LARGE SCALE URBAN SIMULATIONS WITH MILES

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Abstract. Airborne contaminant transport in cities presents challenging new requirements for CFD. The unsteady flow physics is complicated by very complex geometry, multi-phase particle and droplet effects, radiation, latent, and sensible heating effects, and buoyancy effects. Turbulence is one of the most important of these phenomena and yet the overall problem is sufficiently difficult that the turbulence must be included efficiently with an absolute minimum of extra memory and computing time. This paper describes the Monotone Integrated Large Eddy Simulation (MILES) methodology used in NRL’s FAST3D-CT simulation model for urban contaminant transport (CT). We also describe important relevant extensions of the underlying Flux-Corrected Transport (FCT) convection algorithm. Validation studies and issues raised are discussed.

1 INTRODUCTION

The Urban airflow accompanied by contaminant transport presents new, extremely challenging modeling requirements. Reducing health risks from the accidental or deliberate release of Chemical, Biological, or Radiological (CBR) agents and pollutants from industrial leaks, spills, and fires motivates this work. Configurations with very complex geometries and unsteady buoyant flow physics are involved so the widely varying temporal and spatial scales exhaust current modeling capacities. Crucial technical issues include turbulent fluid transport and boundary condition modeling, and post-processing of the simulation results for practical use by responders to actual emergencies.

Relevant fluid dynamic processes to be simulated include complex building vortex shedding, flows in recirculation zones, and approximating the dynamic subgrid-scale (SGS) turbulent and stochastic backscatter. The model must also incorporate a consistent stratified urban boundary layer with realistic wind fluctuations, solar heating including shadows from buildings and trees, aerodynamic drag and heat losses due to the presence of trees, surface heat variations and turbulent heat transport. Because of the short time spans and large air volumes involved, modeling a pollutant as well mixed globally is typically not appropriate. It
is important to capture the effects of unsteady, buoyant flow on the evolving pollutant concentration distributions. In typical urban scenarios, both particulate and gaseous contaminants behave similarly insofar as transport and dispersion are concerned, so that the contaminant spread can usually be simulated effectively based on appropriate pollutant tracers with suitable sources and sinks. In some cases, the full details of multigroup particle distributions are required. In such cases, additional physics includes the deposition, resuspension and evaporation of contaminants.

1.1 The Established Approach: Gaussian Plume Models

Contaminant plume prediction technology currently in use is based on Gaussian similarity solutions (“puffs”). This class of extended Lagrangian approximations is only appropriate for large scales and flat terrain. Separated flow and vortex shedding from buildings, cliffs, or mountains is absent. Diffusion is used in plume/puff models to mimic the effects of turbulent dispersion caused by the complex building geometry and by wind gusts of comparable and larger size. Detailed comparisons using actual “common use” puff/plume models show a range of results depending on how much of the 3D urban boundary layer information from the detailed simulation is incorporated in the Gaussian model. Gaussian models seem to predict too rapid a lateral spread in the vicinity of a source to provide a plume that is approximately the correct width downwind.

1.2 The Urban Aerodynamics Approach

Since fluid dynamic convection is the most important physical process involved in CBR transport and dispersion, the greatest care and effort should be invested in its modeling. The advantages of the CFD approach and LES representation include the ability to quantify complex geometry effects, to predict dynamic nonlinear processes faithfully, and to treat turbulent problems reliably in regimes where experiments, and therefore model validations, are impossible or impractical.

1.1.1 Standard CFD Simulations

Solving for the motion and dispersion of airborne contaminants in the downtown area of a city is a problem for time-dependent, aerodynamic CFD methods. Since fluid dynamic convection is the most important physical process involved in CBR transport and dispersion, the greatest care and effort should be invested in its modeling. The advantages of the CFD approach and LES representation include the ability to quantify complex geometry effects, to predict dynamic nonlinear processes faithfully, and to treat turbulent problems reliably in regimes where experiments, and therefore model validations, are impossible or impractical. This computing urban aerodynamics accurately is a time-intensive, high-performance computing problem. But using this technology for the emergency assessment of industrial spills, transportation accidents, or terrorist attacks (biological or chemical) requires very tight time constraints that suggest simple approximations, which unfortunately produce inaccurate results. The trade-off has been to choose between a fast, but inaccurate model or a much slower, but highly accurate model.
1.1.2 The LES Approach for Contaminant Transport

