Mesoscale to Microscale Simulations over Complex Terrain with the Immersed Boundary Method in the Weather Research and Forecasting Model

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ABSTRACT

Improvements to the Weather Research and Forecasting (WRF) Model are made to enable multiscale simulations over highly complex terrain with dynamically downscaled boundary conditions from the mesoscale to the microscale. Over steep terrain, the WRF Model develops numerical errors that are due to grid deformation of the terrain-following coordinates. An alternative coordinate system, the immersed boundary method (IBM), has been implemented into WRF, allowing for simulations over highly complex terrain; however, the new coordinate system precluded nesting within mesoscale simulations using WRF's native terrain-following coordinates. Here, the immersed boundary method and WRF's grid-nesting framework are modified to seamlessly work together. This improved framework for the first time allows for large-eddy simulation over complex (urban) terrain with IBM to be nested within a typical mesoscale WRF simulation. Simulations of the Joint Urban 2003 field campaign in Oklahoma City, Oklahoma, are performed using a multiscale five-domain nested configuration, spanning horizontal grid resolutions from 6 km to 2 m. These are compared with microscale-only simulations with idealized lateral boundary conditions and with observations of wind speed/direction and SF₆ concentrations from a controlled release from intensive observation period 3. The multiscale simulation, which is configured independent of local observations, shows similar model skill predicting wind speed/direction and improved skill predicting SF₆ concentrations when compared with the idealized simulations, which require use of observations to set mean flow conditions. Use of this improved multiscale framework shows promise for enabling large-eddy simulation over highly complex terrain with dynamically downscaled boundary conditions from mesoscale models.

1. Introduction

Current numerical weather prediction (NWP) codes have been extensively validated and designed for mesoscale

simulations with horizontal resolutions ranging from tens of kilometers to several kilometers (i.e., >3 km). Advances in computational resources have enabled microscale simulations of the planetary boundary layer at large-eddy simulation (LES) resolutions (i.e., <100 m) that are beyond the original design space of available NWP codes. Downscaling of information from mesoscale to microscale resolutions requires the accurate simulation of phenomena with temporal and spatial scales spanning many orders of magnitude. Multiscale NWP models, if designed to properly simulate scales spanning the mesoscale and microscale, have the potential to greatly improve many applications of NWP, including air quality modeling, emergency response dispersion modeling, and wind energy forecasting.

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Several methods have been developed to enable microscale NWP simulations to ingest downscaled mesoscale information. A common approach involves the coupling of separate mesoscale and microscale models. With this method, variables of interest are interpolated from a coarse mesoscale grid onto a high-resolution microscale grid. The coarse time step of mesoscale models and a lack of resolved submesoscale motions often necessitates special treatments to mimic the effect of developed turbulence at inflow boundaries of the microscale model. Using different models for the mesoscale and microscale is further complicated by differences in governing equations, coordinate projections, grid systems, advection schemes, and parameterizations (Baklanov et al. 2002). Despite the potential shortcomings of this approach, coupling of mesoscale and microscale models has been found to improve results relative to microscale-only simulations of urban flow and dispersion (Park et al. 2015; Li et al. 2018).

An alternative to coupling separate mesoscale and microscale models is a grid-nesting approach in which information is dynamically downscaled from a coarse-resolution “parent” domain that provides initial and lateral boundary conditions to a fine-resolution “child” domain. A multiscale NWP simulation configured with grid nesting is therefore composed of a telescoping sequence of increasingly higher-resolution domains. The Weather Research and Forecasting (WRF) Model, which is used in this research, has a grid-nesting approach to downscaling that has been previously validated and applied to nested LES simulations (Moeng et al. 2007; Marjanovic et al. 2014; Taylor et al. 2018).

Multiscale modeling with grid nesting may be impaired by poor grid quality (e.g., extreme aspect ratios and skewed cells), a lack of suitable parameterizations at intermediate scales, and difficulty in generating small-scale turbulent motions after grid refinements. Despite these challenges, multiscale modeling with grid nesting holds many advantages over the model-coupling approach, such as the ease of updating lateral boundary conditions at each time step, conveniently aligned grids that are configured with a common projection, and compatible numerical methods for each grid.

Many NWP codes, including the WRF Model, were originally designed for mesoscale simulations and require extensive development to permit multiscale modeling. WRF’s terrain-following vertical coordinate is problematic for high-resolution simulations over complex terrain because grid distortion resulting from steep terrain slopes leads to numerical errors (Klemp et al. 2003; Zangl et al. 2004; Klemp 2011). When grid resolution is refined, steeper terrain slopes are sampled, thus restricting microscale simulations to application over shallow sloping terrain. Our solution to the challenges

associated with complex terrain in microscale simulations is an alternative gridding technique that does not require a terrain-following coordinate, namely the immersed boundary method (IBM). The IBM implementation in WRF used here builds on the work of Lundquist et al. (2010, 2012) and Bao et al. (2018). WRF-IBM enables the simulation of microscale flow over complex terrain, such as urban street canyons or mountains. Microscale-only urban simulations using WRF-IBM with idealized boundary conditions by Lundquist et al. (2012) have shown model skill that is comparable to other computational fluid dynamics codes such as the Finite Element Model in 3-Dimensions and Massively Parallelized (FEM3MP; Chan and Leach 2007) and “QUIC-LES” (Neophytou et al. 2011). Previous WRF-IBM simulations by Lundquist et al. (2012) were performed with the ghost point method (GPM) version of the IBM algorithm. The velocity reconstruction method (VRM) version of the IBM algorithm, which has been validated by Bao et al. (2018), is used in these multiscale simulations because it facilitates nesting of a microscale IBM domain within a mesoscale terrain-following parent domain, a functionality that was not possible with the GPM.

Over complex terrain, a nested IBM domain will use a different vertical grid than a terrain-following parent domain, which necessitates vertical interpolation during nesting (see Fig. 1). Vertical gridding in the simulations presented here is managed with the vertical grid refinement method detailed in section 2b (Daniels et al. 2016; Mirocha and Lundquist 2017). This method provides control of the grid aspect ratio and placement of vertical grid levels for each domain in a nested simulation, which Mirocha et al. (2013) found to be critical for nested LES in WRF. The combination of vertical grid refinement and IBM enable simulations over complex terrain that capture effects across a wider range of scales than previously possible. A single simulation may now contain nested domains with grid resolutions ranging between the mesoscale (kilometers) to the microscale (meters). To the authors’ best knowledge, the simulations presented here are the first to dynamically downscale from a mesoscale NWP model to a microscale urban simulation within a single NWP code.

