Urban Dispersion Modeling: Comparison with Single-Building Measurements

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(Manuscript received 8 September 2005, in final form 8 September 2006)

ABSTRACT

Two models have been developed to predict airflow and dispersion in urban environments. The first model, the Realistic Urban Spread and Transport of Intrusive Contaminants (RUSTIC) model, is a fast-running urban airflow code that rapidly converges to a numerical solution of a modified set of the compressible Navier–Stokes equations. RUSTIC uses the k–ω turbulence model with a buoyancy production term to handle atmospheric stability effects. The second model, “MESO,” is a Lagrangian particle transport and dispersion code that predicts concentrations of a released chemical or biological agent in urban or rural areas. As a preliminary validation of the models, concentrations simulated by MESO are compared with experimental data from wind-tunnel testing of dispersion around both a multistory rectangular building and a single-story L-shaped building. For the rectangular building, trace gas is forced out at the base of the downwind side, whereas for the L-shaped building, trace gas is forced out of a side door in the inner corner of the “L.” The MESO–RUSTIC combination is set up with the initial conditions of the wind-tunnel experiment, and the steady-state concentrations simulated by the models are compared with the wind-tunnel data. For the multistory building, a dense set of detector locations was available downwind at ground level. For the L-shaped building, concentration data were available at three heights in a lateral plane at a distance of one building height downwind of the lee side. A favorable comparison between model simulations and test data is shown for both buildings.

1. Introduction

Urban airflow models have traditionally fallen into one of two categories: 1) high-fidelity computational fluid dynamic (CFD) models or 2) fast-running low-fidelity models. The CFD methods include large-eddy simulation models [e.g., the Finite-Element Method, Version Massively Parallel (FEM3MP; Chan and Leach 2004) and Finite-Element Flow Solver—Urban (FEFLO-URBAN; Camelli et al. 2004) models], direct numerical simulation models, and Reynolds-averaged Navier–Stokes (RANS) models [e.g., the “Fluent” (Fluent 2005) and Flame Acceleration Simulator (FLACS; Hanna 2004) models]. The CFD models attempt to solve for the flow at relatively high resolution to capture eddy formation using intensive calculations, and they take significant amounts of computer time for fairly small geographic regions. These models are very useful for examining the time-averaged structure of the flow at fairly small scales and for describing the turbulent shedding that occurs, but, in general, they take too long for fast-response situations or in parametric studies.

The faster-running lower-fidelity approach to airflow modeling generally uses either empirical fitting schemes or mass-consistent flow techniques (or a combination of both) to generate quickly a rudimentary estimate of the flow patterns and turbulence parameters (most often an eddy viscosity) in the region of interest. The U.K. Urban Dispersion Model (UDM) code (Brook et al. 2003, Hall et al. 2003) and the Finnish Meteorological Institute (FMI) UDM-FMI code (Karppinen et al. 2000) are representative of this approach, both using Gaussian puffs. An example of the use of mass-consistent flow is given by Kaplan and Dinar (1996). This type of modeling is useful for very quick response situations, but the lack of fidelity restricts the technique to situations in which no other solution method is practical.

Under recent Defense Advanced Research Projects Agency (DARPA) sponsorship, a fast-running urban...
airflow model [the Realistic Urban Spread and Transport of Intrusive Contaminants (RUSTIC) model] has been developed. RUSTIC was created to provide a midrange solution in terms of speed and fidelity when compared with typical CFD codes, yet with more physical modeling than the fast-running mass-consistent flow codes. In specific terms, RUSTIC represents an effort to simplify and optimize a RANS CFD method to a relatively short run-time regime, as opposed to adding rules to a fast-running model in an attempt to address phenomena like turbulence empirically. In terms of run time, the desire is for RUSTIC to be able to create a description of the airflow with the turbulent kinetic energy (TKE) and turbulent dissipation for a 1 km $\times$ 1 km urban area in less than 1 h on a standard personal computer with accuracy that is acceptable for calculating a prediction of contaminant dispersion.

