Computational Fluid Dynamic Simulations of Plume Dispersion in Urban Oklahoma City

JULIA E. FLAHERTY

Laboratory for Atmospheric Research, Department of Civil and Environmental Engineering, Washington State University, Pullman, Washington

DAVID STOCK

Department of Mechanical and Materials Engineering, Washington State University, Pullman, Washington

BRIAN LAMB

Laboratory for Atmospheric Research, Department of Civil and Environmental Engineering, Washington State University, Pullman, Washington

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ABSTRACT

A 3D computational fluid dynamics study using Reynolds-averaged Navier–Stokes modeling was conducted and validated with field data from the Joint Urban 2003 dispersion study in Oklahoma City, Oklahoma. The modeled flow field indicated that the many short buildings in this domain had a relatively small effect on the flow field, whereas the few tall buildings considerably influenced the transport and diffusion of tracer gas through the domain. Modeled values were compared with observations along a vertical profile located about 500 m downwind of the source. The isothermal base case using the standard $k-\varepsilon$ closure model was within 50% of the concentration measurements, and a convective case with ground and building surfaces 10°C hotter than ambient temperatures improved the modeled profile to within 30% of observations. Varying wind direction and source location had a marked effect on modeled concentrations at the vertical profile site. Ground-level concentrations were 6 times the observed values when the approach flow wind direction was changed by $\pm 15^\circ$ and were nearly zero when the wind direction was changed by $-15^\circ$. Similar results were obtained when the source was moved 50 m to the east and to the west, respectively. All cases underestimated wind speed and turbulent kinetic energy near the surface, although adding heat significantly improved the magnitude of the modeled turbulent kinetic energy. Model results based upon a Reynolds stress closure scheme were also compared with the vertical concentration profiles. Neither the isothermal case nor the thermal buoyancy case resulted in an improvement over the standard $k-\varepsilon$ model.

1. Introduction

Urban air-quality modeling and measurements pose many interesting challenges for atmospheric scientists and environmental engineers. The urban environment is characterized by particularly complex flow patterns that include separation, recirculation, channeling, and chimney effects. As such, pollutant plumes in the urban landscape can often travel nonintuitive paths. Britter and Hanna (2003) summarized the important features in urban areas and highlighted research on moisture, heat, and roughness, as well as other parameters that affect urban flow patterns.

Urban environments are especially important in air-quality studies because there is both a high occurrence of pollutant sources (such as vehicles) and receptors (people). According to a United Nations (2004) report, 48% of the world’s population lived in urban areas in 2003. To protect these people from urban air pollutants,
regulatory agencies require monitoring stations to ensure cities do not exceed pollutant standards. However, improperly sited monitoring stations may report less-than-typical concentrations, allowing urban populations to unknowingly experience unhealthy levels of pollutant. Alternately, monitors may report higher-than-typical concentrations, which cause cities to invest unnecessary funds into attainment plans.

As computing power has become more affordable, computational fluid dynamics (CFD) has become an increasingly valuable tool for studying urban flow. These models explicitly account for building geometry and require minimal parameterizations as compared with a Gaussian model. Knowledge gained from computational efforts can be used for guidance in urban design to explore pollutant “hot spots,” minimizing personal exposure, and ensuring proper positioning of air intakes for building heating–ventilation–air conditioning systems.

In recent years, researchers have conducted CFD studies on various geometries. For example, there have been numerous investigations with single buildings, such as the work of Brzoska et al. (1997), Gao and Chow (2005), Meroney et al. (1999), Cowan et al. (1997), and Calhoun et al. (2004), ranging from a simple cube to a complex building. There has also been a great deal of study involving single street canyons. This work lends itself easily to two-dimensional investigations, such as the work of Jeong and Andrews (2002), Kim and Baik (2001), and Chan et al. (2002). In addition, other groups, such as Lien and Yee (2004) and Chang and Meroney (2003) have examined generic arrays of building obstacles, while small groups of buildings have been modeled by Guenther et al. (1990) and Riddle et al. (2004), Scaperdas and Colvile (1999) have used CFD to investigate monitoring station data at an urban intersection.

The objective of this paper is to present flow field and tracer dispersion results from a 3D CFD analysis based on data collected from the Joint Urban 2003 field campaign conducted in Oklahoma City, Oklahoma. Although previous researchers have investigated a variety of urbanlike configurations, only a small number of CFD modeling studies have been conducted for real urban geometries. This manuscript describes the investigation of the transport and dispersion of a tracer gas released north of the central business district of Oklahoma City. Section 2 briefly describes the field measurements used for comparison. Section 3 presents modeling details, which include information on the computational domain, turbulence modeling, boundary conditions, modeling cases, and grid uncertainty. The results of this modeling investigation are presented in section 4. Conclusions and future work are presented in section 5.