DNS is prohibitively expensive for most practical flows at moderate-to-high Reynolds number, and especially so for urban CT studies. On the other end of the CFD spectrum are the standard industrial methods such as the RANS approach, e.g., involving $k$-$\varepsilon$ models, and other first- and second-order closure methods, which simulate the mean flow and approximately model the effects of turbulent scales. These are generally unacceptable for urban CT modeling because they are unable to capture unsteady plume dynamics. LES constitutes an effective intermediate approach between DNS and the RANS methods. LES is capable of simulating key flow features that cannot be handled with RANS or Gaussian plume methods such as significant flow unsteadiness and localized vortex shedding, and provides higher accuracy than the industrial methods at lower cost. The main assumptions of LES are: (i) that transport is largely governed by large-scale unsteady convective features that can be resolved, (ii) that the less-demanding accounting of the small-scale flow features can be undertaken by using suitable subgrid scale (SGS) models. Given its potential for computational efficiency, the Monotone Integrated LES (MILES) approach (see [xi] for a recent review) is ideally suited to CFD-based urban-scale plume simulations, an application where RANS methods are inadequate and classical LES methods are too expensive.

2 MILES FOR URBAN SCALE SIMULATIONS

The three-dimensional FAST3D-CT MILES model is based on a scalable, low dissipation, 4th order phase-accurate FCT convection algorithm. Other than changes described below, the FCT used in FAST3D-CT is documented in Boris et al. xvii

![Figure 1: Contaminant dispersion from an instantaneous release in Times Square, New York City as predicted by the FAST3D-CT MILES model. Concentrations shown at 3, 5, 7, and 15 minutes after release.](image)

A practical example of urban-scale MILES is given in Figure 1, showing contaminant dispersion in Times Square, New York City. The figure demonstrates the typical complex unsteady vertical mixing patterns caused by building vortex and recirculation patterns, and the endangered region associated with this particular release scenario. In particular, the figure depicts the so-called fountain effect occurring behind three tall buildings. The fountain effect is the systematic migration of contaminant from ground level up the downwind side of tall buildings followed by continuous ejection into the air flowing over the tops of these buildings. This phenomenon has also been seen in experiments in Los Angeles and has been reported in wind tunnel studies. It is important because the contaminant can be transported downwind much faster than might be otherwise expected during this process. This effect appears to be driven by arch vortices lying behind the buildings – e.g., as in the well-
studied problem of flow past a surface mounted cube. It is important to note that this is a process that puff/plume models cannot capture directly.

FAST3D-CT has models for a number of additional physical processes. Incorporating specific models for these processes in simulation codes is always a challenge but has been accomplished with reasonable fidelity. The primary difficulty is the effective calibration and validation of these physical models since much of the input needed from experimental measurements of these processes is typically insufficient or even nonexistent. Further, even though the individual models can all be validated separately, the larger problem of validating the overall simulation code has to be tackled as well.

A typical run with the FAST3D-CT model for a complex urban area of 30 square km resolved with 6 m cells takes 24 hours on a 32-processor SGI system. This is significantly faster per square km than classical CFD models, due to the savings achieved by MILES as well as other algorithmic improvements. However, first responders and emergency managers on site to cope with contaminant release threats cannot afford to wait while actual simulations and data post-processing are carried out. An operational solution of this problem carries out unsteady CFD simulations in advance and pre-computes compressed databases for specific urban areas incorporating suitable assumed weather and a full set of wind conditions and distributed test-sources. The relevant information is summarized as Dispersion Nomograf™ datasets so that it can be readily used through portable devices, with sensors providing current observational information regarding local contaminant concentrations and winds. With this new approach, implemented in a system called CT-Analyst®, the accuracy of CFD simulations can be recovered instantly with little loss of fidelity.

2.1 Atmospheric Boundary Layer Specification

The planetary boundary layer characterization upstream of the finite computational domain directly affects the boundary-condition prescription required in the simulations. The weather, time-of-day, cloud cover and humidity all determine if the boundary layer is thermally stable or unstable and thus determine the level and structure of velocity fluctuations. Sensitivity studies show that the fluctuating winds affect urban dispersion. The strength of the wind fluctuations, along with solar heating are shown to be major determinants of how quickly the contaminant density decreases in time. This in turn is extremely important in emergency applications as it determines overall dosage.

In FAST3D-CT the time average of the urban boundary layer is specified analytically with parameters chosen to represent the overall thickness and inflection points characteristic of the topography and buildings upstream of the computational domain. These parameters can be determined self-consistently by computations over a wider domain, since the gross features of the urban boundary layer seem to establish themselves in a kilometer or so. Including this extra area, however, this increases the cost of simulations considerably.