For contaminant dispersal, RUSTIC is normally run in conjunction with “MESO,” a Lagrangian tracer dispersion code, which for urban calculations is based on the random-walk technique of Diehl et al. (1982). Also, again under DARPA sponsorship, MESO has been modified to accept the 3D flow and turbulence fields from RUSTIC and has been given special features needed for accurate urban (building aware) dispersion modeling. The two codes can be used separately, which allows a single RUSTIC solution to be used for many MESO dispersion simulations. Because MESO runs much faster than RUSTIC does, the source location and strength in MESO can be varied 1) to perform fast parameter studies, 2) for training, or 3) for identification of a threat source location.

After providing short overviews of RUSTIC and MESO, this paper outlines a preliminary validation effort for the two codes using wind-tunnel data for two single buildings: one is a simple rectangular building and the other is an L-shaped building. The overview of the RUSTIC code is abbreviated, because greater detail is given in a companion article by Burrows et al. (2007). However, a brief summary of the model including a description of the numerical method can be seen in an older paper by Burrows et al. (2004a). Additional comparisons can be seen in another companion paper by Hendricks et al. (2007) using dispersion and meteorological data from Oklahoma City, Oklahoma, from the large Joint Urban 2003 field test. An overview of the field test is given by Allwine et al. (2004).

2. RUSTIC flow model overview

To simplify computation, RUSTIC combines the continuity and thermodynamic equations into a single pressure tendency equation. The prognostic equation for pressure is then written in a form with the speed of sound $c$ identified in a manner that allows it to be greatly reduced to permit a large time step. Experimentation has confirmed that the exact value of $c$ has little or no effect on the final velocity and turbulence fields predicted (Burrows et al. 2004a, 2007). RUSTIC includes a $k$–$\omega$ turbulence model (Wilcox 1998, p. 121) with a buoyancy production term for TKE, permitting the study of atmospheric stability effects. Execution speed is further enhanced with an expanding grid capability and with the ability to allow cells far from the most turbulent regions to “coast” for $n$ cycles whenever the acceleration is found to be below a preset criterion. The coasting technique, however, is still under investigation and was not used for this study. Solutions are obtained with finite-volume techniques based on a modified Cartesian grid structure. Although the cells are rectangular for increased computation speed, partial cells are used at building edges to improve the accuracy.

A technique for running RUSTIC with several different grids of increasing resolution is being developed with the goal of providing rapid convergence to a “useful” solution within as short a period of time as possible. A useful solution is defined here as one that results in a dispersion prediction that is accurate to within a factor of 2 with a resolution smaller than the size of the smallest building of interest. To initialize the grid and to supply the wind profile and turbulence energy and dissipation at the inflow boundary, a 1D numerical algorithm that contains the $k$–$\omega$ turbulence equations is included. The algorithm computes the flow as a function of altitude over a rough surface based on the sensible heat flux and surface roughness. RUSTIC can be run with an upwind heat flux that differs from the heat flux value around the larger buildings.

3. MESO Lagrangian tracer model overview

To model transport and dispersion of contaminants, RUSTIC flow and turbulence fields are passed to MESO, which is based on Lagrangian tracer techniques. MESO has been primarily sponsored by the Naval Surface Warfare Center Dahlgren Division for general-purpose “rural” transport and dispersion applications and can ingest 3D forecast predictions. For non-urban dispersion predictions, MESO contains a sophisticated convective boundary layer model and uses the stochastic Lagrangian tracer technique of Franzese et al. (1999) for unstable conditions and Luhar and Britter (1989) for stable conditions.