Simulations of a continuous tracer release from the Joint Urban 2003 (JU2003) field campaign in Oklahoma City, Oklahoma (Allwine and Flaherty 2006), are used here to systematically evaluate the performance and potential benefits of the VRM algorithm and the multiscale modeling framework. Previous JU2003 studies (Chan and Leach 2007; Hanna et al. 2011; Neophytou et al. 2011; Nelson et al. 2016; García-Sánchez et al. 2018) have examined wind flow and tracer transport and

FIG. 1. A vertical slice through a fictional nested domain with two grids using the VRM immersed boundary method and grid refinement. The immersed boundary is shown in red.

dispersion using many different models including diagnostic wind flow models, Reynolds-averaged Navier–Stokes simulations, and large-eddy simulations. The simulations presented here include a multiscale configuration of five nested domains with resolutions ranging from 6.05 km to 2 m. The NCEP North American Regional Reanalysis is used for initial conditions and lateral boundary updates for the outermost domain of the multiscale simulation. Because current models cannot replicate this multiscale configuration, we validate the multiscale modeling framework developments by comparison with observations and with idealized simulations. The two idealized setups (GPM and VRM) evaluated here are similar to previous modeling efforts by Golaz et al. (2009) and Lundquist et al. (2012) with a two-domain nested setup, grid resolutions of 10 and 2 m, periodic lateral boundary conditions on the outer domain, and a pressure gradient forcing scaled according to JU2003 observations. Configurations for the idealized and multiscale simulations are detailed in sections 3a and 3b, respectively. Predictions of velocities and passive tracer concentration from the three simulations are compared with the JU2003 observations using several statistical measures of model skill proposed by Chang and Hanna (2004) and Calhoun et al. (2004) that are described in section 4. Comparison of model skill from the idealized simulations provides insight into the benefits of a more sophisticated IBM while comparison of the idealized VRM and multiscale simulations provides insight into the benefits of downscaling using a multiscale grid-nesting approach.

2. Improved multiscale modeling framework

The multiscale simulations presented here rely upon use of two major improvements to the WRF Model: the immersed boundary method (section 2a) and vertical grid refinement (section 2b).

a. The immersed boundary method

The immersed boundary method is a technique for imposing the effects of a physical boundary on fluid flow.

The method is especially useful for the simulation of flow over complex shapes or flexible surfaces because it does not require complicated meshing and it provides a convenient way to determine forces exerted by fluid on boundaries (Peskin 1972). IBM has the additional benefit of using a structured grid, which makes spatial discretization easier and eliminates numerical errors associated with grid transformations. Previous applications of the IBM are diverse and examples include simulations of flow over vehicles, fluid–particle interactions, and geophysical flows (Iaccarino and Verzicco 2003; Senocak et al. 2004; Mittal and Iaccarino 2005).

As simulations of environmental flows advance to higher resolutions, implementations of the immersed boundary method are increasingly common and are recently undergoing substantial research and improvement (Bao et al. 2018; Li et al. 2016). For atmospheric applications, the immersed boundary method can eliminate grid transformation errors where terrain-following coordinates are traditionally used or simplify meshing where a more traditional computational fluid dynamics model would be used with a conforming grid, such as simulations in urban terrain. Immersed boundary methods have been implemented for a variety of atmospheric simulations that notably include simulations of the Bolund Hill complex terrain test case (Jafari et al. 2012; Diebold et al. 2013; Bao et al. 2016; Ma and Liu 2017; Bao et al. 2018; DeLeon et al. 2018), flow over fractal trees (Chester et al. 2007), and urban simulations of transport and dispersion (Lundquist et al. 2012).

Figure 1 shows a slice through a grid with the immersed boundary (IB) shown in red. Boundary conditions are enforced at the IB through the addition of a forcing term to the governing equations. Several IBMs appear in the literature and can be categorized based upon whether the forcing term is introduced to the continuous or discretized governing equations. WRF-IBM falls within the latter category, also known as a discrete forcing approach, and includes a body force term in the conservation equations for momentum and scalars [Eq. (1)]. These body force terms are not computed directly but are instead implicitly applied by modifying variables at grid points near the immersed boundary:

$$\partial_t \mathbf{V} + \mathbf{V} \cdot \nabla \mathbf{V} = -\alpha \nabla p + \nu_t \nabla^2 \mathbf{V} + \mathbf{g} + \mathbf{F}_B \quad \text{and} \quad (1a)$$

$$\partial_t \phi + \mathbf{V} \cdot \nabla \phi = \kappa_t \nabla^2 \phi + F_\phi. \quad (1b)$$

In Eq. (1a) $\mathbf{V}$ is the velocity vector, α is the specific volume, p is pressure, $\mathbf{g}$ is gravitational acceleration, ν_t is turbulent viscosity, and $\mathbf{F}_B$ is the body force term. In Eq. (1b) ϕ is a scalar quantity, which could represent potential temperature, moisture, or a passive tracer, κ_t is the scalar diffusivity,

and F_ϕ is the additional scalar forcing; $\mathbf{F}_B$ and F_ϕ modify the conservation equations near the IB and assume values of zero away from the IB. The conservation equations, Eqs. (1a) and (1b), are presented in a simplified form for illustrative purposes. Further information regarding the implementation of an IBM on the WRF governing equations can be found in [Lundquist et al. \(2010\)](#).

The immersed boundary method in WRF (WRF-IBM) has previously been used for a variety of microscale and large-eddy simulations. [Lundquist \(2010\)](#) developed WRF-IBM in two dimensions and coupled the IBM to a suite of atmospheric parameterizations, allowing for surface fluxes of heat and moisture at the immersed boundary. [Lundquist et al. \(2012\)](#) extended the method to three dimensions and simulated flow and dispersion within the central business district of Oklahoma City. [Arthur et al. \(2018\)](#) enabled topographic shading at immersed boundaries and evaluated the development of thermally driven downslope flow on an isolated mountain during the Mountain Terrain Atmospheric Modeling and Observations (MATERHORN) field campaign. [Bao et al. \(2018\)](#) implemented a surface stress parameterization at the IB and compared simulations with observations from the Askervein (Scotland, United Kingdom) and Bolund (Denmark) field experiments. Each of these previous simulations used idealized initial conditions and forcing at lateral boundaries, preventing representation of time-varying weather effects on these smaller-scale simulations.

In previous applications of WRF-IBM, idealized initial conditions and lateral boundary conditions were used because domains using the immersed boundary method could not easily be nested within those using WRF's native terrain-following coordinate. This was due to the GPM version of the IBM algorithm requiring computational grid points below the immersed boundary. These additional grid points introduce a discontinuity in grid heights at the interface between nested terrain-following and GPM domains, which is incompatible with the WRF Model equations. VRM is an alternative to the GPM that does not require grid points beneath the IB, which greatly simplifies the nesting of a domain using VRM within a terrain-following parent grid. WRF-IBM uses a nonconforming structured grid that can optionally be independent of the IB or, if using VRM, the grid may optionally and selectively align with the IB. An example grid, shown in [Fig. 1](#), illustrates the approach used in these multiscale modeling efforts using VRM where the grid is allowed to conform to the underlying ground topography while complex features, such as buildings, are represented by the immersed boundary.