The important length scales (tens of meters to kilometers) and time scales (seconds to minutes) in wind gusts can be resolved easily by CFD models that accurately resolve the buildings. Since they can be resolved, the gusts, must not be averaged out. To address this, a deterministic model for an evolving realization of these fluctuations is included as part of the...
boundary conditions with input parameters to approximate particular atmospheric conditions being simulated. The model for these boundary condition wind fluctuations that we have used is a complicated analytic function defined throughout the computational domain; this fluctuation provides the initial and boundary conditions of a run.

Three types of motion are superimposed at several different wavelengths to construct this function. A coherent shearing motion transverse to the average wind direction, typical of meanders, is impressed with a sinusoidal structure. Superimposed on this are horizontal pancake vortices at several scales to represent a type of flow possible in stratified fluids. The third motion is due to longitudinal vortices with finite vertical and horizontal extent to represent wind-induced hairpin vortices found in typical boundary layers. The space and time scales for each of these motions were made incommensurate, permitting the nonlinear interactions to guarantee an overall chaotic boundary condition representation. In addition, a nonlinear term was included in all sinusoidal dependences to force a broad spectrum of fluctuations.

The vertical dependence of these resolved-scale fluctuations is a superposition of two functions, one for the unobstructed flow and one to provide additional fluctuations due to buildings upstream of the domain. The unobstructed component is largest away from the ground and below the atmospheric boundary layer. The building component is largest near the tops of the assumed buildings upstream whose general disposition and height is incorporated in the shape of the average inflow urban boundary layer. When this (turbulent) flow field is allowed to evolve by flowing over 0.5 to 1.0 kilometers of actual city geometry, initial inconsistencies are replaced by a more self-consistent flow. Several research issues remain unresolved in this area, both observationally and computationally. So deterministic\textsuperscript{xx} and other\textsuperscript{xxi} approaches to formulating turbulent inflow boundary conditions are being investigated.

2.2 Turbulent Stochastic Backscatter

The spatial and temporal distribution of subgrid-scale (SGS) viscosity is a distinct feature characterizing the ability of different LES models to capture the underlying unresolved physics, ranging from purely dissipative scalar to tensorial scale-similarity models. An overall positive SGS viscosity implies that energy is transferred from resolvable flow structures towards small, unresolved scales via a cascade process (outscatter). Conversely, a negative SGS viscosity implies that energy is overall transferred in the opposite direction by a reverse cascade process, i.e. backscatter. Backscatter can become important in complex geometries such as these when appreciable turbulent kinetic energy may be present in the unresolved scales. Backscatter, both systematic and stochastic, can occur at select wavelengths and for certain nonlinear triads of modes even when the overall cascade corresponds to outscatter. Modeling how the unresolved features of the flow contribute to the large scales through this stochastic backscatter process presents a difficult challenge: how are these effects to be predicted based on the resolvable scale information?

Because of the anisotropic features of the implicit SGS modeling incorporated,\textsuperscript{xxii} MILES offers an effective approach for the simulation of the inherently inhomogeneous turbulent
flows in complex CT geometries. This SGS modeling is not purely dissipative, and some degree of desirable systematic backscatter is actually incorporated implicitly in MILES. Historically, additional (explicit) backscatter effects have been modeled by incorporating suitable source terms in the actual flow equations being solved. The approach used here has some points of contact with the work by Leith, in which stochastic backscatter was modeled through source terms in the momentum equations, and unresolved SGS information was parameterized in terms of a conventional Smagorinsky SGS model. The approach used here also prescribes such source terms, but takes advantage of the flux-limiter information computed by the FCT convection algorithms to determine where SGS backscatter information effects are strongest and must be supplied.

When the FCT algorithm detects structure in the flow that it “knows” cannot be resolved on the grid, only a fraction of the anti-diffusion flux can be applied. The fraction of the flux that cannot be used is an explicit estimate of this unresolved flow and is coupled on the grid scale to the specifics of the fluid dynamic convection. FAST3D-CT uses these “stochastic backscatter fluxes” by pseudo-randomly perturbing the resolved flow velocity in each cell by an amount proportional to the unused flux velocities. The unused high-order momentum flux is accumulated at each grid point during the direction-split convection stages of the integration. This backscatter source is measured in terms of its absolute value summed over all three directions for each timestep and suitably normalized by the density, i.e.,

\[ \eta = \sum (1 - \Gamma) \left| \rho v'_j - \rho v'_{j3} \right| / \langle \rho \rangle . \] (1)