New urban capabilities have been recently added to MESO under DARPA sponsorship. Tracer techniques
have a number of advantages over standard grid advection methods. One is the reduction of advection errors in highly sheared flow, which is very important when using coarse grid cells to reduce run time. Another is the elimination of artificial diffusion, which is of particular importance for biological agents that can cause fatalities even with extremely small quantities. A third advantage is the ability to handle large size distributions and droplet settling naturally. MESO contains a full suite of tools for handling chemical and biological agents, including droplet evaporation and surface evaporation.

Of particular importance for small biological particles, MESO contains a state-of-the-art model for estimating the rate of particle deposition including canopy “filtration.” The model, which is based on similarity curve fits (Seinfeld and Pandis 1998; Slinn 1977), is a function of particle size and density, surface characteristics, surface layer meteorological conditions, and vegetation characteristics. Each ground cell of the flow grid can have its own surface/vegetation qualities, including canopy type, a condition that allows the deposition rate to be modeled on a cell-by-cell basis. The primary limitation of the model is the assumption that the boundary layer is fully developed, implying a long upwind fetch that is seldom the case in an urban setting. As yet, MESO does not model chemical reactions or surface absorption.

MESO also includes a sophisticated heat flux algorithm that uses the heat budget at the surface/canopy to estimate the sensible heat flux. The algorithm also computes the Obukhov length $L$ and the friction velocity $u^*$, which are needed for estimating the deposition. For urban runs the heat flux model ignores the turbulence predicted by RUSTIC and instead computes its own surface-layer properties based on the local flow speed and surface type. The heat flux model, which is based on an iteration technique similar to that of van Ulden and Holtslag (1983), has been found to reproduce accurately the 24-h heat flux histories taken during the First International Satellite Land Surface Climatology Project Field Experiment (FIFE) field trials (Strebel et al. 1998) in the Kansas prairie. The model accuracy is limited, however, by the fact that MESO–RUSTIC does not yet take into account shading behind the buildings. This limitation will be corrected in the near future. For urban simulations, the output of the heat flux model is only used to compute particle deposition, and the dispersion is computed with the turbulence predicted by RUSTIC.

To move tracers with the flow, MESO first determines the cell in which the tracer is located. MESO uses a grid that is offset by one-half of a RUSTIC cell such that each of the eight corners of the MESO cell has its own velocity vector. The tracer velocity is then estimated by interpolating among the eight corners of the cell. The interpolation scheme assumes the flow is detached at the building edges and corners. To improve the flow accuracy around corners and in tight eddies, the tracers are advanced with a predictor–corrector numerical scheme. When one or more of the eight corners is located inside a building, boundary conditions are set to force the flow normal to the surface to be zero.

MESO includes a terrain-tracking capability to prevent tracers from artificially depositing or impacting building walls as a result of advection errors. This is of particular importance in turbulent flow in which the tracers are also moved in a stochastic manner. The ground surface, which is defined by a terrain grid passed to MESO from RUSTIC, includes the buildings themselves. In other words, MESO treats the buildings as ground elevation changes. For tracers that are moving toward the surface and reside within a vertical distance of one cell height from the surface, the normal component of the velocity is linearly interpolated to zero at the surface from the first adjacent node. Thus, the closer to the surface that the tracer resides, the more parallel its flow vector becomes to the surface. Based on numerical studies with urban geometries, this approach has been found to affect the predicted concentrations by only a few percent or less over the regions of the plume with concentrations above 10% of the peak value.

To model urban dispersion, each tracer undergoes numerous random-walk excursions in each coordinate direction as the tracers travel with the flow. As discussed in detail by Diehl et al. (1982), the random-walk technique satisfies the well-mixed condition, which in effect means there is no artificial drifting of the tracers in areas of high diffusion gradients. For improved accuracy, the diffusivity $K$ between cells is modeled with linear segments rather than as a series of step changes. Although stochastic in nature, the random-walk method is in effect a gradient transfer process. For example, at the limit of large numbers of tracers, the vertical random-walk movements in each RUSTIC layer result in a tracer flux $F(z)$ of the form

