of observations paired in time and space with simulations.

The statistics for IOP2 and IOP8 are presented in Tables 3 and 4, respectively.

b. Dispersion results for IOP2

All IOP2 simulations show very similar characteristics, with common features similar to those described by Brown et al. (2013). For brevity, in Fig. 9 we only present concentration plots from the Brown case (the case yielding the best statistics in terms of fraction of points within a factor of 2 and 5), the mean expert profile, and the two WRF-driven cases. The flow patterns for all cases can be found in the appendix.

During the first 30 min, all of the simulations show similar channeling in north–south direction and a concentration drop of three orders of magnitude north of the release point, as well as the overestimation of the concentration south of the release point and just north of the release point. Despite these similarities, the simulations differ in terms of the plume width and its boundaries. The simulation driven by the Brown profile provides the narrowest plume among all cases. As a consequence, this simulation managed to reproduce the crosswind concentration drop on the northwestern edge of the plume better than any other (see concentrations at most northern points, near northing \( \approx 1100 \) m on Fig. 9 during the first 30 min). The limited lateral plume extent in the Brown case is associated with high wind speeds that promote effective downwind plume transport. The analysis of the vertically integrated wind profiles (see Table 5) confirms that indeed the flow rate across the QUIC domain is highest under the Brown profile.

Both WRF simulations overpredicted the western plume extent in the northern two-thirds of the plume, and consequently overestimated concentrations in this region. The WRF-simulated wind direction was a couple degrees more southerly than other expert profiles, which most probably led to the observed differences in the northern part of the western plume boundary. It should be noted, however, that closer to the release point—around 850 m to the north—the more southerly flow simulated by WRF resulted in a better representation of the concentration on the western edge (see first 30-min plots in Fig. 9).

As presented in the right column of Fig. 9 during the second 30-min period after the release, all simulations show significantly lower concentrations as compared with the first period. The concentration drop in the core of the plume due to contaminant flushing is generally captured well in all simulations, and generally results are in better agreement with observations. The scatterplots presented in Fig. 10, showing an increase in the number of matched zeros and fewer points outside of the factor-of-5 line, also confirm the improvement. Overall, the WRF simulations perform slightly worse than the expert-driven cases, especially during the first 30 min. The main reason for this is the relatively low ventilation rate in the WRF simulations when compared with the expert profiles. The flow rates across the QUIC domain in both WRF cases were significantly lower than in the cases in which expert profiles were used (see Table 5). Hence, the WRF-driven dispersion simulations generally overestimated concentrations. However, as shown in Table 3, during the second 30-min interval the WRF cases are comparable with the expert cases. During both periods, the FAC2 computed for WRF-driven simulations (all data paired in time and space) was greater than 30%, suggested as an acceptance criterion by Hanna and Chang (2012). The NAD was generally less than 0.5 except for the WRF u0 case during the second 30-min period, which was 0.54. The fractional bias, however, was not as good, with the values exceeding the recommended acceptance threshold of 0.67.

Figure 11 indicates that most of the simulations have similar MOE skills. For the initial 30 min of the release, the MOE computed from both WRF-driven simulations are slightly worse than the expert profiles.
WRF-simulated plumes had a larger number of false positives compared to the expert profiles, which seems to be a result of overestimated crosswind plume dispersion. This is most probably due to generally low WRF-simulated winds and an overly strong southerly component of the flow.

During the second 30-min period, both WRF simulations seem to have the same perfect false negative

<table>
<thead>
<tr>
<th>IOP2 1st 30 min</th>
<th>IOP2 2nd 30 min</th>
</tr>
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<tbody>
<tr>
<td><strong>Brown</strong></td>
<td></td>
</tr>
<tr>
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<td><img src="image7" alt="Image" /></td>
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</table>

**Fig. 9.** Simulated (color shading) and observed (color filled symbols) concentrations for IOP2 at 1.5 m AGL. Circles and diamonds correspond to street-level and roof-level measurements, respectively.
FIG. 10. Paired scatterplots of the predicted concentrations vs observations for IOP2 release 1 (2 Jul 2003). The first 30 min corresponds to the release [1100–1130 central daylight time (CDT)], and the second 30 min corresponds to the period right after the release shut off (1130–1200 CDT). Circles and diamonds correspond to street-level and roof-level measurements, respectively. For plotting purposes, the model-computed zero concentrations were set to $1 \times 10^{-9}$ g m$^{-3}$. The inner dashed lines indicate that the modeled results are within a factor of 2 of the measurements, and the outer dashed lines mark results that are within a factor of 5.
component of MOE as the expert profiles, but show more false positives. This suggests that the WRF plume extent is slightly over predicted. However, for both periods, the WRF results lie within the 95% confidence intervals of the expert profiles. This suggests that in terms of the MOE, the WRF-driven and expert-driven simulations are statistically similar.