1) GHOST POINT METHOD

GPM enforces desired boundary conditions by applying forcing at computational nodes considered to be within the “solid” portion of the domain. Nodes where forcing is applied are referred to as “ghost points.” The procedure to modify each ghost point begins by reflecting the ghost point across the immersed boundary, which creates an “image point.” The image point's magnitude is calculated based upon the magnitudes of nearby computational nodes using an interpolation scheme, which in this case is the inverse distance weighting (IDW) scheme, the details of which are discussed later in this section. An example illustrating this procedure is shown in [Fig. 2a](#). The magnitude of ϕ at a ghost point is then determined using Eq. (2a) for a Dirichlet boundary condition or Eq. (2b) for a Neumann boundary condition:

$$\phi_G = 2\phi_\Omega - \phi_I \quad \text{or} \quad (2a)$$

$$\phi_G = \phi_I - \overline{GI} \frac{\partial \phi}{\partial \mathbf{n}} \Big|_\Omega, \quad (2b)$$

where ϕ_G is the value at the ghost point, ϕ_I is the value at the image point, and ϕ_Ω is the value at the IB. The $\overline{GI}$ is the distance between the ghost and image points and $\partial \phi / \partial \mathbf{n}|_\Omega$ is the surface-normal gradient value assigned at the IB for a Neumann boundary condition. For the simulations presented here using the GPM, a no-slip boundary condition is applied to velocities.

Because the GPM requires ghost points and at least two vertical grid levels positioned beneath the IB, the grid's bottom level is lowered relative to a WRF grid using terrain-following coordinates. This mismatch complicates nesting between terrain-following and GPM domains because it creates a discontinuity in domain height across the nest interface. For this reason, we have modified another WRF-IBM algorithm, the velocity reconstruction method first introduced by [Bao et al. \(2018\)](#) and described below, which is suited to our needs for multiscale modeling because it does not require ghost points, and thus is capable of being used on a domain nested within a parent domain using terrain-following coordinates. Additionally, [Bao et al. \(2018\)](#) found improved model performance when using IBM algorithms that use log-law boundary conditions, such as the velocity reconstruction method.

2) VELOCITY RECONSTRUCTION METHOD

VRM follows a similar approach to that of [Senocak et al. \(2004\)](#), in which a log-law boundary condition at the IB is enforced by applying forcing at the computational nodes in the fluid domain that are adjacent to the immersed boundary, which are referred to here as

FIG. 2. Two-dimensional examples of point selection by the (a) GPM and (b) VRM algorithms. The immersed boundary is shown in green, reconstruction points (VRM) and ghost points (GPM) are in purple, interpolation points (VRM) and image points (GPM) are in blue, and nearest neighbors are in red. The solid and dashed gray lines represent the Arakawa-C staggered grid used by WRF, with mass points located at the intersections of the dashed lines.

reconstruction points (RP). Extensive validation of the VRM in WRF-IBM was performed by Bao et al. (2018), which includes simulation of flow over flat terrain, idealized hills, and Askervein and Bolund Hills.

Boundary conditions at the IB are enforced by modification of each RP according to the following procedure, an example of which is illustrated in Fig. 2b. First, a vector is calculated that connects the RP and the nearest section of the IB. The “interpolation point” (IP) is then located by projecting away from the IB along this vector until reaching a cell face. The u , v , and w velocities at the IP are calculated using the IDW interpolation scheme described in section 3. The coordinate orientation at the IP is then rotated to be surface normal to the IB, aligning with the vector used earlier. The log-law for flow over a rough surface, Eq. (3) as written by Panofsky and Dutton (1984), is then used to relate velocities at the IP and RP:

$$U = \frac{u_*}{\kappa} \ln \left(\frac{z}{z_0} \right). \quad (3)$$

Here z is the surface normal distance from the IB, z_0 is the roughness height, u_* is the friction velocity, κ is the von Kármán constant, and U is the magnitude of the velocity. Note that relating the IP and RP using Eq. (3) assumes that the friction velocity is constant in the surface normal direction within the region that contains both the IP and RP. With this assumption the relationship between the IP and RP can be represented as follows, where d_{RP} and d_{IP} are the surface normal distances between the IB and the RP or IP:

$$U_{RP} = U_{IP} [\ln(d_{RP}/z_0)/\ln(d_{IP}/z_0)]. \quad (4a)$$

The w_{RP} is calculated by assuming $w = 0$ at the IB and a linear relationship of w with d , which yields

$$w_{RP} = w_{IP} (d_{RP}/d_{IP}). \quad (4b)$$

The U_{RP} is then separated into u and v velocities, where θ is the horizontal wind direction defined using geographic convention:

$$\theta = \arctan(u_{IP}/v_{IP}) \quad \text{and} \quad (5a)$$

$$u_{RP} = U_{RP} \sin \theta, \quad v_{RP} = U_{RP} \cos \theta. \quad (5b)$$

Last, the u , v , and w velocities at the RP are rotated from being surface-normal to the IB back to the coordinate orientation of the grid.

3) INVERSE DISTANCE WEIGHTING INTERPOLATION SCHEME

The IDW interpolation scheme is used to determine values for image and interpolation points when using GPM and VRM, respectively. First, the nearest-neighboring grid points to the image/interpolation point are located by searching a box of grid points centered on the

image/interpolation point. The simulations presented here search for nearest neighbors within either a $4 \times 4 \times 4$ or $6 \times 6 \times 6$ box of grid points for simulations using the GPM or the VRM, respectively. Each point in searched region is ranked based upon distance from the image/interpolation point. Points beneath the IB are removed from consideration. For the VRM, reconstruction points are also removed from consideration. The nearest n points are used as the nearest neighbors to the image/interpolation point, where $n = 8$ for the GPM and $n = 7$ for the VRM. Image/interpolation points will occasionally have fewer than n valid nearest neighbors, especially if the point is located over extremely complex terrain. The simulations presented below have been configured such that all image/interpolation points have at least two valid nearest neighbors.