$$F(z) = -(K_0 + K_1 z) \frac{\partial \chi}{\partial z},$$

where $\chi$ is the tracer concentration and the diffusivity $K_0 + K_1 z$ is a linear function of the height $z$, with the constants $K_0$ and $K_1$ chosen so that a linear change in the diffusivity smoothly spans between each RUSTIC grid value. Thus, with 3D RUSTIC flow fields, MESO predictions are numerical solutions to the 3D advec-
tion–diffusion equation. As shown by Diehl et al. (1982), a linear diffusivity of this form requires tracer random-walk movements given by

$$
\ell(z) = \pm [2\Delta t(K_0 + K_1z) + (\Delta tK_1)^2]^{1/2} + \Delta tK_1, \tag{2}
$$

where the ± sign is determined by a random-bit generator and $\Delta t$ is the time step. Even though each tracer is independent of the others, by integrating to determine the flux across a boundary it can be shown that Eq. (2) will, in the limit of an infinite number of tracers, give the flux $F(z)$ in Eq. (1). If near a surface where $K_0$ is zero, the negative sign generates movements toward the surface that are much smaller than those produced by the positive sign. In fact, as a tracer becomes progressively closer to the surface the negative movements go to zero.

As shown in Fig. 1, the vertical diffusivity predicted by RUSTIC is modeled as a series of connected linear diffusivity segments, which is much more accurate than a series of step changes between levels. Small abnormal net fluxes can, however, occur near junctions if the particle movements are not handled correctly. As illustrated in Fig. 2, this problem is easily resolved by extending the adjoining diffusivities, $K$ and $K'$, at the junction at $z_0$ to levels $z_1$ and $z_2$ above and below $z_0$. These levels correspond to the maximum distance from which tracers above and below $z_0$ can penetrate the junction at each time step. The heights of $z_1$ and $z_2$ are given by

$$
z_1 = z_0 - [2\Delta t(K_0 + K_1z_0)]^{1/2} \quad \text{and}
$$

$$
z_2 = z_0 + [2\Delta t(K_0 + K_1z_0)]^{1/2}. \tag{3}
$$

These expressions for $z_1$ and $z_2$ could as easily have been written using $K_0' + K_1'z_0$ instead of $K_0 + K_1z_0$ because at $z_0$ the two are equal. Tracers in the overlap region above $z_0$ are moved upward according to $K'$ but are moved downward according to $K$. The converse is required for tracers in the overlap region below $z_0$. If one assumes that the time step $\Delta t$ is sufficiently small that the overlap regions do not extend more than halfway across the layer, the resulting flux $F(z)$ is strictly proportional to the concentration gradient. Even without the overlap regions, the net drift at cell junctions is small relative to the treatment of diffusivity in a stepwise manner.

For the random-bit sequence needed for Eq. (2), the numerical method of Press et al. (1988) is used, based on the work of Watson (1962). Because the random bits can be obtained in a numerically fast manner, the random-walk movements in general take less computer time than do other stochastic techniques that require a normally distributed random-number generator. [See, e.g., Marsaglia and Bray (1964), McGrath and Irving (1975), and Luhar and Britter (1989).] Furthermore, when a tracer nears a surface where the diffusivity goes toward zero, the technique does not require a small time step. For the random-walk method, the time step criteria is $\Delta t < \Delta z^2/(8K_{\text{max}})$, where $\Delta z$ is the layer thickness and $K_{\text{max}}$ is the maximum diffusivity in the layer. The random-walk step size is usually smaller than the advection step, which is limited to one-half of the travel time across a RUSTIC cell. Many stochastic Lagrangian models set the time step to a small fraction of the Lagrangian time scale, which becomes very small near the surface as the dissipation becomes very large. [See, e.g., Luhar and Britter (1989).] Thus, tracers can in effect become trapped near the surface, eating up
CPU time. To solve this problem, various model developers have limited the time step to a finite value; however, this occasionally results in tracer penetration of the ground surface. Thus, various schemes have been suggested to “reflect” tracers back above the surface in a manner that does not overly distort the underlying physics. For example, Thomson and Montgomery (1994) suggest a method that relates the reflected velocity to the incident velocity and the normal velocity distribution.