The WRF simulations with the multilayer urban model (WRF u2) and bulk parameterization (WRF u0) show similar results, but generally the multilayer urban parameterization yields slightly better results, especially during the second 30-min period. This is likely a result of the higher wind speeds predicted at the average building height (see Fig. 4), which is directly used to scale the building wake and recirculation velocity parameterizations in QUIC. This results in increased mixing in the plume dispersion simulations.

c. Dispersion results for IOP8

The comparison between the observed and simulated concentrations for IOP8 is presented in Fig. 12. Similar to the daytime IOP2 case, during the nighttime IOP8, both WRF-driven simulations show results close to those driven by the expert profiles. During the first 30 min following the release start, all simulations tend to overestimate concentrations at the center of the plume. The biggest difference is noticeable in the western plume extent, which in the case of the Brown simulation is the greatest and closest to the observations. The Mean simulation shows the narrowest plume, not reaching as far west as observed. The WRF simulations seem to perform better than these two expert runs, with the WRF u0 case showing a western plume boundary that closely matches the Brown case and the observations. The paired plots presented in Fig. 13 show that the number of matched zeros for this case is actually greater than for the Brown case, and equal to the results obtained using the mean expert profile. Similar to IOP2 cases, all IOP8 simulations show general overestimation of the concentration during the initial 30-min period. However, contrary to IOP2, during IOP8, the WRF-driven simulations often

![Fig. 11. MOE for the IOP2 simulations driven by various wind profiles for (left) the first 30 min and (right) the second 30 min. The x axis represents a measure of false negatives, with 1 corresponding to perfect agreement and 0 to no agreement. The y axis represents a measure of false positives, with 1 corresponding to no false positives (the best score) and 0 being the worst score. The error bars represent 95% confidence levels computed using jackknife sampling.](http://journals.ametsoc.org/jamc/article-pdf/54/10/2119/3579457/jamc-d-15-0020_1.pdf)

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match observations better than the expert cases. The quantitative statistics shown in Table 4 confirms this observation. The paired plots presented in Fig. 13 show fewer outliers, and more points near the 1–1 line for the WRF cases than for the expert cases. The WRF simulations for IOP8 generally meet the acceptance criteria suggested by Hanna and Chang (2012): \( \text{FAC2} > 30\% \), \( \text{NAD} < 0.5 \), and \( \text{NMSE} < 6 \) (second 30 min only), which suggests that mesoscale WRF simulations have a potential as a source of forcing for fast-response urban models.

The MOE plots also show significant improvement in results from WRF-driven IOP8 (Fig. 14) simulations relative to IOP2 (Fig. 11). Both WRF u0 and WRF u2 MOE scores are as good as the Brown case, which had the best MOE score among all expert profiles. Depending on the inflow wind profile, some of the QUIC cases underestimated the plume area during the initial period (Gowardhan and Sykes), while others overestimated it (Brown, Hanna, and the WRF). It should be noted that all of the results are very similar and lie within the 95% confidence interval of each other. During the period after the end of the IOP8 release, all cases underpredicted the plume extent (more false negatives) but still remained within the 95% confidence intervals. In general during the first 30 min, all cases slightly underdisperse the plume and overpredict concentrations at the plume core but capture the plume shape well. During the second 30 min period after the release, the modeled winds tend to ventilate the pollutants and reduce the concentrations closer to the observed levels. However, most of the simulated plumes become narrower, resulting in a slightly larger number of false negatives when compared with the initial period after the release. The WRF results with the multilayer urban model (WRF u2) and without it (WRF u0) are similar, but, as in IOP2, the run with the multilayer urban parameterization provided slightly better results.