The value at each image/interpolation point ϕ is calculated using Eq. (6a), which is a weighted average of the nearest neighbors to the image/interpolation point. Weights of nearest neighbors are calculated using Eq. (6b) where $r_{\max}$ is the maximum distance between a nearest neighbor and the image/interpolation point, and W_i is the weight of the i th nearest neighbor, which is a distance r_i from the image/interpolation point. Image/interpolation point locations, nearest neighbors, and weights are recalculated at each time step to avoid complications that may arise if the WRF gridpoint heights shift during runtime because of the model's mass-based vertical coordinate:

$$\phi = \frac{\sum_{i=1}^n W_i \phi_i}{\sum_{i=1}^n W_i} \quad \text{and} \quad (6a)$$

$$W_i = \left(\frac{r_{\max} - r_i}{r_{\max}} \right)^{1/2}. \quad (6b)$$

b. Vertical grid refinement

A key feature required for multiscale simulations is vertical refinement of nested domains. Prior to WRF, version 3.8.1, the only available method of vertical grid refinement was “ndown,” a separate program that ingests parent grid output files and generates boundary updates for a nest. Because ndown processes output files, the parent simulation must be run to completion before the nested simulation can be run. In addition, the boundary update frequency is limited to that of the parent grid output, which can prohibit downscaling of resolved turbulent flows.

We previously developed an improved vertical grid refinement method that has been included within the WRF public release since version 3.8.1 (Daniels et al. 2016) and is used here in version 3.6.1. This capability

allows for nested domains with different vertical grids to be run concurrently without requiring a separate program like ndown. The lateral boundary conditions of a nest are updated at every time step using an interpolation between bracketing time steps from the corresponding parent. We have also included the ability to specify unique vertical grid levels for every domain in a sequence of nested grids. Additional details regarding the capabilities, implementation, and validation of the vertical nesting framework can be found in Daniels et al. (2016).

The vertical grid refinement capability is a critical component of the multiscale modeling framework described here. The ability to refine vertically provides control over each domain's grid aspect ratio ($\Delta x/\Delta z$), an important variable for accurate large-eddy simulations (Mirocha et al. 2013; Mirocha and Lundquist 2017). Note that our multiscale simulation, detailed in section 3b, successfully applies the vertical grid refinement method to a sequence of five nested grids, a considerably more complex configuration than simulations from Daniels et al. (2016).

3. Simulations for Joint Urban 2003 dispersion study

During July of 2003, the Defense Threat Reduction Agency (DTRA) and the U.S. Department of Homeland Security (DHS) worked together to facilitate the JU2003 atmospheric dispersion study in Oklahoma City. Investigators from universities, government laboratories, and private industry participated in the field campaign and analysis. Some of the primary objectives of this field campaign included the investigation of flows downwind of tall buildings and in street canyons and the investigation of tracer dispersion around and downwind of tall buildings. More details can be found in the study overview (Allwine and Flaherty 2006).

Joint Urban 2003 consisted of 10 intensive observational periods (IOPs), each with 8-h duration, throughout the 34-day span of the field campaign. A tracer gas—sulfur hexafluoride (SF_6)—was released during each IOP as either a puff or continuous release. Meteorological conditions and tracer concentrations were measured at sites throughout the central business district. The locations of the SF_6 release site and the instruments used in this analysis are displayed in Fig. 3. Observations from several instruments have been used for configuration and analysis of the simulations presented here, including a minisodar deployed by Argonne National Laboratory (ANL), 11 Dugway Proving Ground (DPG) Portable Weather Information Display Systems (PWIDS) with propeller-vane anemometers, 15 DPG “super PWIDS”

FIG. 3. A map of the Oklahoma City business district showing measurement stations used during the analysis of simulation results. The SF_6 release location was located at UTM coordinates (634603, 3925763). The ANL minisodar was located at UTM coordinates (634451, 3925592). The plot's limits are coincident with the lateral boundaries of the innermost domain with 2-m horizontal resolution.

with sonic anemometers, 19 Lawrence Livermore National Laboratory (LLNL) “bluebox” integrating gas samplers, and 25 NOAA/Air Resources Laboratory (ARL) Field Research Division (FRD) programmable integrating gas samplers (PIGS).

The simulations and analysis presented in this paper are limited to the first continuous tracer release of IOP 3 from 1600 to 1630 UTC 7 July 2003. During IOP 3 the SF_6 release location was at the northeast corner of the botanical gardens at 2 m above ground level (AGL) and universal transverse Mercator (UTM) coordinates (634603, 3925763; meters easting and then northing), marked by the yellow star in Fig. 3. This particular tracer release was selected for analysis because it was previously simulated in Chan and Leach (2007) and Lundquist et al. (2012), and therefore there are previous modeling studies to which we can compare our results. IOP 3 was selected for these previous studies because the wind direction was consistent over the 30 min release

period and the atmospheric stability was near neutral, which are benefits when using idealized lateral boundary conditions or a computational fluid dynamics model without atmospheric stability effects. While these attributes are beneficial for our idealized simulations, our multiscale simulation is capable of simulating a case with shifting wind conditions and nonneutral atmospheric stability. Demonstration of this ability will be the subject of future work.

Simulations are configured to enable comparisons between the GPM and VRM IBM algorithms as well as the idealized and multiscale configurations. Three simulations are analyzed here; two idealized configurations (section 3a) and one multiscale configuration (section 3b). In the two idealized simulations, the GPM and VRM IBM algorithms are used, which builds on the work presented in Lundquist et al. (2012), where the GPM IBM algorithm was used in an idealized simulation of JU2003 IOP 3. Although the VRM algorithm

was validated in Bao et al. (2018), its use here is presented as validation for urban applications, and allows for the quantification of differences between the GPM and VRM algorithms. The multiscale configuration is then presented, which uses both terrain-following grids and the VRM-IBM. Comparisons between the idealized and multiscale simulations provide insight into the performance of the multiscale setup.

a. Idealized configuration

The idealized simulations are configured similar to previous JU2003 modeling efforts at building-resolving scales that used simplified boundary conditions and forcing scaled to generate agreement with observations. Reynolds-averaged Navier–Stokes (RANS) simulations by Chan and Leach (2007), Chow et al. (2008), along with both the RANS and LES simulations by Neophytou et al. (2011) used inflow boundary conditions based upon steady velocity profiles constructed by fitting a log-law profile to sodar and weather station observations. The idealized simulations presented here adopt a similar configuration to simulations by Golaz et al. (2009) using the COAMPS-LES model and WRF-IBM simulations by Lundquist et al. (2012) and Bao et al. (2018) that use a two-domain nested configuration to produce turbulent inflow for the nested domain. This configuration simulates only the microscale and both domains use the 3D Smagorinsky turbulence closure. The parent domain uses periodic boundary conditions and a pressure gradient forcing term is applied to achieve agreement between the simulated and observed time-averaged velocity profiles. Figure 4 shows the grid layout for the idealized simulations.

Vertical grid refinement was used to maintain a near-surface grid aspect ratio $\Delta x/\Delta z = 2.0$ for each domain. Aloft, the vertical grid levels are spaced increasingly far apart with a constant stretching coefficient, $(z_{k+1} - z_k)/(z_k - z_{k-1})$, of 1.016 for D1 and 1.028 for D2. Upon reaching $\Delta x/\Delta z = 0.5$ the grid aspect ratio is maintained for the remaining vertical grid levels. The coarsening of vertical resolution aloft was used to reduce computational costs without sacrificing high-resolution and grid quality in the region of interest (near surface). Because of the need for ghost points beneath each point of the immersed boundary, the WRF-IBM-GPM simulations have two additional levels located approximately 2 and 4 m beneath the ground level.