For horizontal diffusivity, standard interpolation techniques are used to compute the diffusivity in an arbitrary location in a cell based on the values at the eight corners. First, horizontal diffusivity values are estimated by vertical interpolation at the tracer height at the four horizontal corners. Next, as shown in Fig. 3, interpolation in both x and y produces the diffusivities \( K_{x1}, K_{x2}, K_{y1}, \) and \( K_{y2} \) on the lines intersecting at the tracer location, which are then used to interpolate a diffusivity value at the tracer location and to estimate the horizontal diffusivity gradients. For example,

\[
\frac{\partial K}{\partial x} = \frac{(K_{x2} - K_{x1})}{\Delta x},
\]

and, in the spirit of Eq. (2), the tracer random-walk motion in the x direction is computed using

\[
\ell(x) = \pm \left[ 2\Delta t K + \left( \Delta t \frac{dK}{dx} \right)^{1/2} + \Delta t \frac{\partial K}{\partial x} \right].
\]

As is done for the velocities, when one of the corners is located inside a building, the diffusivity in the building is set to a value that forces the diffusivity to zero at the surface.

In contrast to the vertical random-walk movements, overlap regions near diffusivity junctions have not been included for the horizontal tracer movements. However, the net artificial flux decreases as the size of the overlap region decreases, which is a function of the time step. To limit the problem, the horizontal time step is kept small in comparison with the vertical time step. Numerical experimentation has shown that the drift error is often small relative to the statistical fluctuations from the use of a finite number of tracers. Furthermore, it can be argued that the drift only occurs where the gradients are high near building walls. Additional research is under way to find a more numerically efficient solution to the problem. As will be shown in the next two sections, in its current form the model does a respectable job of matching experimental data.

4. Comparison with wind-tunnel data for a rectangular building

For this dispersion comparison, the wind-tunnel setup represented a midsized rectangular structure that resembles a multistory building with a parking garage at the base. A full description of the experiment and results, listed as case A1-5, could be found at the Compilation of Experimental Data for Validation of Micromodel dispersion models (CEDVAL) Internet site maintained by Hamburg University (Schatzmann 2005). Although the wind-tunnel building was at 1/200 scale, the model represents a full-scale height of 25 m with a frontal width of 30 m and a thickness of 20 m. The boundary layer flow in the tunnel corresponded to a surface roughness of 0.14 m and a friction velocity of 0.377 m s\(^{-1}\), yielding a wind velocity at the roof height of 5 m s\(^{-1}\). On the downwind side of the building are four openings of size 4.6 m\(^2\) that are emission sources with a flow rate of 3 m s\(^{-1}\).

The building was modeled with cubic cells 1 m in size out to 20 m away from the building in each horizontal direction, at which point the grid was then expanded. Prior to expanding vertically, the cell dimensions were held at 1 m in size until a height of 40 m. The total number of cells was 527,904 and required 112 min of CPU time on a 2.2-GHz Pentium IV processor for RUSTIC to reach convergence. For the MESO simulation, 20,000 tracers were employed, requiring about 4 min of CPU time on a 2.8-GHz Pentium IV. Because of statistical fluctuations, the MESO results have a normalized rms error of about 5% in the central body of the plume near the buildings. The error estimate was based on a series of runs, each with 20,000 tracers but with a different starting seed for the random-number generator.