2. Field measurements

The Joint Urban 2003 (JU03) campaign was a major field study conducted in the summer of 2003 in Oklahoma City, Oklahoma (Allwine et al. 2004). Meteorological data were collected continuously throughout Oklahoma City, while tracer releases were performed during 10 main intensive operating periods (IOPs) and one mini-IOP. These 10 primary IOPs included 6 daytime experiments and 4 nighttime experiments, while the mini-IOP was conducted during the daytime. The primary IOP dates were selected based on predicted winds from the south or southeast. The Washington State University (WSU) Laboratory for Atmospheric Research participated in the JU03 field campaign by measuring tracer concentrations approximately 1 km from downtown tracer release locations. Continuous 5-min-averaged concentrations of sulfur hexafluoride (SF₆) tracer gas were measured at seven heights along a crane, from 10 to 75 m above ground level. Eight sonic anemometers also collected data at this site continuously throughout the month-long study. Researchers from Lawrence Livermore National Laboratory (LLNL) collected the sonic anemometer measurements and processed 10-min-averaged values. Additional details regarding the vertical concentration profile measurements are given by Flaherty et al. (2007).

The present study investigates the mini-IOP tracer release period. The predicted wind direction on the day of the mini-IOP was not favorable for conducting a regular IOP with all the field participants; instead, a release location was selected specifically to observe the plume at the crane site. This case was selected for CFD study primarily because the tracer release position was approximately five blocks, or 500 m, upwind of the WSU–LLNL crane as compared with the nearly 1-km distance between the source and receptor during other IOPs. With this source–receptor arrangement, the CFD domain was minimized relative to that needed for other IOPs.

The mini-IOP involved three 20-min-long tracer releases. The tracer was released from a tank via a tube attached to a parking meter located about 1/3 of a block west of the intersection of NE 4th Street and Hudson Avenue. There were no buildings directly to the north of the release site; however, there were two fairly short (4–7 m) buildings on the western half of the block (see Fig. 1). This modeling study investigates a 10-min period during the second of the three releases, which was conducted from 1230 to 1250 central daylight time (CDT).

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3. Numerical modeling

a. Computational domain

The computational domain utilized for this study was 900 m wide, 1200 m deep, and 300 m tall. It incorporated about 40 city blocks: 5 east-west and 9 north-south. Negligible changes were observed in the flow field results when these domain dimensions were extended. The buildings within this domain were created using GAMBIT 2.2.30 (Fluent Inc. 2003), a preprocessing program for modeling geometry and creating mesh. Approximately 150 buildings with 1-m resolution were incorporated in this domain. The domain was located north of the central business district of Oklahoma City (see Figs. 1 and 2). The buildings were irregularly spaced, and many of the buildings had fairly small footprints. The tallest building was the 70-m Regency Tower, which was located near the center of the domain. There was a cluster of buildings that were about 50 m tall in the southeast corner of the domain, but most of the buildings were less than 10 m tall. The black circle in Figs. 1 and 2 represents the location of the tracer release, while the triangle represents the crane location.

Fig. 1. Map of Oklahoma City with streets and building footprints. The heavy black rectangle represents the area of the computational domain. The black circle and triangle within the domain represent the release and crane locations, respectively. The four black stars that appear to the south of the domain indicate the locations of the tracer releases during the 10 regular IOPs.
The domain was meshed with 3-m tetrahedral cells near the ground and faces of the buildings. These cells were allowed to grow at a rate of 1.05 away from these surfaces to minimize the computational effort associated with excess cells. Although hexahedral cells are preferred for computational accuracy and efficiency, the geometry of the domain made it particularly difficult to utilize hexahedral meshing. The meshing scheme created approximately 2,995,000 cells in the domain.

b. Model details

To gain insight into the transport and dispersion of atmospheric pollutants in this urban environment, a computational fluid dynamics analysis with a Reynolds-averaged Navier–Stokes (RANS) model was conducted. Although the instantaneous Navier–Stokes equations exactly define all fluid flow, it is essentially impossible to solve these equations for turbulent flows over domains of significant spatial scale. Therefore, the exact equations are often Reynolds averaged to create a set of equations that can be solved for the spatial scales of interest. FLUENT 6.2.16 (Fluent Inc. 2003) was employed in this modeling study. Steady-state computations with the standard $k$–$\varepsilon$ turbulence closure (where $k$ is turbulent kinetic energy and $\varepsilon$ is turbulent dissipation rate) and Reynolds stress closure models were utilized. The $k$–$\varepsilon$ models are known to have weaknesses in complex flows, and incorrectly assume the dispersion coefficients are isotropic. However, it was an appropriate model to begin the computation, as it required less computational effort relative to that of the Reynolds stress model (RSM) or large eddy simulation (LES).