Our idealized WRF-IBM simulations use a two-domain setup with a periodic parent domain (D1) at $\Delta x = \Delta y = 10$ m and a nested domain (D2) at $\Delta x = \Delta y = 2$ m, with a grid refinement ratio of 5. The domains use time steps of 0.05 s for D1 and 0.01 s for D2. In the east–west, north–south, and bottom–top dimensions, D1

FIG. 4. A plan view of the two-domain nested configuration used for idealized WRF-IBM simulations. The outer domain is marked with UTM coordinates.

has dimensions $241 \times 241 \times 146$ grid points and D2 has dimensions $351 \times 401 \times 243$ grid points. D1 has flat terrain, and D2 includes building geometries. Both domains use a 3D Smagorinsky turbulence closure with coefficient $C_s = 0.18$. Domain D1 was run for seven hours to develop statistically steady turbulence prior to initialization of D2. Domain D2 was initialized prior to the tracer release by 10 min, roughly double the time required to traverse the domain at 3 m s^{-1} and a sufficient amount of time for the flow to fully develop around the complex urban terrain.

The idealized GPM and VRM simulations are forced by a uniform pressure gradient that is adjusted to generate agreement between the time-averaged velocity profile from D2 and the time-averaged minisodar observations at approximately 40 m AGL, shown in Fig. 5. Both domains have a model top at 400 m AGL and a Rayleigh relaxation layer applied to W velocities within the top 40 m with a damping coefficient of 0.2 s^{-1} .

The observed velocity profile used for our idealized WRF-IBM simulations is the combination of data from several closely located instruments that measure at different heights. A similar method for inflow profile generation was also used by Hanna et al. (2011) and Lundquist et al. (2012). The instruments used here include an ANL minisodar, two DPG PWIDS (P10 and P11), two DPG super PWIDS (SP17 and SP20), and the NOAA/ARL FRD sonic anemometer located at the SF₆ release location. The ANL minisodar data from the 30 min SF₆ release window was temporally averaged to provide velocities at 5 m increments from 15 to 135 m AGL, shown in Fig. 5. Each of the DPG PWIDS (P10 and P11) and DPG super PWIDS (SP17 and SP20) was temporally averaged over the SF₆ release window. An average of these four stations, with each station given equal weight, was used as an estimate of velocities at 8 m AGL. Additionally, an ARL FRD

FIG. 5. Vertical profiles of horizontal wind speed and direction at the ANL minisodar location (634451, 3925592). Profiles have been time averaged over the 30-min SF_6 release period. Observations from the ANL minisodar are included along with results from the idealized VRM, idealized GPM, multiscale simulation, and multiscale simulation with added roughness elements on the 10-m domain (cubes).

sonic anemometer collocated with the SF_6 release site was similarly temporally averaged to provide an estimate of velocities at 2 m AGL.

The GPM simulation uses a no-slip bottom boundary condition for velocities and the VRM simulation uses the log-law boundary condition with roughness length $z_0 = 0.1$ m. Both GPM and VRM simulations use the traditional WRF boundary condition for scalar variables, which is a no-flux condition applied at the model bottom. No treatment is applied for scalars at the IB (i.e., building surfaces); however, this has minimal effect on our results because the wind fields prevent advection of scalars through the IB and diffusion of scalar across the IB is negligible. A scalar immersed boundary condition exists for the GPM but was not used to maintain similarity between the GPM and VRM configurations. A scalar immersed boundary condition that does not require

ghost points is currently under development for use with the VRM.

b. Multiscale configuration

The multiscale WRF-IBM simulation uses five nested domains with horizontal resolutions of 6.05 km and 550, 50, 10, and 2 m. Resolutions are selected to optimize computational resources while properly resolving flow features at scales of interest. Horizontal dimensions of the 10- and 2-m domains are identical to the dimensions of the corresponding domains in the idealized simulations. Because the predominant wind direction (south-southwest) is known, the 10- and 2-m domains are positioned in the northeast quadrant of their respective parent domains. This offset increases the fetch prior to inflow boundaries, which promotes the development of turbulence without increasing the domain extents and computational costs. The multiscale grid layout is depicted in Fig. 6. The five domains are initialized in a cascading fashion with start times of 0300, 0600, 1200, 1500, and 1550 UTC. Conditions on the 2 m domain are saved every two seconds during the release window between 1600 and 1630 UTC. Ideally, studies would be conducted to evaluate the optimal number of nests, grid refinement ratios, the necessary spatial extents of each domain, and domain start times, however the computational costs of such studies currently exceed available resources.

Lateral boundary conditions and initial conditions for the outermost 6.05-km domain are prescribed using data from the NCEP North American Regional Reanalysis (Mesinger et al. 2006), which has horizontal resolution of 32 km. The VRM IBM algorithm is used on the 10- and 2-m domains while the standard WRF terrain-following coordinate is used on the 6.05-km, 550-m, and 50-m domains. Domains run with the VRM use a constant roughness length of $z_0 = 0.1$ m. The 6.05-km and 550-m domains use the Mellor–Yamada–Janjić (MYJ) planetary boundary layer scheme (Mellor and Yamada 1982; Janjić 2002) while the 50-, 10-, and 2-m domains use the 3D Smagorinsky turbulence closure scheme with $C_s = 0.18$. A summary of grid configuration and physics options is included in Table 1.

A model top of 200 hPa is used for all domains of the multiscale simulation. Near-surface vertical grid levels for the multiscale 10- and 2-m domains are selected to match, as closely as possible, those used in the comparable domains of the idealized simulations. Above the model top of the idealized simulations (400 m AGL), vertical grid levels stretch in height at a constant rate of $(z_{k+1} - z_k)/(z_k - z_{k-1}) = 1.05$. This greatly reduces the number of grid points, and correspondingly the computational costs, of the microscale domains while

FIG. 6. Configuration of domains used in the multiscale simulation centered over the business district of Oklahoma City. The five domains have resolutions of 6.05 km and 550, 50, 10, and 2 m. The 550-, 50-, and 10-m domains include contour levels of topography. The 2-m domain includes contours of the building heights AGL (the color bar is not shown). Dimensions of each domain and other configuration information are included in Table 1.

maintaining an optimal grid aspect ratio near the surface in the region of interest.

c. Urban geometry

Urban geometry represented by the immersed boundary was created by sampling, at each grid point, a “shapefile” containing vectorized building information. Narrow gaps between buildings and other insufficiently resolved features were manually adjusted to ensure that each of the VRM interpolation points had a minimum of two nearest neighbors for the IDW interpolation. WRF-IBM currently uses a two-dimensional array to store the immersed boundary height at each grid point, which restricts the model topography to solid shapes without void space. Because of this restriction, an elevated walkway at UTM coordinates (634850, 3925800) was omitted from the model topography because WRF-IBM

is currently unable to resolve flow in the free space beneath the suspended structure. In addition, several buildings near inflow boundaries, specifically the southern edge, were removed because of spurious interactions with the inflow conditions. Nonphysical behavior around buildings near the inflow boundaries of the 2-m domain is not unexpected because these buildings are not represented on the 10-m parent domain and the flow on the parent domain is unobstructed. Identical building geometry representations were used for both the idealized and multiscale simulations.