Examples of typical distributions of the quantity \( \eta \) in the context of a representative FAST3D-CT urban flow simulation are reported in Patnaik et al. In some geometries, these additional grid-scale fluctuations break symmetries and initiate three-dimensional instabilities via stochastic backscatter that otherwise would have to grow up from computer round-off. Physically they also transport small particles and droplets to material surfaces because of unresolved turbulence even though the resolved flow field has a zero velocity normal to the walls. This means that particles and droplets can deposit on a ceiling as well as the floor. Finally, the numerical limiting of the imposed stochastic fluctuations, caused by the nonlinear flux limiter, provides a small additional macroscopic (resolved scale) transport right where the FCT algorithm has detected subgrid structure. Each of these expected realistic effects requires further theoretical analysis and careful calibration by experiment.

### 2.3 Tuning the Implicit SGS model for Urban Street Crossings

Historically, flux-limiting (flux-correcting) methods have been of particular interest in the MILES context. The properties of the implicit SGS model in MILES are related to the choice of flux limiter, high- and low-order schemes, and specifics of the implementation of the algorithm. This corresponds to choosing/adjusting an (explicit) SGS model in conventional LES. An approach using the freedom here to control unwanted numerical diffusion through appropriate choice of low order transport algorithms is now discussed.

In our simulations of urban areas, a typical grid resolution is 5 to 10 meters. While this resolution is adequate to represent the larger features of the city, many of the smaller features
are resolved with only one to two cells. This is true of smaller streets found in cities, which are about 20 m wide. Alleyways are even smaller. These smaller streets, represented by only one or two cells in our computations, put a tremendous demand on the numerical convection not to diffuse and retard the flow. By using rough-wall boundary conditions instead of no-slip boundary conditions, the flow can proceed unhampered down a street only one cell wide. However, if there is another street intersecting the first, it was found that the flow tends to stagnate at this intersection. The problem only occurs when dealing with streets which are 1–2 cells wide and not with wider streets. After careful inspection, it was determined that this problem arose due to the form of the diffusion term in the low-order solution in the standard FCT algorithm, LCPFCT, used in the FAST3D-CT code.

The traditional low-order component of FCT introduces numerical diffusion even when the fluid velocity goes to zero (as in the cross street). In normal situations, the flux limiter is able to locate an adjacent cell that has not been disturbed by the diffusion in the low-order method and is able to restore the solution to its original undiffused value. However, when the streets are 1–2 cells wide, the region of high velocity is diffused by low-order transport and there are no cells remaining at the higher velocity. Thus the flux limiter cannot restore the solution in these cells to the original high value.

A solution to this problem is to change the form of the diffusion in the low-order method. In LCPFCT, The algorithmic diffusion coefficient for the low-order scheme is given by \( \nu = \frac{1}{6} + \frac{1}{3} \epsilon^2 \), where the Courant number is \( \epsilon = |U| \Delta t / \Delta x \). Note that \( \nu \) does not go to zero even when \( U \) goes to zero (as in the cross street). The simplest less-diffusive low-order algorithm which ensures monotonicity is the upwind method previously used in the formal MILES analysis (e.g., Fureby, Grinstein & DeVore 2005) for which the diffusion coefficient is given by \( \nu_{\text{upwind}} = \frac{1}{2} |\epsilon| \), which has the desired form for \( \nu \). When the diffusion coefficient in the low-order component of FCT is replaced by \( \nu_{\text{upwind}} \), the flow no longer stagnates at the intersection of streets. With this modification of the low-order method, the global properties of the transport algorithm were altered sufficiently to address this problem peculiar to under-

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Figure 2: A, (Left): Contaminant dispersion at ground level for release close to Chicago River using LCPFCT (conventional low-order method). B, (Right): Contaminant dispersion using modified low-order method.
resolved flows in urban areas. This approach also has the added advantage of retaining the 4th order phase properties of the high-order convection algorithm. In practice, the particular choice of low-order scheme is used only for the momentum equations; the usual low-order scheme is used for the mass density convection, since the density is almost constant everywhere. Lowered numerical diffusion in the cross-stream direction and consequent lowering of numerical diffusion overall allows for significantly larger predicted lateral contaminant spreading and for faster downstream plume propagation. Comparative results are shown above in Figure 2a-b.