The Reynolds-averaged Navier–Stokes equations include the continuity and momentum equations:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0 \quad \text{and} \quad \frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = \frac{\partial p}{\partial x_i} \rho (T - T_0) g_i + \mu \frac{\partial^2 u_i}{\partial x_j^2} + \frac{\partial}{\partial x_j} (-\rho u_i u_j). \tag{1b}
\]

The variables in these equations are defined as follows: $\rho$ is the density; $t$ is time; $u_i$ and $u_j$ are the mean velocity components in the $x_i$ and $x_j$ directions, respectively; $g_i$ is gravity; $\beta$ is the thermal expansion coefficient; $T$ and $T_0$ are the temperature and reference temperature; and $\mu$ is viscosity. The overbar and prime denote the mean and fluctuating components of the velocity, respectively.

The Reynolds stresses, the final term in Eq. (1b), must be modeled to develop a closed set of equations. For the $k$–$\varepsilon$ model, the Boussinesq hypothesis is utilized and the Reynolds stresses are modeled in terms of the mean velocity gradients:

\[
-\rho u_i u_j' = \mu_j \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \left( pk + \mu_j \frac{\partial u_i}{\partial x_j} \right) \delta_{ij}. \tag{2}
\]

Here, $\mu_j$ is the turbulent viscosity, $k$ is the turbulent kinetic energy, and $\delta_{ij}$ is the Kronecker delta. The turbulent kinetic energy $k$ and turbulent dissipation rate $\varepsilon$ are obtained from the following transport equations:

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_j}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho e - Y_M + S_k \quad \text{and} \tag{3}
\]

\[
\frac{\partial}{\partial t} (\rho e) + \frac{\partial}{\partial x_i} (\rho e u_i) = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_j}{\sigma_e} \right) \frac{\partial e}{\partial x_i} \right] + C_{1_e} \frac{e}{k} (G_k + C_{2_{e_k}} G_b) - C_{2_{e_k}} \frac{e^2}{k} + S_e. \tag{4}
\]
Here, \( G_k \) and \( G_b \) are the generation of \( k \) due to the mean velocity gradients and to buoyancy, respectively; \( Y_M \), known as the dilatation dissipation, is neglected for incompressible flows; \( C_{1e} \), \( C_{2e} \), and \( C_{3e} \) are constants; \( \sigma_k \) and \( \sigma_b \) are the turbulent Prandtl numbers for \( k \) and \( b \); and \( S_k \) and \( S_b \) are user-defined source terms (Fluent Inc. 2003).

The turbulent viscosity is modeled as

\[
\nu_t = \rho C_{\mu} (k^{2/3}/e).
\]  

(5)

The constants in the standard \( k-e \) model were from Lauder and Spalding (1972): \( C_{\mu} = 0.09 \), \( \sigma_k = 1 \), \( \sigma_b = 1.3 \), \( C_{1e} = 1.44 \), and \( C_{2e} = 1.92 \). The final constant \( C_{3e} \) represents the effect of buoyancy on \( e \):

\[
C_{3e} = \tanh(\nu/e).
\]  

(6)

We designate \( C_{3e} \) to be 1 for buoyant shear layers where the main flow is aligned with the direction of gravity and 0 when the flow is perpendicular to gravity.

The Reynolds stress model, on the other hand, solves for turbulence closure with six transport equations for the Reynolds stresses and one equation for the dissipation rate. In general, the Reynolds stress model requires about 50%-60% more computing time and 15%-20% more memory than the \( k-e \) model (Fluent Inc. 2003). The transport equation for the Reynolds stress is

\[
\frac{\partial}{\partial t} (\rho \bar{u}_i \bar{u}_j) + \frac{\partial}{\partial x_k} (\rho \bar{u}_i \bar{u}_j \bar{u}_k) = - \frac{\partial}{\partial x_k} \left[ \rho \bar{u}_i \bar{u}_j \bar{u}_k + p(\delta_{ik} \bar{u}_j + \delta_{ij} \bar{u}_k) \right] + \frac{\partial}{\partial x_k} \left[ \mu_t \frac{\partial}{\partial x_k} (\bar{u}_i \bar{u}_j) \right] + \rho \beta (g \bar{u}_i \bar{\theta} + g \bar{\theta} \bar{u}_i) + p \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) + 2 \rho \Omega_k (\bar{u}_i \bar{u}_j \bar{\omega}_{ikm} + \bar{\omega}_{ikm} \bar{u}_j) + S_{user}.
\]  

(7)

The convection (II), molecular diffusion (IV), stress production (V), and production by system rotation (IX) terms are known, but the turbulent diffusion (III), buoyancy production (VI), pressure-strain (VII), and dissipation (VIII) terms must be modeled to close the equation. The turbulent diffusion transport is modeled as

\[
\frac{\partial}{\partial x_k} \left( \mu_t \frac{\partial \bar{u}_i}{\partial x_k} \right).
\]  