Variations in the ground elevation within the microscale modeling domain are small in magnitude, with minimum and maximum elevations of 360 and 365 m MSL. Because of restrictions from periodic boundary conditions, the idealized simulations ignore the underlying ground topography and only building heights

TABLE 1. Multiscale model configuration for JU2003 simulations for domains 1–5 (TF = terrain-following coordinate, KF = Kain–Fritsch cumulus parameterization, Smag = 3D Smagorinsky turbulence closure, WSM3 = WRF single-moment 3-class, RRTM = Rapid Radiative Transfer Model, and MM5 = Fifth-generation Pennsylvania State University–National Center for Atmospheric Research Mesoscale Model).

	D1	D2	D3	D4	D5
Δx and Δy (m)	6050	550	50	10	2
Coordinate	TF	TF	TF	IBM	IBM
Time step (s)	30	3	0.25	0.05	0.01
East–west grid points	221	232	254	241	351
South–north grid points	221	232	254	241	401
Bottom–top grid points	51	51	76	146	243
Turbulence	MYJ	MYJ	Smag	Smag	Smag
Microphysics	WSM3	WSM3	WSM3	None	None
Longwave radiation	RRTM	RRTM	RRTM	None	None
Shortwave radiation	Dudhia	Dudhia	Dudhia	None	None
Surface layer scheme	MM5	MM5	MM5	None	None
Land surface model	Noah	Noah	Noah	None	None
Cumulus parameterization	KF	KF	None	None	None

FIG. 7. Instantaneous horizontal wind speed at 8 m AGL at 16:16:52 UTC from the 2-m domain of the multiscale simulation. Arrows are included at every fifth grid point. An animation of horizontal wind speed at 8 m AGL from the innermost four domains of the multiscale simulation is included in the online supplemental materials.

above ground level are included in the immersed boundary height. An advantage of the multiscale simulation, in contrast, is that no periodic boundary conditions are used and the underlying ground topography can be included. For the multiscale simulation, the building heights above ground level are combined with the underlying ground topography interpolated from the parent domain. To maintain flat rooftops, the IB height is averaged at points within each building footprint, which results in minor adjustments within each building geometry.

4. Simulation results and discussion

The WRF-IBM simulations illustrate the complex behavior of atmospheric flows within urban environments. Both the idealized and multiscale simulations display channeling effects in street canyons and many other microscale flow features including separation

zones, return flows, and recirculation in the lee of buildings. Contours of instantaneous wind speed, Fig. 7, illustrate many of these intricacies seen in all three simulations. The analysis presented below includes qualitative comparisons of observations and simulation results of wind speed, direction, and SF_6 concentration that have been time averaged over the SF_6 release period. In addition, quantitative analysis is performed using measures of model skill to evaluate the accuracy of various model configurations in predicting winds and SF_6 concentrations compared to observations.

During IOP 3, the ANL minisodar was located within the botanical gardens and sampled flow that was relatively unobstructed upstream. Figure 5 compares time-averaged vertical profiles of horizontal wind speed and direction from the simulations with the time-averaged minisodar measurements. Both idealized simulations (GPM and VRM) overestimate the horizontal wind speed, sometimes by up to 2.5 m s^{-1} , in the region

between ground level and approximately 40 m AGL, despite tuning the pressure gradient to match the observations at 40 m AGL. The multiscale simulation, which does not include a priori knowledge of the JU2003 observations (i.e., tuning), shows improved agreement between 5 and 30 m AGL and from 100 to 140 m AGL with an overestimation from the surface until 100 m AGL. Unlike the idealized simulations, the multiscale simulation produces a profile with similar shape to that seen from the minisodar, possibly due to the large-scale flow features downscaled from the mesoscale domains. All of the simulations show excellent agreement with the measured wind direction. This agreement is expected in the idealized simulations because the pressure gradient forcing is tuned to generate agreement with the observations, but the multiscale model has no such tuning and yet shows comparable agreement to the observed wind direction.

A possible explanation for the overestimation of the near-surface wind speed in all three simulations is the omission of terrain-features upstream of the minisodar. To test this theory, the multiscale simulation was run a second time with roughness elements added to D4, the 10-m domain. Ideally we would add the actual building geometries to the 10-m domain; however, the great majority of structures within the 10-m domain have too few grid points per building to be properly resolved. According to Tseng et al. (2006), a minimum of six–eight grid points is necessary across a bluff body to achieve reasonable results when using an IBM in a LES. For this reason, we have instead used a regular pattern of large roughness elements to represent the urban terrain. These elements have footprints of $80\text{ m} \times 80\text{ m}$ and are 10 m in height with the element center-points described by an array with 320-m spacing and 30° offset between rows to roughly align with the predominant wind direction. Figure 8 shows the immersed boundary height on the 10-m domain (D4) of this modified multiscale simulation.

Figure 5 shows that the addition of these roughness elements to the 10 m domain resulted in noticeably improved agreement between the 2-m domain (D5) and the observed near-surface wind speed profile, particularly between 15 and 40 m AGL. If future computational resources allow, the 2-m domain could be extended southward to provide additional fetch and resolve flow around more buildings upstream from the minisodar and the SF₆ release location. Another solution could be to add artificial drag at grid points that fall within poorly resolved terrain features. While these modifications could potentially yield improvements, the current simulation configurations are sufficient for the focus of this paper, which is analyzing the performance and benefits

FIG. 8. Topography from the multiscale-simulation 10-m domain with cubes ($80\text{ m} \times 80\text{ m} \times 10\text{ m}$) added to mimic the effects of the urban terrain.

of the multiscale configuration. Investigation and analysis of treatments for poorly resolved terrain features will be the focus of future research as it appears to be of importance for improving future multiscale models.

A quantitative analysis of model skill is discussed below; however, visual comparison of model results to time-averaged wind speed/direction from DPG PWIDS (P) and super PWIDS (SP), shown in Fig. 9, indicate that all three simulations have similar behavior to observations within the street canyons, in the lee of buildings, and on rooftops. Importantly, all three simulations agree reasonably well with P11 and SP17, which are collocated at the SF₆ release location.