Figure 4 shows the results of a RUSTIC simulation.
for flow around the structure in which cells on the downwind side have been set up as sources of additional flow. Surface vectors at a height of 2 m and iso-surfaces of TKE are plotted. The effluent openings were modeled with not only the correct flow rate, but also with estimated values of the TKE and dissipation, as determined from a simple 1D numerical channel flow model containing the $k-\omega$ turbulence model. The flow near the surface at the rear corners is apparently disrupted by the flow out of the rear openings, preventing the formation of large corner eddies. A comparison between dispersion measurements and data is shown in Fig. 5 at heights of 2 and 7 m. Here, the dimensionless concentration $K^*$ is plotted, defined by normalizing the concentration by $Q/(\mu h^2)$, where $Q$ is the source strength, $h$ is the building height, and $\mu$ is the wind speed at $z = h$. The diffusivity $K$ for the simulation was set to $K = 2.5k/\omega$, where $\omega$ is the dissipation coefficient in the $k-\omega$ turbulence model. More will be said about this choice for $K$ in the next section.

For the main plume located behind the structure, the comparison between the measurements and the model simulations is within a factor of 2 or better. For a given contour, both the width and length of the plumes are of similar size. At a height of 2 m, the regions of similar contour value are approximately the same length, but the model underpredicts the plume width. At both levels the model underpredicts the degree to which the effluent is pushed upwind along the sides of the building. This is likely the result of the use of cells that are too large in this region to allow correct simulation of the narrow eddies along the sides of the buildings. The results could be improved with finer cells in this region. Nevertheless, the model simulated the movement of effluent roughly halfway upwind along the building walls. The inability to handle correctly the dispersion along the sides of the structure might also be linked to the fact that the plume is too narrow downwind. The model did a respectable job of simulating the change in size and shape of the high-concentration region (red) between the 2- and 7-m levels at the rear of the building. In other words, even though the release was near ground level, the model simulated the relatively high values of concentration at the 7-m level.
5. Comparison with wind-tunnel data for an L-shaped building

For this comparison, the wind-tunnel setup was the “Project EMU” A1 case as described by Cowan et al. (1997) and by Castro et al. (1999). Project EMU was a study funded by the European Union to assess CFD solution variability. For case A1, an L-shaped building with an inner side door was placed in a boundary layer flow with a surface roughness $z_0$ of 0.12 m. Although the model was tested at 1/200 scale, only full-scale values will be given here. As shown in Fig. 6, the full-scale building was 10 m in height with the wind direction head on toward the long end of the building. The wind speed at a height of 10 m was 5 m s$^{-1}$. Flow was also

Fig. 5. Comparison between (left) measured and (right) simulated dimensionless concentration $K^*$ for a rectangular building with effluent holes near ground on the lee side. The comparison is shown at two heights: (bottom) 2 and (top) 7 m. Measurements were available only at the locations of the colored squares.

Fig. 6. The L-shaped building geometry used in EMU wind-tunnel test A1.
forced out of the door at 1 m s\(^{-1}\) with a trace gas added to allow dispersion estimates downwind of the building. Because the door was fairly large, 4 m wide \(\times\) 5 m high, the door flow had a substantial influence on the flow.

To investigate the effect of grid size on the results, three simulations were made using cell sizes in the region of the building of 0.75, 1.0, and 1.5 m. For each of the three cases, the cell size was slowly increased in all directions away from the building, creating a domain size approximately 100 m upwind of the building, 170 m downwind of the building, and 100 m on either side. The horizontal grid for the 1.0-m case is shown in Fig. 7. In the vertical direction, the cells were held constant in size up to the height of the roof and then expanded up to a height of over 40 m. Near the ground, the vertical cell sizes were 0.4, 0.4, and 1.0 m corresponding to the minimum horizontal cell sizes of 0.75, 1.0, and 1.5 m, respectively. For the 1.0-m case the total number of cells was 108 \(\times\) 94 \(\times\) 43 and required 67 min on a 2.2-GHz Pentium IV processor for RUSTIC to reach convergence.