3 URBAN SIMULATION MODEL VALIDATION

Establishing the credibility of the solutions is one of the stumbling blocks of urban CFD simulations. The goal of validating a numerical model is to build a basis of confidence in its use and to establish likely bounds on the error that a user may expect in situations where the correct answers are not known. Validation with experiments requires well-characterized datasets with information content suitable to initiate and evaluate unsteady simulation models as well as the cruder steady-state models. Unfortunately, current full-scale field studies do not provide all this information: the data acquired is typically too sparse to fully characterize the flow conditions; the number of trials is limited; and trials cannot be repeated under the same conditions. Two possible validation approaches are to: 1) compare urban flow simulations with carefully controlled laboratory-scale wind tunnel experiments, and, 2) carry out detailed comparisons with actual urban field experimental databases as they become available.

3.1 Benchmarking with Wind-Tunnel Urban Model Data

Figure 3: USEPA Meteorological Wind Tunnel: 3-d Array of Buildings. Courtesy, Michael Brown, LANL.

Comparisons with laboratory measurements of flow and contaminant over a simple urban model were made to evaluate and validate the ability of FAST3D-CT to model contaminant transport. Brown et al. measured velocity distributions and tracer concentrations associated with the flow over an array of cubes in the USEPA wind tunnel facility (Figure 3) under controlled conditions. The experiments were conducted in an open-return wind tunnel, with a working test section of length 18.3 m, width 3.7 m, and height approximately 2.1 m. The
wind-tunnel experiment simulated a neutrally stratified atmospheric boundary-layer flow over an array of buildings. The array consisted of 7 x 11 cubes (0.15 x 0.15 x 0.15 m) with one cube-height spacing between cubes. The reference velocity at one cube height is 3 m/s. These datasets provide high quality, spatially dense (but not time-resolved) data. In addition to velocity data, the measured volume fraction data of a \( \text{C}_2\text{H}_6 \) tracer released continuously at the centerline just behind the first cube was also reported. The laboratory profiles used as basic reference for the FAST3D-CT model benchmarking purposes were measured in the vertical symmetry plane of the building array (Figure 4).

Figure 4: Instantaneous distributions of the tracer concentration at the 2cm-height plane; release occurred at a location behind the first cube in the vicinity of the centerline plane; flow direction is from bottom to top.

Previous reported studies used the USEPA wind-tunnel data to test flow simulation models but did not address their effects on CT. One such study\(^{\text{xxxi}}\) of this data used the HIGRAD code, which is used to predict the evolution of atmospheric phenomena. HIGRAD is second-order in time and space and uses a Smagorinsky type or one-equation turbulent kinetic energy based sub-grid closure. Advection is done with the MPDATA scheme. These simulations reproduce the mean longitudinal velocity, including the recirculation patterns in the canyons behind the blocks. The turbulent kinetic energy is modeled well, except for some under prediction in the canyons. Another study\(^{\text{xxxi}}\) modeled the USEPA wind-tunnel experiment on the cube array using a RANS STREAM code. The Kato–Launder model was also used as an alternative to the standard Jones and Launder model. The agreement between the predicted mean velocity profiles and the experimental data is generally very good, with the greatest discrepancy occurring in the recirculation zone immediately downstream of the leeward face of the array. This study indicates that a RANS model is sufficient to predict the mean flow
features.

Table 1 summarizes the various runs performed with the FAST3D-CT MILES model. Baseline simulations were carried out on a 371x350x60 mostly-uniform grid (R1), with 1 cm resolution (corresponding to 15 cells per cube height). It is important to note here that the resolution considered is on the fairly-coarse side, if simulations of flow over a single (surface-mounted) cube are performed. On the other hand, this resolution is representative of what we can afford to resolve practically in urban simulations relative to typical building dimensions.

<table>
<thead>
<tr>
<th>Run</th>
<th>Cube Array?</th>
<th>Inflow Fluctuations?</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>R4</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>R5</td>
<td>Yes</td>
<td>No</td>
</tr>
</tbody>
</table>

Table 1: Runs performed with the FAST3D-CT MILES model. Runs 2 and 3 omitted for brevity.

The inflow velocity consisted of a mean profile and superimposed fluctuations prescribed at $y=-0.5$ m (the front of the first cube is located at $y = 0.0$, see Figure 4). Including some finite-level fluctuation component at the inflow turns out to be crucial as will be shown further below. The deterministic model of wind fluctuations discussed above was included as part of the inflow boundary conditions (at $y=-0.5$ m). The strength of the model velocity fluctuations was calibrated to match the experimentally observed $rms$ values at $y = -0.225$ m. Agreement was achieved visually by adjusting amplitude, spatial wavelength and temporal frequency of the imposed wind fluctuations in the unsteady-wind model in FAST3D-CT. This approach provided a practical approximation to the turbulent inflow boundary condition specification problem (consistent with the available laboratory data). However, the actual fluctuation modeling and calibration is inherently difficult, given that there is no unique way to prescribe such fluctuations based on the available mean and standard deviation of the velocity components. In particular, it is well known that a simple inflow velocity model based on white noise perturbations is not adequate to emulate large-scale unsteadiness.²²

![Figure 5: Average $rms$ streamwise velocity fluctuation profiles upstream of the first cube, at the matching](image)
location \((y = -0.225)\). Note that the cubes enhance fluctuation levels upstream.