(8)

The first term, with \(-C_1\) as the leading coefficient, represents the return to isotropy. The second term, with \(-C_2\), was the rapid pressure strain, and the final two terms with \(C'_1\) and \(C'_2\) are the wall reflection terms. The final transport equation in the Reynolds stress model solves the dissipation rate with an expression similar to that of the \( k-e \) model:

\[
-\frac{\mu_t}{\rho Pr_t} \left( \frac{\partial \rho}{\partial x_j} + \frac{\partial \rho}{\partial x_i} \right).
\]  

(9)

The pressure-strain term (VII) is modeled in the classical approach as

\[
-\frac{C_1}{K} \left( \frac{\partial \rho}{\partial x_j} + \frac{\partial \rho}{\partial x_i} \right).
\]  

(10)
The Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) pressure–velocity coupling algorithm was utilized to enforce mass conservation. To minimize numerical diffusion, the second-order upwind discretization scheme was used for this computation. Gradients were computed using the node-based option, which is known to be more accurate than a cell-based scheme for tetrahedral cells. Last, standard wall functions (Lauder and Spalding 1974), modified for rough walls (Cebeci and Bradshaw 1977), were used to account for the effect of the walls.

After the flow field was determined, the concentration of a trace gas \( Y_i \) was computed using the following conservation equation:

\[
\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho u_i Y_i) = -\nabla \cdot J_i + R_i + S_i. \tag{12}
\]

Here, \( R_i \) is the rate of production by chemical reaction, and \( S_i \) is the rate of creation by addition from the dispersed phase, plus user-defined sources. Both of these terms were zero for this study. For turbulent flows, the mass diffusion term \( J_i \) is computed as

\[
J_i = -\left( \rho D_{l,m} + \frac{\mu_t}{\sigma_c} \right) \nabla Y_i. \tag{13}
\]

Here, \( D_{l,m} \) is the diffusion coefficient for species \( i \), and is the laminar diffusion portion that arose because of concentration gradients. The second term in Eq. (13) is the turbulent diffusion, which, in this study, used a turbulent Schmidt number \( \sigma_c \) of 0.7.

c. Boundary conditions

We simulated a continuous release of SF\(_6\) tracer that was conducted at 1240 CDT 15 July 2003. The wind speed and wind direction above the mean building height of the city were fairly consistent during this release period. The 10-min-average wind direction (from 1240 to 1250 CDT) was 197\(^\circ\), and the sides of the domain were parallel to the mean wind direction. This allowed symmetry conditions to be used for the east and west boundaries. The south and north boundaries were velocity inlet and outflow conditions, respectively. The ground and walls of the buildings were defined as stationary walls with appropriate roughness applied. Aerodynamic roughness lengths \( z_0 \) were approximated from Stull (1988) as 0.1 and 0.05 m for the ground and building surfaces, respectively. The corresponding roughness heights are 1.95 and 0.98 m. The ceiling was set as a moving wall.

The velocity inlets were defined with wind speed, turbulent kinetic energy (TKE), and turbulent dissipation rate profiles. An initial wind speed profile was defined by fitting a logarithmic profile to the 10-min-averaged data from the eight sonic anemometers that were mounted on the crane. This profile compared well to the 15-min data from a sodar that was deployed a few blocks north of the crane. The wind direction and wind speed (for 45 min on either side of the study period of 1240–1250 CDT) were generally within 5\(^\circ\) and 2 m s\(^{-1}\) of the profile from the crane, respectively. This gave us confidence that the profile chosen was representative of the mean flow over this region of the city. Turbulent kinetic energy and turbulent dissipation rate profiles were adapted from Detering and Etling (1985). These initial inlet profiles were adjusted to physically match each other by running it through a section of the Oklahoma City urban landscape. Figure 3 gives the inlet profiles used for these computations.

d. Model cases

To characterize urban dispersion in this landscape, several model cases were investigated. The base case was an isothermal investigation of the 197\(^\circ\) wind direction. The flow field was computed with a total of 600 iterations on four nodes of a Linux cluster. This required approximately 45 s per iteration for a total of 7.5 h. The SF\(_6\) tracer was released from a 4.4-m volume approximately 100 m south of the crane.

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The Regency Tower was a significant obstacle between the source location and the crane site. Therefore, we also considered a case in which this large building did not exist. This showed the effect that this particular obstacle had on flow and dispersion and illustrated the importance of including all the buildings in the domain. When the Regency Tower was removed, the significant obstacle that remained upwind of the crane location was the new Federal Building. (In Fig. 2, the new Federal Building is the building with the V-shaped notch removed from the north part of the structure, located approximately 100 m south of the crane.)
To explore both the sensitivity of the tracer concentration at the crane site to wind direction and the potential effect of wind direction variability over this 10-min period, two additional wind direction cases were considered. Field measurements indicated that the standard deviation of the wind direction was approximately 15°. Therefore, 182° and 212° wind direction cases were also computed. The computational domain for each of the wind direction cases involved rotating the geometry so that the wind direction was again parallel to the sidewalls.