Figure 10 shows time series of horizontal wind speed and wind direction at 8 m AGL above the SF₆ release location. All simulations, idealized and multiscale, display similar behavior of the time-averaged horizontal wind speed, but differences between simulations are clearly visible in the time series of wind direction. Fluctuations in wind direction from the idealized GPM and idealized VRM simulations are of lower magnitude than those in the multiscale simulation, which includes larger deviations from the mean wind direction and lower-frequency variations. These characteristics indicate the presence of large-scale features from the coarse-resolution parent domains transitioning into the 2-m domain of the multiscale simulation. The effects of increased meandering of the flow in the multiscale simulation are evident in Fig. 11 where the time-averaged plume of the idealized VRM simulation is considerably more spatially constrained compared to that from the multiscale simulation. As hypothesized by Nelson et al. (2016), our

FIG. 9. Horizontal wind speed and direction, time averaged over the 30-min SF₆ release period, at the locations of DPG PWIDS (P) and DPG super PWIDS (SP). Arrows are included for observations and the three simulations (idealized GPM, idealized VRM, and multiscale).

multiscale simulation appears to reproduce some of the transient flow interactions within the urban topography that are driven by oscillations in the prevailing wind direction.

Quantitative performance measurements of the simulations compared to JU2003 observations are calculated using methods suggested by [Chang and Hanna \(2004\)](#): fraction of predictions within a factor of x (FAC x), fractional bias (FB), geometric mean bias (MG), geometric variance (VG), and normalized mean square error (NMSE). Differences in wind direction are evaluated using the scaled average angle (SAA) skill test devised by [Calhoun et al. \(2004\)](#). Combinations of these performance metrics have previously been applied to Joint Urban 2003 simulations by [Chan and Leach \(2007\)](#) and [Chow et al. \(2008\)](#) using the FEM3MP model, [Hanna et al. \(2011\)](#) when comparing four diagnostic urban wind flow models with Lagrangian particle dispersion models, and by [Lundquist et al. \(2012\)](#) using the WRF-IBM-GPM model. The calculations for the above statistics are

$$\text{FAC}_x = \text{fraction of data that satisfies } 1/x \leq X_p/X_o \leq x, \quad (7a)$$

$$\text{FB} = 2(\overline{X_o} - \overline{X_p}) / (\overline{X_o} + \overline{X_p}), \quad (7b)$$

$$\text{MG} = \exp[\overline{\ln(X_o)} - \overline{\ln(X_p)}], \quad (7c)$$

$$\text{VG} = \exp\{\overline{[\ln(X_o) - \ln(X_p)]^2}\}, \quad (7d)$$

$$\text{NMSE} = \overline{(X_o - X_p)^2} / (\overline{X_o X_p}), \quad \text{and} \quad (7e)$$

$$\text{SAA} = \sum (|U_i| |\phi_i|) / (N |\overline{U}|). \quad (7f)$$

In the above equations, X_o is the set of observational data and X_p are the corresponding predictions from the simulation, N is the number of observations, ϕ_i is the difference between observed and predicted wind directions, and $|U_i|$ is the predicted wind speed. Here we use values for X_o and X_p that are time averages

FIG. 10. A time series of horizontal wind speed and wind direction at 8 m AGL at the SF_6 release location for the idealized GPM, idealized VRM, and multiscale simulations. Also plotted are DPG PWIDS (P11) and super PWIDS (SP17), which are collocated at 8 m AGL at the release location. Data from SP17 are shown after the application of a rolling-average filter with window length of 10 s.

over the 30-min release period. An overbar indicates averaging of all locations.

The methods above are chosen to provide a broad analysis of model performance. FACx, MG, and FB provide insight into the systematic bias of the predictions. NMSE and VG provide insight into the scatter of the data and indicate whether there is agreement between the distributions of predictions and observations. Some skill metrics, such as FB and NMSE, are more heavily influenced by data points with large magnitudes versus small, which is fine for variables such as wind speed that do not vary over many orders of magnitude. The time-averaged observed and predicted SF_6 concentrations span several orders of magnitude (from 0.001 to 100 ppbv), so the logarithmic forms of mean bias and variance, MG and VG, are more appropriate for analysis of SF_6 concentrations because these metrics evenly weigh the under- and overpredictions (Hanna et al. 1993).

Concentration floors are applied to the LLNL bluebox samplers and the NOAA/ARL FRD PIGS because each dataset has a minimum concentration that could be accurately measured given errors from the instruments and analysis procedures. Additionally, several of the skill-test calculations are mathematically valid only for predictions and observations that are nonzero. PIGS data points of SF_6 concentration less than the method limit of detection (MLOD) have a quality control flag. Flagged PIGS data points are modified to 1 pptv, which corresponds to one-half of the minimum analyzed

concentration used during calibration. Instrument limit of detection and MLOD are not available from the LLNL bluebox samplers. A 5-pptv floor to the LLNL bluebox concentrations is introduced by modifying data points that are below the lowest reference concentration from the calibration curves of the gas chromatograph used to analyze the samples, 9.3 pptv. To maintain consistency, the concentration floors are also applied to the predicted time-averaged station concentrations.

Graphical representations of model skill for predicting wind speed/direction and concentration are shown in Fig. 12. The simulations display excellent FAC2 scores for predicting horizontal wind speed with all three simulations reporting a score of 0.91 relative to PWIDS and the lowest score relative to super PWIDS being an impressively high value of 0.73. Despite at least one of the idealized simulations matching or slightly outperforming the multiscale simulation in every wind speed/direction skill test, it is important to remember that both idealized simulations (GPM and VRM) were provided with an initialization constructed using JU2003 observations. Additionally, the pressure gradient forcing used for the idealized simulations was tuned to maintain agreement with minisodar velocity profile observations. While the idealized simulations rely upon a priori knowledge of the local meteorology, the multiscale simulation is run as a forecast and uses initial conditions and forcing that are independent of the JU2003 observations and are provided by external datasets, as is typical in mesoscale

FIG. 11. The SF_6 concentrations at 2.5 m AGL from the (left) idealized WRF-IBM-VRM simulation and (right) multiscale simulation. Both the observed and predicted concentrations are time averaged over the 30-min release period. Large circles represent time-averaged measurements from LLNL bluebox stations. Small circles represent time-averaged measurements from NOAA/ARL FRD PIGS stations. Only LLNL stations with a height of 2.5 m AGL and NOAA stations with a height of 8 m AGL are shown. An animated version of this plot is available in the online supplemental materials.

forecasting. Thus, the agreement of the multiscale simulation with observations of wind speeds/directions and SF_6 concentrations is quite remarkable considering the absence of model tuning.