Typical instantaneous distributions of a simulated tracer concentration are visualized in a horizontal plane at the 2-cm height as shown in Figure 4. The simulated tracer modeled the continuous release in the laboratory experiments at a location behind the first cube on the centerline. The comparisons with experimental results shown in Figure 5–8 are located in a vertical plane along the centerline. Figure 5 focuses on the \(rms\) streamwise velocity profiles at the \(y = -0.225\) m location (selected as the location for matching with the experiments). By comparison with a case run with steady inflow conditions (no superimposed fluctuations, R5), the figure clearly shows that the imposed unsteady velocity components account for a large fraction of the velocity fluctuation upstream of the cube array location. Also shown, is a curve for velocity \(rms\) for flow without the cube arrangement (R4) with exactly the same time-dependent inflow boundary conditions as in the simulations with the cube array present (R1). Interestingly, there is feedback from the cube array that adds to the prescribed velocity fluctuations, even at a reasonable distance upstream of the first cube.

![Figure 6: Average velocity in the canyon between the second and the third cube (second canyon). Symbols are experimental results at the corresponding profile location.](image)

Figure 6 shows profiles of the mean (time-averaged) streamwise velocity in the second canyon between cube rows. The mean velocity shows that the simulation model is able to capture the recirculation zone that is formed. In the experiments, the reverse velocity is highest at the first measurement location above the floor. This detail is not well captured by the simulations, especially in the first canyon (not shown). In the canyon between the second and the third cube (second canyon) the simulations show better agreement with the experimental results. In this canyon, the flow is strongly conditioned by the effects of the two rows of cubes upstream, and the relative influence of the assumed structure of the inflow velocity fluctuations is diminished in both in the experiments and in the simulations. Thus, the agreement is better.

Figure 7 compares \(rms\) streamwise velocity fluctuation profiles in the second canyon. Corresponding profiles from the runs carried out with the steady inflow conditions (R5) and
without the cube arrangements (R4) are also shown for reference. The comparison shows the influence of the unsteady inflow on the velocity fluctuations in the canyon between the second and third row of cubes. It is apparent that fluctuations are largely due to the cube array up to about 1.5 cube heights.

Figure 7: Average *rms* streamwise velocity fluctuations in the canyon between the second and the third cube (second canyon). Absence of inflow fluctuations causes significant under-prediction of fluctuation levels.

A comparison of the average tracer concentration profiles from simulations and experiments is shown in Figure 8 at selected stations located in the first three canyons. In all cases, agreement is within a factor of two, with agreement somewhat worse in the first canyon – perhaps reflecting questions in resolving the precise details of the release there. Agreement gets better as we move downstream. This also may occur because the mean velocity and fluctuations agree better as we move downstream. In the simulations, the contaminant is found to rise somewhat higher in the boundary layer, due to higher velocity fluctuations above one cube height in the numerical simulations (Figure 7).

Figure 8: Average concentration profiles are profiles are shown at selected stations located in the first three
The crucial need for a finite level of inflow fluctuations in the simulations is very clearly indicated in Figure 8. Disagreements with the laboratory data are significantly larger when steady inflow conditions (R5) are used. Unsteady fluctuations help condition the flow to enable it to resemble the experimental conditions more quickly downstream. Although the unsteady inflow specifications are important, they are not the main controlling factor once the geometry of the buildings (blocks) have had sufficient chance to influence the flow.

To summarize, we have found very good agreement between the simulations and the laboratory data with respect to the mean velocities, and fair agreement with respect to the \( \text{rms} \) velocities and the tracer concentrations. While agreement could presumably be improved with better calibration of the unsteady component of the prescribed inflow conditions, this calibration is very difficult since it must be based on laboratory (or field) databases, which typically provide single-point statistics, insufficient to characterize the unsteady structure of the flow. However, a particularly valuable insight is that, despite these inherent difficulties in calibrating the inflow boundary conditions, the fluid dynamics within the cube arrangement (i.e., beyond the first canyon) seems to be partially insulated by the flow events in the boundary rows, and thus appears to be less dependent on the exact details of the inflow conditions. The results indicate that reasonable agreement can be achieved with benchmark laboratory data with current MILES CT models using resolutions achievable in actual larger urban contexts. Indeed for cities we find also that a few city blocks of buildings strongly control the flow and the resulting contaminant even when the boundary flow is steady.