In addition to variability in wind direction, the effects of perturbing the source location were investigated. For these cases, the release was moved 50 m to the east and the west and 15 m vertically from the base-case location. A final source location case moved the source just 2 m downwind from the base case. This was conducted to see if there is a significant effect, at this mesh resolution, to moving the source to a position in which the size of the cell (or pair of cells, in this case) nearly matches the estimated size of the plume. With the base-case configuration, the source cell was larger than the actual source in the field. Therefore, the source was moved so that the virtual point source associated with the 2-m downwind release volume corresponded with the actual source position. The Pasquill–Gifford Turner dispersion curves for urban landscapes and the variability in wind speeds from the field data were used as guidance for determining the width of the downwind cells necessary to produce the desired virtual point source position.

Last, the particular field case that we modeled was conducted at 1240 CDT on a fairly hot summer day. Since the building surface temperature was greater than that of the surrounding air temperature, a case with thermal buoyancy was considered. A slightly unstable temperature profile was prescribed for the inlet air, and the ground and building surfaces were assumed to be 10° hotter than the ground-level air temperature. Berdahl and Bretz (1997) show surface temperatures can exceed air temperatures by between 5° and 50°C, depending on the color and type of material. Since this was a simple case to test the effect of convection, we estimated that 10° was the average temperature for the ground and building surfaces. (Unfortunately, no building-surface temperature measurements were available, and we only had our personal experience under the hot Oklahoma sun for guidance.) In reality, the building rooftops would have the highest surface temperature, and the building walls and ground would have spatially varying temperatures depending on the sun angle, shading, and surface type. The Boussinesq approximation, which assumes that density is a function of temperature in the buoyancy term of the momentum equation, and constant for all other terms, was utilized for this model case.

The base and heat-added cases were both computed with the standard $k$–$\varepsilon$ model as well as the Reynolds stress model, while the remaining cases were modeled with $k$–$\varepsilon$ closure only. The RSM computation was started from the converged $k$–$\varepsilon$ solution to minimize the overall computational effort as well as the potential for divergence. In summary, the following cases were conducted: 1) base case ($k$–$\varepsilon$ and RSM), 2) Regency Tower removed ($k$–$\varepsilon$), 3) changes in wind direction of 15° ($k$–$\varepsilon$), 4) changes in source location of 50 m east, 15 m vertically, and 2 m north ($k$–$\varepsilon$), and 5) add heat ($k$–$\varepsilon$ and RSM).

e. Grid uncertainty

Although the general patterns of flow parameters developed from this CFD analysis indicated that it produced physically realistic results, a more quantitative analysis of the computational error was necessary.
Richardson extrapolation (Richardson 1910) was used to determine the error associated with the computational grid. Celik and Karatekin (1997) provided a concise Richardson extrapolation procedure that was utilized as a guide for this analysis. Three mesh sizes, nominally of 3-, 4.2-, and 6-m-resolution tetrahedral cells, with 2,995,000, 1,415,000, and 664,000 cells, respectively, were used for the error analysis. The plume width at half maximum was selected as a parameter for the quantification of the grid error because it was an integral quantity that exhibited monotonic convergence between the three mesh sizes. The error in the grid, as calculated from the plume width at half maximum, included the errors in the wind field and the turbulence, as these quantities were incorporated in the computation of the plume. Since second-order upwind discretization was used in the CFD modeling, a value of two was used to calculate estimates of the computational error. The grid convergence index, which is a conservative estimate of the error band (Celik and Karatekin 1997), was 6% for the tracer plume half-maximum width. The errors associated with the base-case grid size were relatively small, and the mesh resolution was sufficient.

4. Results

a. Base case

First, we considered the flow field of the base case with the wind at 197°. Figure 4 shows the velocity vec-
tors on a plane 10 m above the ground; a level that is above many of the buildings. The velocities (wind speed and direction) above the shorter buildings do not appear to be perturbed by the presence of these buildings. Vectors on the western half of the domain generally maintain a uniform direction. The taller buildings, however, significantly alter velocity vectors in the eastern half of the domain.