Figure 8 shows the simulated velocity vectors for the 1.0-m cell case at 2.5 m above the ground after the flow has reached steady state. Also shown at this level are TKE contours (m\(^2\) s\(^{-2}\)). As expected, the TKE values are high in the strong shear regions at the front corners and weak in the slow eddies behind the building. The TKE is also moderately high well away from the building because of the boundary layer. Two eddies can be seen at the rear of the structure, with the stronger of the two coming off the far rear corner. Although not shown in this particular figure, a relatively strong eddy also forms at the rear corner of the roof.

Streamlines are shown for a series of starting locations at the door. Although the streamlines would suggest that most material is carried over the roof rather than around the building, as will be shown, a significant amount of the trace gas goes out around because of the turbulence. A few of the streamlines follow small eddies in the region of the door that carries them to the front of the building prior to flowing over the roof. At about one building height behind the structure, many of the streamlines curve back toward the building in the small rear eddy. Even a small difference in the starting location can result in an entirely different path relative to its neighbors. However, the turbulence is sufficiently strong to disrupt the path of a tracer along any given streamline.

A contour plot of simulated dimensionless concentration \(K^*\) is shown in Fig. 9, again for the 1.0-m cell size. For the simulation, a series of 20 Gaussian-shaped clusters were released 0.5 m from the door in a pattern four across and five high. Improving the fidelity of the door source to an even greater degree was found to have little effect on the concentrations. As seen in the figure, turbulent eddies near the inside corner by the effluent source carry trace gas upwind to near the front end of the structure. Primarily because of turbulence created at both upwind corners on the door side, trace gas at low levels is carried well away from the building side section.

For this same simulation, a plot of measured versus simulated concentration is shown in Fig. 10 for three different scaled heights \(z/h\). The measurements were taken in a plane directly behind the building at a downwind distance \(x/h = 1\). The crosswind distance has also been normalized by the building height. Thus, as indicated in the diagram in the upper-right corner of the plot, the location \(y/h = +1\) aligns with the long wall of the building, and \(y/h = -1\) aligns with the small wall of the side extension. At all three altitudes, the peak value on the simulated curves is within about 30% of the peak value of the test data. The main difference between the simulated and measured values is for the simulated \(z/h = 0.16\) curve, which does not extend as far out from the building toward negative \(y\) as the measured curve does. The MESO dispersion simulations were made with 30,000 tracers, resulting in a normalized rms error of about 5% in the region of the peak concentration.

The diffusivity \(K\) used in this calculation was set to \(K = (k/\omega)/Sc_t\), where \(k/\omega\) is the kinematic eddy viscosity in the \(k-\omega\) turbulence model, as simulated by RUSTIC for each cell. A value for the turbulent Schmidt number \(Sc_{t}\) of 0.4 was found to give the best overall comparison to the data, and is the same value that was used for the rectangular building. Although a more standard value for \(Sc_t\) is about 0.7, Riddle et al. (2004) found for at-
mospheric flow that an even smaller value of 0.3 gave the best results with a CFD code containing the $k$–$\varepsilon$ model. Increasing values of $K$ do not substantially widen the peaks, suggesting the effect of the higher diffusivity primarily reduces the residence time of the tracers circulating in eddies behind the building. A somewhat lower value for $Sc_t$ than that found by other investigators might be in part the result of lower artificial diffusion due to the use of tracers.

The smaller values of $Sc_t$ needed here to improve the comparison to measurements might be simply compensating for artificially low values of $k$ simulated by the $k$–$\omega$ turbulence model when used for urban geometries. For example, Lien and Yee (2004) and Lien et al. (2004) reported that CFD models using the standard $k$–$\varepsilon$ as well as modified $k$–$\varepsilon$ models often underpredicted $k$ by a factor of 1.5–2.0 for urban flow. Burrows et al. (2004b) also noted that RUSTIC underpredicts TKE near ground level by roughly a factor of 2 relative to urban measurements; however, this may also be due to the presence of large-scale atmospheric turbulence in the measurements.