### 3.2 Los Angeles Simulations: Validation with Actual Urban Field Data

This section discusses validation of FAST3D-CT, using full-scale field trial data for acute (short duration) releases in urban settings. Rappolt\textsuperscript{xviii} conducted a series of short duration SF\(_6\) releases in downtown Los Angeles, California. The SF\(_6\) was released continuously for five minutes in each trial. Fifty synchronized samplers each took twelve 2.5-minute duration samples for a total experimental trial duration of 30 minutes. The region instrumented was about one kilometer square as shown by the square sampler locations in the panels of Figure 9. Summary results from one of these field trials are presented in shortened form.

FAST3D-CT was run for the same conditions as field trial #8 (as closely as could be determined). Moderate wind fluctuations were specified and the sun angle was set to correspond to mid morning. Eight independent realizations of the experimental release were computed, all taken from the same fluctuating wind distribution. These realizations correspond to releases five minutes apart in a continuously computed flow field. Five minutes was established as an adequate de-correlation time for the computational experiments.

Cross-sections of the contaminant concentration for four of the eight realizations are shown in Figure 9 for the tenth sampling interval, 22.5 to 25.0 minutes. This interval begins 25 minutes after the SF\(_6\) release commenced. The differences from one realization to another are substantial, as evidenced by comparing the four outer panels. Obtaining equivalent multiple realizations of the experimental plumes is not realistically possible at city scale so there is no direct experimental yardstick for comparing a measured to a computed concentration. This is
an acknowledged drawback to field trials. How close two different solutions actually are depends on the natural variability to be expected in the measured contaminant distribution.

By computing multiple realizations, however, we can measure the expected concentration variance computationally and this provides a quantitative yardstick - as long as background conditions, including the wind fluctuations, are well characterized. When impressed wind gusts were turned off completely in the simulations, only a small reduction in the overall computed concentration variability was observed because building vortex shedding still provides turbulence and the boundary layer is unstable from solar heating. In each of the four realizations shown in Figure 9, the set of 50 experimental sampler values (squares) is shown for comparison, colored with the same concentration scale as used for the FAST3D-CT simulations. The blow-up of one realization in the center of the figure shows this comparison of the experimental and simulated values more clearly.

Several of the accepted techniques for comparing a simulation with a single experimental realization were applied to these data. Scatter plots on a log-log scale were constructed for the experimental measurements plotted versus the ensemble of simulated measurements. The main result is that when one simulated realization is plotted against all the others, as if it were the experiment, the scatter plots are very similar to those showing the experimental data against all the realizations. Congruency counts are also used to compare model results with a single field trial. For the eight computational realizations of a baseline simulation (wind from 170° at 3 m/s) the percentage of simulation data points within 20% of the experimental values, within a factor of 2, within a factor of 5, and within a factor of 10 were computed. Table 2 summarizes these results for the field trial and for one
computational realization compared to the full set of simulated realizations.

<table>
<thead>
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<th>Wind 170° @ 3 m/sec</th>
<th>± 20%</th>
<th>0.5 to 2x</th>
<th>0.2 to 5x</th>
<th>0.1 to 10x</th>
<th>Counts</th>
</tr>
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<tr>
<td>Field Trial vs. Simulations (Avg.)</td>
<td>14.5%</td>
<td>39.5%</td>
<td>73.8%</td>
<td>88.4%</td>
<td>1147</td>
</tr>
<tr>
<td>One Realization vs. Simulations (Avg.)</td>
<td>19.5%</td>
<td>53.6%</td>
<td>84.4%</td>
<td>90.0%</td>
<td>1496</td>
</tr>
</tbody>
</table>

Table 2: Congruency counts

About 160 of the possible 600 field trial values were above the experimental threshold of 20 parts per trillion. The total number of counts is about eight times this number because there were eight realizations. It is seen that almost 90% of all observations (center row of Table 2) were within a factor of ten, almost 75% within a factor of five, but barely 40% were within a factor of two. Only about 15% of the number pairs were within 20% of each other. Is this good or bad agreement? Exactly the same congruency count test was performed by comparing the numerical realizations with the ensemble comprised of the set of the remaining seven realizations. In this case we know each of the realizations is coming from the same distribution so the lack of perfect agreement must be attributed to the natural variability from one realization to another. It cannot be the result of any error in the solutions or systematic differences between distributions. A typical result is also given in the bottom row of Table 2. Less than 20% of the number pairs are within 20% of each other, a little over 50% with a factor of two, less than 85% with a factor of five, and about 90% within a factor of ten.