By examining the velocity vectors closely, we see that the smaller buildings have a much more subtle impact on the flow field when compared with the overwhelming changes in flow direction observed near large buildings. Figure 5 presents the velocity vectors on a horizontal plane, 3 m above the ground. With the exception of the Regency Tower, located in the upper portion of the figure and marked with an X, all of these buildings are small and short. The flows around these small buildings tend to wrap gently around the obstructions, and quickly return to the mean wind direction behind the buildings. There are no visible recirculation zones near the source. A 3D sonic anemometer was deployed at the release location at about 2 m above the ground level. The 10-min vector averages of the wind components from the sonic were 247° and 2.8 m s\(^{-1}\). However, near the source location, the model predicts a wind direction from 198° to 208° and wind speeds between 1.4 and 1.8 m s\(^{-1}\) at the 2-m height (interpolated from 3 m). The model overestimates the velocity deficit that exists near the release from the upwind buildings, and fails to capture the streamline curvature. The k-\(\varepsilon\) models are known to be weak for flows with separation, secondary flows, and streamline curvature.

Figure 6, on the other hand, shows a dramatic modification in the flow field caused by the obstruction of the Regency Tower. Flow approaching the building is nominally parallel to the mean wind direction, and separates around the building to create two counterrotating vortices in the lee of this building. These flow features as well as the channeling seen between the buildings northeast of the Regency Tower play a significant role in determining the size and shape of the tracer plume.

To develop a more three-dimensional view of the flow pattern over the Regency Tower, velocity vectors on a vertical plane are presented in Fig. 7. This vector plot depicts flow features that are expected over such a building (Brzoska et al. 1997). There is a relatively small recirculation zone near the ground upwind of the building, which corresponds to velocity vectors moving down the upwind face. Conversely, the larger vortex downwind of the building corresponds to winds flowing up the downwind face. This figure indicates how tall buildings can very effectively mix the tracer plume.

Figure 8 presents concentration contours from 1 to \(1 \times 10^5\) parts per trillion by volume (ppt). This figure reflects the flow field observed in previous graphs, with
the plume centerline appearing to follow the above-city wind direction initially, and then displaying some asymmetry due to the mixing by the taller buildings toward the east of the plume centerline. The contours are very close together on the western half of the plume, while there are large spaces between contour lines on the eastern half. This shape was created initially by the Regency Tower and was exacerbated by the channeling and mixing from the tall buildings to the northeast of the tower.

Vertical profiles of velocity, turbulent kinetic energy, turbulent dissipation, and tracer concentration from the model at the WSU–LLNL crane site are presented in Fig. 9. The range on the vertical axis in both the dissipation rate and concentration plots goes only to 100 m in order to show more near-surface detail. The profiles of velocity, TKE, and turbulent dissipation rate have general shapes that we expect in an urban environment. These general shapes include low velocities, high TKE, and high turbulent dissipation rate near the ground, where the buildings affect the flow the most. For examples of modeled velocity and TKE profiles in an
urbanlike geometry, see Lien and Yee (2004). Buildings upwind of this site depress the velocities at low elevations, but comparisons with the field data suggest that the model has overestimated the effect of the buildings and/or ground. Near the ground, the model predicted about half of the observed wind speed. Although the size of the wake behind the Regency Tower and the new Federal Building appear to be appropriate, the model is not allowing the flow to speed up to the values observed with the sonic anemometers. It appears that, in general, the model is producing excessive drag along the no-slip ground surface.

The modeled turbulent kinetic energy peaked at about 50-m height with a value of about 1.5 m$^2$ s$^{-2}$. Although the shape of the TKE profile compared well to the field data, the magnitude of TKE was underestimated. The TKE from field data peaked at a value of about 3.6 m$^2$ s$^{-2}$. The upwind buildings, and in particular the Regency Tower, likely defined both the magnitude and height of the TKE peak. The modeled turbulent dissipation rate profile also had a local maximum at around 50 m. Generally, the dissipation rate decreased with increasing height. The modeled tracer concentration profile compared well to observations. Modeled values were generally within 50% of the observations, with the model performing best for the receptors below about 50 m, and performing worst above 50 m.

b. Regency Tower removed

For comparison, the profiles at the crane site for the case without the Regency Tower are presented with the base case in Fig. 9. The velocity defect was not as severe for this case, and compared well to the upper half of the sonic anemometer measurements. The shape of the TKE curve was similar to the base case; however, the maximum value of about 1.2 m$^2$ s$^{-2}$ occurs at about 30 m, nearly half the height of the base case. Correspondingly, the turbulent dissipation rate profile had smaller values at high vertical positions than in the base case. There was less turbulent kinetic energy generated in this case, and therefore less energy to dissipate as well. As one would expect, removing the Regency Tower had a significant effect on the concentration observed at this downwind position. At the top receptor, the concentration was very similar to the observations; however, with decreasing height, the concentration was increasingly higher with the Regency Tower removed. Near the ground, the concentrations were nearly four times higher with the Regency Tower removed. This single, large obstacle mechanically mixed the plume in the vertical direction to decrease the gradient of the concentration profile.