Equation (7b) can be rearranged to yield Eq. (8), from which it becomes clear that the negative fractional bias scores in Fig. 12 indicate that all three models are slightly overestimating wind speeds relative to both PWIDS and super PWIDS:

$$\frac{\overline{X_p}}{\overline{X_o}} = \frac{1 - \frac{\text{FB}}{2}}{1 + \frac{\text{FB}}{2}}. \quad (8)$$

The idealized VRM simulation shows the least overestimation of wind speeds with FB scores of -0.05 (PWIDS) and -0.09 (super PWIDS), which implies overprediction by factors of 1.05 and 1.09. FB scores from the idealized GPM and multiscale simulations are clustered around -0.25 ± 0.01 , which roughly corresponds to a factor of 1.29 overprediction. Earlier, when evaluating the vertical profiles of wind speed, it was suggested that the omission of terrain features could be responsible for the overestimation of the near-surface

wind speed. The negative FB scores are another indication that the simulations presented here are missing some important small-scale features of the terrain that would produce additional drag and slow the near-surface winds. When compared with the idealized GPM simulation, the improved FB score of the idealized VRM simulation indicates that the log-law bottom boundary condition used by the VRM yields less bias in the magnitude of wind speeds than the no-slip bottom boundary condition used by the GPM. Drawing conclusions about the multiscale simulation from the differences in FB scores is complicated by variations in the idealized and multiscale model configurations, such as the lateral boundary conditions and forcing methods.

Skill tests evaluating the prediction of SF_6 concentrations, displayed in the second row of Fig. 12, show the multiscale simulation produced the highest model skill followed by the idealized VRM simulation, which outperformed the idealized GPM simulation. For each simulation, the FAC5 agreement with the bluebox samplers is higher than that of the FRD samplers, likely because of the FRD samplers being sited further downwind from the release location. FAC5 comparing to the bluebox samplers was 0.68, 0.74, and 0.95 for the

FIG. 12. Results of model skill tests evaluating (top) horizontal wind speed and wind direction and (bottom) SF₆ concentration for the idealized VRM, idealized GPM, and multiscale simulations in comparison with DPG PWIDS and super PWIDS (for top row) and LLNL bluebox and NOAA/ARL FRD integrated tracer samplers (for bottom row). Thick horizontal black lines indicate a perfect model score.

idealized GPM, idealized VRM, and multiscale simulations, respectively, and 0.44, 0.56, and 0.64 relative to the FRD samplers. The multiscale simulation's exceptional skill-test results show that we can achieve admirable predictions of urban dispersion by appropriately downscaling mesoscale forecasts to force microscale simulations.

Both the idealized and multiscale simulations display model skill that exceeds the minimum performance for an acceptable model as noted in many previous studies, such as [Chang and Hanna \(2004\)](#) and [Tewari et al. \(2010\)](#). These standards include greater than 50% of predictions within a factor of 2 ($\text{FAC2} \geq 0.5$) and less than 30% mean bias ($0.7 \leq \text{MG} \leq 1.3$). Relative to previous microscale simulations of transport and dispersion during JU2003, ([Chan and Leach 2007](#); [Hanna et al. 2011](#); [Lundquist et al. 2012](#); [Li et al. 2018](#)), the model skill of the multiscale simulation for prediction of SF₆ concentrations is exceptional, with FAC2 scores of

0.58 and 0.56 relative to the bluebox and FRD samplers, respectively, as well as FAC5 scores of 0.95 and 0.76 relative to the bluebox and FRD samplers, respectively. The simulation of transport and dispersion during IOP 3 by [Li et al. \(2018\)](#), which used coupled mesoscale and microscale models, offers an excellent comparison with the multiscale model presented here and produced a FAC2 and FAC5 of 0.37 and 0.84, respectively, relative to the bluebox samplers. The favorable FAC2 and FAC5 scores of the multiscale simulation indicate that transport and dispersion models can obtain substantial improvements in model skill by dynamically downscaling meteorological fields from the mesoscale to microscale.

5. Summary and conclusions

The expansion of WRF's multiscale framework presented here enables simulations over complex terrain

with resolutions ranging from the mesoscale to the microscale and forcing supplied by an operational forecast. The velocity reconstruction method version of the immersed boundary method algorithm is designed such that a domain run with VRM can be nested within a terrain-following parent domain. Using VRM, microscale domains can accurately simulate flow over complex terrain, such as dense urban environments. The vertical grid refinement functionality of Daniels et al. (2016) facilitates transitioning from terrain-following domains in the mesoscale to IBM domains in the microscale. The vertical refinement method also enables control over the grid aspect ratio of each domain in a sequence of nests, which is critical for producing high quality simulations across a range of scales.

The performance of the multiscale model was evaluated here by comparison to idealized simulations of a continuous tracer release from IOP 3 of the Joint Urban 2003 field experiment in Oklahoma City. The idealized simulations use a two-domain nested configuration with resolutions of 10 and 2 m, periodic lateral boundary conditions (parent domain only), simplified terrain, and forcing based upon local measurements taken during JU2003. Two idealized simulations were also analyzed, one using the ghost point method version of the IBM algorithm of Lundquist et al. (2012) and another using the VRM. The idealized simulations share many features with configurations of previous JU2003 modeling efforts by Chan and Leach (2007), Neophytou et al. (2011), and Lundquist et al. (2012). The multiscale simulation consisted of five nested domains with horizontal resolutions of 6.05 km and 550, 50, 10, and 2 m. Initial conditions and boundary conditions were supplied by the NCEP North American Regional Reanalysis dataset. Unlike the idealized simulations, the multiscale simulation did not use large-scale forcing parameters dependent on observations from the JU2003 field experiment. Terrain-following coordinates were used on the 6.05-km, 550-m, and 50-m domains and VRM was used for the 10- and 2-m domains.

Evaluation of the three simulations included a suite of statistical measurements of model skill for the prediction of wind speeds and SF₆ concentrations, as suggested by Chang and Hanna (2004). All three simulations displayed excellent skill at predicting wind speeds/directions, including the multiscale simulation, which was run in a forecasting mode. For prediction of SF₆ concentrations, the multiscale simulation outperformed the idealized simulations by displaying the highest skill in nine out of the ten metrics calculated. These impressive skill scores may be a result of increased plume meandering caused by downscaled motions with scales larger than those produced in the idealized

simulations. The high level of skill shown by the multiscale simulation implies that microscale simulations over complex terrain, especially transport and dispersion simulations, may greatly benefit from downscaled meteorology.

Future studies of the multiscale modeling framework will focus on the development and quantification of turbulence and the impacts of improved representation of land surface heterogeneity at resolutions between the mesoscale and microscale. Additionally, these studies will evaluate the multiscale modeling framework's applicability to nonneutral atmospheric conditions, such as those observed during nighttime IOPs of JU2003.

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