**Fig. 8.** Flow vectors and TKE ($m^2 s^{-2}$) contours at a height of 2.5 m as simulated by RUSTIC for the L-shaped building. (Only every other vector is shown along the wind direction.) The flow was 5 m s$^{-1}$ at the roof level with a boundary layer corresponding to $z_0 = 0.12$ m. Also shown are streamlines originating at various locations at the door.

**Fig. 9.** Dimensionless concentration $K^*$ simulated by MESO–RUSTIC near the ground ($z/h = 0.16$).
A comparison between the simulated and measured concentrations for the 1.5-m cell size is shown in Fig. 11. As the cell size is increased, the near-ground concentration increases and the roof-level concentration decreases. The reverse is true for the 0.75-m grid. It is apparent that the artificial diffusion produced by advection through the larger cells plays a significant role in the simulations. For the L-shaped building, Cowan et al. (1997) likewise reported that a smaller cell size made the simulations grow worse in comparison with experiment and suggested that artificial diffusion might be responsible for improving the simulations. Because the design goal for RUSTIC is a fast-running medium-accuracy tool, setting the various coefficients for diffusion of momentum, $k$, and $\omega$ as a function of cell size and flow curvature is under consideration for urban simulations. Table 1 lists the computer time needed for each of the three simulations of the L-shaped building at the three different cell sizes based on a 2.2-GHz Pentium IV processor.

Current research is involved with investigating the effects on dispersion-related improvements to the $k-\omega$ turbulence model. In its standard form, the $k-\omega$ turbulence model overestimates the TKE in the vicinity of a

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**Fig. 10.** Comparison between measured and simulated trace gas concentrations at a distance of one building height $h$ behind the L-shaped building. The simulations were based on the standard $k-\omega$ turbulence model with the 1.0-m grid. The curves represent normalized concentration data for Meso–Rustic (no symbols) and for measured data (no symbols) taken in a downwind plane ($x/h = 1$ behind the building) at three heights: $z/h = 0.16$ (blue), $z/h = 1.02$ (magenta), and $z/h = 1.47$ (teal).

**Fig. 11.** As in Fig. 10, but with simulations made using the 1.5-m grid.
stagnation point in front of a wall. This was investigated by Durbin (1996) as the stagnation point anomaly, with a solution to the problem later refined by Medic and Durbin (2002). Burrows et al. (2007) found better comparisons to urban measurements with both the adjustment to handle the stagnation point problem and small adjustments to the coefficients in the $k - \omega$ model. Preliminary results for the 1-m grid indicate that these modifications do not necessarily improve the dispersion for the L-shaped building. In particular, the dispersion near the ground still does not extend out away from the building wing (toward $-y$) as far as the measurements, and at the roof level the peak concentration is overpredicted by almost a factor of 2.

6. Conclusions

The RUSTIC and MESO models were designed to generate predictions many times faster than typical CFD codes with accuracy on the order of a factor of 2. For the two buildings modeled for this study, the code solutions match the overall features of the dispersion data reasonably well—in particular in view of the complicated emission source geometries and conditions. Particularly satisfying was the modeling showing 1) effluent moving up the back wall of the rectangular building, 2) agreement with experiment in the high-concentration region at the rear of the rectangular building, and 3) the rough agreement of the relative amount of effluent going over the L-shaped building as opposed to going around it. Less satisfying is the result that the simulated curve for the $z/h = 0.16$ level does not extend as far out from the L-shaped building as the measured values do and that the results are sensitive to the model cell size. Additional research is needed to resolve the sensitivity to cell size and to understand better the need for a small Schmidt number $Sc$ to obtain good comparison to measurements. Even though some compromises were made to decrease model run time, the models appear comparable in accuracy to other RANS CFD models.

Acknowledgments. This effort was sponsored by the Defense Advanced Research Projects Agency under Contract SPO700-98-D-4000.

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REFERENCES