The concentration contour lines on the plane 10 m above the ground for the case without the Regency Tower are shown in Fig. 10. The contour lines on the east half of the plume are farther apart than on the west half, indicating that this feature was indeed a result of the channeling between and mixing by the taller buildings in this part of the plume. However, the plume is significantly more symmetrical about the centerline than the base case that included the Regency Tower (Fig. 8). The narrower, more symmetrical plume that is computed when the Regency Tower is removed is a result of the decreased turbulent kinetic energy in the near field. Without the energetic vortices behind the building, the plume travels a more direct line of transport with less diffusion.

c. Changes in wind direction

Figure 11 presents the concentration contour plots on the 10-m plane for the two additional wind direction cases. For the 182° case, the large and tall buildings were well to the right of the plume centerline, which allowed for a narrow plume overall. The crane location was near the edge of this plume, so very low concentrations were expected. When the wind direction was
212°, however, the tallest buildings were very near the centerline of the plume, which resulted in a wide plume.

The vertical profiles at the crane position for the three different wind direction cases are compared in Fig. 12. Of interest is that the velocity magnitude profiles for all three cases were very similar to each other (although the two new wind directions resulted in slightly higher winds near the ground). The crane was located in a clearing, with about 100 m of empty space upwind. Therefore, it appears that the velocity profile develops over the length of this clearing, so any southerly wind results in nominally the same profile. The turbulent kinetic energy profile, on the other hand, still revealed dependence on the upwind building characteristics. The 182° case had a TKE profile very similar to the 197° base case. The 212° case, on the other hand, was more similar to the “no Regency” case, a result of shorter buildings upwind of the receptor. The turbulent dissipation rate profiles were very similar between the three cases, with slight differences between 40 and 100 m above the ground. Last, the tracer concentration profile showed exactly what we expected from these three wind direction cases. The base case resulted in the best comparison to field data, while concentrations were overpredicted and underpredicted by the 212° and 182° wind directions, respectively.

d. Changes in source location

Figure 13 presents the vertical concentration profiles for the four cases in which the source location was moved. When the source position was moved 50 m to the east and west, along the length of the street, the effect on the concentration profile at the crane site was similar to the varying wind direction cases. Although

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Fig. 9. Vertical profiles of (a) velocity magnitude, (b) turbulent kinetic energy, (c) turbulent dissipation rate, and (d) SF6 concentration at the crane position for the base case (197°) and no-Regency case. The vertical scale in (c) and (d) extends only to 100 m to show near-surface detail.
not shown here, the contour plots of these two source location cases also look very similar to the two wind direction cases. Both the $212^\circ$ wind direction and the positive 50-m source shift result in much wider plumes than do the $182^\circ$ wind and negative 50-m source shift cases. Fifty meters is about one-third the length of the city block, so this indicates that it is very important to know the position of a point source as precisely as possible. When a hazardous spill or intentional release occurs, this may be one of the most difficult parameters to determine, but can easily account for two orders of magnitude difference in concentration at a particular receptor. In addition, the maximum concentration, independent of location, was higher when the source was moved to the east rather than west.

Moving the source vertically by 15 m, on the other hand, had a smaller effect on downwind concentrations at the WSU–LLNL profile site. Concentrations were 50% larger than the concentrations from the base case near the ground, but approached the base-case profile with increasing height. The higher concentrations were a result of fewer obstructions to the plume in the first few meters of transport. The original source height of about 2 m was below the tops of the closest buildings, but the 17-m height of the elevated source was well above these near-source buildings.

The final source position was the 2-m downwind shift that moved the source into two cells to match the ap-
proximate width of a typical urban plume. Very little change was seen between the shapes of the concentration profiles for the base case and this source shift case. Releasing the tracer from the downwind cells reduced the agreement with the field data by about 10% at the lower receptors. This small difference was likely due to the convenient orientation of the original source cell. The tip of the tetrahedral source cell was near the true source location, while the base of the cell was north of the tip. This shape mimics the spreading of the plume, so that moving the source downwind to a wider pair of cells does little to improve the release volume.

e. Add heat

Figure 14 compares the velocity magnitude, turbulent kinetic energy, turbulent dissipation rate, and concentration profiles from the base case with the thermal buoyancy case in which surface temperatures were higher than the air temperature. The heavy black lines in this figure represent the \( k-c \) cases. Adding heat slightly improved the velocity magnitude predictions over the base case; however, wind speeds near the ground were still underpredicted. The turbulent kinetic energy profile, however, showed a significant improvement over the isothermal base case. The two cases were similar in that the peak TKE occurred at the same height, but TKE values were much higher when heat was added. Additionally, TKE values were larger than 1 m² s⁻² for much of the upper half of the vertical profile when heat was added, whereas the TKE value was essentially zero above 150 m in the base case. This case also showed improved agreement of tracer concentration between the field measurements and the base case, with the change in the slope of the concentration profile attributable to thermal mixing lifting the plume. The highest three receptors, which showed the largest error, had modeled concentrations that were 20%–30% smaller than the field data. Although only an approximate average surface temperature was applied, the slight qualitative improvement in the tracer profile comparison indicates that detailed building shading
schemes may not be as important as simply prescribing the average differential temperature between the surface and the air.