5. Conclusions

Despite the problems capturing the complex structure of the low-level jet, the coupled WRF–QUIC system showed similar skill in terms of concentration predictions as QUIC dispersion computations driven by expert wind profiles. The WRF-simulated wind profiles for IOP2 matched the observations very well (in fact better than did the expert wind profiles). However, the WRF-driven dispersion results during IOP2 were not as good as for IOP8, for which the WRF wind profiles did not match observations that well, but were close to the expert profiles (especially Brown and Gowardhan). One possible explanation for this surprising result is that the assumption of a neutral atmosphere in the QUIC computations worked better for the nighttime IOP8 than for the daytime IOP2, during which the assumed neutral stratification

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Table 5. Flow rates per unit width (m² s⁻¹) for the different cases obtained by vertically integrating wind speed profiles over the depth of QUIC domain for IOP2 and IOP8.
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</table>

**Fig. 12.** As in **Fig. 9**, but for IOP8.
FIG. 13. As in Fig. 10, but for IOP8 release 2 (25 Jul 2003) with the first 30 min corresponding to the release (0100–0130 CDT) and the second 30 min corresponding to the period right after the release shut off (0130–0200 CDT).
could limit convective mixing and lead to the observed overestimation in the concentrations at the plume core.

In terms of the plume overlap (MOE), WRF–QUIC performed as well as expert-driven QUIC. In both IOP2 and IOP8, the WRF–QUIC MOEs were within the 95% confidence interval computed from expert-driven simulations. That suggests that the basic plume properties may be captured adequately with WRF forcing, which is of special importance for dispersion forecasting.

Even though the wind profile analysis did not provide any conclusive evidence of the superiority of the simple bulk parameterization over the multilayer scheme, the later one provided slightly better dispersion results especially during the nighttime IOP8. It seems that stronger shear at the surface, as well as wind veering (turning clockwise with height) captured by the multilayer parameterization, helped to widen the plume and reduce the general overestimation of the concentration. In the urban canopy layer, the width of the plume is governed not just by turbulent mixing, but by channeling as well. Hence, even small changes in wind directions away from perpendicular to the buildings may result in much wider plumes or so-called topological dispersion (Belcher 2005).

Similarity between the simulations performed with various expert profiles also suggests that the system is rather robust with respect to the inflow wind speed, but quite sensitive with respect to the inflow wind direction. The dispersion results suggest that coupled system benefits from better representation of the UCL (multilayer vs bulk parameterization), which encourages further work on a two-way coupled system in which the WRF wind field could be directly affected by the UCL processes captured at very high horizontal resolutions by QUIC. However, additional improvements could be made to both QUIC and the coupled system to improve results. For example, currently mean velocity is coupled from WRF to QUIC, but turbulence is not. As a result, large-scale turbulence features above the city are not advected into the QUIC domain. In addition, buoyancy parameterizations should be added to QUIC to capture increased mixing during unstable periods.

Acknowledgments. This research was supported by National Science Foundation (NSF) Grant IDR 191 CBET-PDM 113458. The authors are also grateful to Drs. Ian Sykes and Steve Hanna for their “expert profile” contributions. We acknowledge high-performance computing support from Yellowstone (arc:/85065/d7wd3xh) provided by NCAR’s Computational and Information Systems Laboratory, sponsored by the NSF. An allocation of computer time from the Center for High Performance Computing at the University of Utah is also gratefully acknowledged.

APPENDIX

Extended Wind Field and Concentration Analysis

In the main document, we presented and discussed concentration results from the best cases driven by the expert profiles and WRF. Here, we present the flow and concentration fields for all analyzed cases. The results for the daytime IOP2 are shown in Fig. A1, while the results from the nighttime IOP8 are shown in Fig. A2.

Clearly, the wind directions are very similar for all IOP2 cases. In fact, all expert profiles were forced with a wind direction of 215°, while the WRF simulations showed only slightly more southerly flow with the wind direction of nearly 209°. As a consequence, the
biggest differences in the flow pattern for IOP2 are associated more with the wind speed than the wind direction. The strongest flow was observed with the Brown profile. In this case, the plume was effectively pushed downwind, with high concentrations in the plume core and limited lateral extent. With these features, the Brown cases compared best to the observations. The WRF-simulated winds were weaker and slightly more southerly than the expert winds. As a consequence, their northwesterly extent was overestimated as compared to the observations.

More variability across the expert profiles was observed during IOP8. In this case, the wind directions varied between 155° (Hanna) and 166° (Sykes). As a consequence, the plume shapes and building recirculation patterns in the northern part of the domain differed significantly across the expert profiles. More southerly flows like Gowardhan and Sykes were associated with the plume splitting into two distinctive branches, which resulted in overpredicted concentrations in the northern part of the domain. The weaker and most easterly flow (Hanna) on the other hand resulted in an overestimated westward plume extent. The
<table>
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wind directions of $\sim 160^\circ$ with relatively strong flows (Brown and WRF) resulted in the best agreement between the simulated and observed concentrations.

REFERENCES