f. Reynolds stress model

Profile comparisons at the WSU–LLNL crane site were also made between the $k-\varepsilon$ and RSM results, and are shown in Fig. 14. The thinner lines in this figure represent the Reynolds stress model computations. The velocity magnitude profiles from the two RSM cases were both very similar to the $k-\varepsilon$ model results. This indicates that the modeled velocity deficit near the ground was not a result of the $k-\varepsilon$ model alone. The turbulent kinetic energy profiles with the RSM model underpredicted values (particularly below 100 m) as compared with predictions from the $k-\varepsilon$ model. The Reynolds stress model does not solve the transport equation for the turbulent kinetic energy; instead, $k$ is derived from the Reynolds stress tensor. The dissipation rate profile remained very similar between the two turbulence models. The profiles of $SF_6$ concentration, on the other hand, varied more between the two RSM cases than the two $k-\varepsilon$ cases. The isothermal RSM run underestimated the $SF_6$ significantly, as a result of a plume centerline that was shifted toward the west and differences in the shape of the recirculation zone behind the Regency Tower relative to the $k-\varepsilon$ case. Adding heat to the RSM resulted in predicted concentrations from about 55%–30% below observations. Although the RSM requires additional computational resources relative to the requirements of the $k-\varepsilon$ model, this does not always translate to improved solutions. This is because RSM is very sensitive to initial conditions and can often result in divergent computations.

5. Conclusions and future work

This paper compared the results of computational fluid dynamics modeling with data collected during the Joint Urban 2003 atmospheric dispersion study. The computed flow field appeared reasonable and exhibited features that were expected in an urban environment. Furthermore, a grid uncertainty analysis conducted with this mesh revealed a grid uncertainty index of approximately 6%. Therefore, the mesh did not heavily influence the solution obtained from this analysis.

These results showed that a single large obstacle can have a substantial effect on the flow field, and that it is most important to model the buildings that exist between the source and receptor. The tracer concentration results showed that large obstacles considerably alter the plume shape. The plume in this study was asymmetric, with a pocket of highly mixed air behind the 70-m-high Regency Tower, as well as channeling between buildings in the east half of the plume. The vertical concentration profile at the crane site was modeled with modest accuracy, with some error in the vertical gradient. Both the near-surface wind speed and turbulent kinetic energy were underestimated in this study, although including elevated surface temperatures showed improvement in the TKE values. The Reynolds stress model, which is employed less frequently than both the $k-\varepsilon$ and large eddy simulation models for urban environments, was utilized in this analysis to compare with the simpler $k-\varepsilon$ model. In this case, the RSM did not reveal a significant improvement over the $k-\varepsilon$ model; therefore, the faster computation from the $k-\varepsilon$ model is preferred. This numerical investigation highlighted the characteristics of flows in urban areas less developed than the urban core. Downtown areas typically contain many tall buildings in a somewhat homogeneous array; however, dispersion in the surrounding areas may be highly sensitive to a few key features in the landscape.

A survey of various modeling cases using the $k-\varepsilon$ model affirmed that the wind direction and source location were very important parameters for defining dispersion patterns. Flow traveling through irregular arrays of obstacles resulted in very different plumes depending on the localized landscape that it traveled.
through. In this case, any plume whose centerline passed through the Regency Tower resulted in a very wide plume, whereas centerlines that missed this obstacle produced much more narrow and concentrated plumes. This is particularly important to consider when providing CFD results to emergency response personnel. In the event of a hazardous release, it is unlikely that the meteorology will be fully characterized, or that the source location will be known to high accuracy. Therefore, multiple modeling cases with varying meteorology should be performed a priori to quickly provide several possible outcomes for consideration. In addition, as the number of CFD investigations using real urban geometries increase, these results can be used to develop parameterizations for fast-response models based on characteristics of the cityscape.

Future work with computational fluid dynamics should include a number of model improvements. First, we observed that including building surface temperatures is important in computing the flow and concentration fields. An improved approach to the convective case would be to apply more realistic temperatures to building and ground surfaces, including sun angle and building shading. Surface temperature measurements from future urban field studies would aid tremendously in this effort. Additionally, a larger modeling domain suitable for investigating more JU03 field experiments could be developed. This will allow for a more thorough evaluation of the model because more data points from the field campaign will be available for comparison. Furthermore, modeling the central business district with its denser array of taller buildings will serve to
contrast the geometry investigated in this paper. Last, time-varying boundary conditions could be applied with either RANS or LES to study more complex flows.

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