Figure 10: Ensemble concentration distribution functions from eight FAST3D-CT simulated realizations at the location of Sampler 25 in run LA#8. The vertical lines denoted with “E” indicate the experimental measurement
and the short crosshatched bar is the threshold value of 20 parts per trillion used for this comparison.

We conclude that the field trial-to-simulation congruency comparison is nearly the same as the simulation-to-simulation comparison. This means that there is no reason to expect any method could give closer congruency between simulation and experiment, given the differences from one simulated realization to another. Therefore, to gain a more quantitative way to look at this comparison, we began the study the distributions of the simulated values in the ensemble of realizations.

Figure 10 shows the distributions of simulated values at the location of Sampler 25 for six of the twelve sampling intervals (2.5 minutes in duration) beginning with the SF₆ release and continuing for half an hour. Sampler 25 was chosen because it had measured concentrations above threshold for all 12 sampling intervals. The horizontal concentration scale is logarithmic in each small figure, as used in other validation studies because of the wide range of meaningful concentration values. Representative concentration values are collected at the experimental sampling sites in the simulation and at nearby points to build up the relatively continuous distributions shown. The distribution of concentration values collected this way is reasonably gaussian in each time interval after a few minutes have elapsed. Therefore, the mean and standard deviations of the concentrations are also meaningful. This standard deviation approximates the concentration variance needed to compare simulated and experimental values quantitatively.

The center of the black bar in each small figure is at the mean value and the bar extends one standard deviation on either side of the mean for each local distribution. This particular statistical comparison shows that the experimental data taken by sampler 25 has a 50% chance of having been drawn from the simulated distributions because the Chi-Square ($\chi^2$) value is about 13 for 12 degrees of freedom. This particular agreement is not very good because the sampler was very close to the source and thus was above threshold for all 12 sampling intervals.

Most of the other samplers that were above threshold for a few of the sampling intervals showed much better agreement using the $\chi^2$ test. When all samplers and time intervals were taken into account, there were 159 degrees of freedom in the experiment and the baseline simulation ensemble showed a 98% Agreement Probability with field trial #8. This means that this level of agreement can be obtained by chance less than one time in fifty. This analysis approach allows us to derive quantitative (probabilistic) results regarding the validity of the FAST3D-CT simulations.

Furthermore, this quantitative analysis permits parameter variations and system sensitivity studies. It was found that the quality of agreement depends at most weakly on the meteorological wind fluctuations assumed because the buildings generate most of the turbulence from vortex shedding. The inflow wind direction and speed were also varied from the nominal baseline run at 170° at 3 m/s for trial #8. Changing the wind 10° in one direction or increasing the speed by 1 m/s gave unacceptably poor results (37% and 2% probability of agreement respectively). However, changing the wind 10° in the other direction or reducing the speed to 2 m/s gives results in somewhat better agreement with the field data than the baseline simulations (99.7% and 99.9% probability of agreement respectively). By way of
contrast, using only the congruency count test to conduct these sensitivity studies, it could not be determined with any confidence that some case other than the baseline simulation conditions might actually be a better fit to the overall experiment.

In closing, we summarize the Los Angeles field trial validation studies to date. The multi-realization FAST3D-CT simulations with 6-meter resolution seem to be virtually indistinguishable from the Los Angeles field trial data. Naturally occurring variations between realizations can be quite large, due to building vortex shedding, even when inflow wind gusts are absent, but multi-realization CFD simulations provide a way to approximate the missing concentration variability data for scientifically quantitative comparison of data sets. The $\chi^2$-probability approach also gives a sensitive way to approximate unknown parameters as well as to validate time-dependent CFD models.

4 CONCLUSIONS

Physically realistic, time-dependent, urban CT simulations are now possible but still require some resolution compromises due to time and computer limitations. Detailed time-dependent wind field observations at key locations can be processed suitably to provide initial and boundary conditions and, at the least, can be used for global validation. We believe that the building and large-scale fluid dynamics effects that can be captured today govern the turbulent dispersion. However, there is room to improve both the numerical implementation and the understanding of the stochastic backscatter that is being included both implicitly and explicitly. We know that the quality of the spatially and time-varying boundary conditions imposed (i.e., the fluctuating winds), require improvement. Inherent uncertainties in simulation inputs and model parameters beyond the environmental conditions also lead to errors that need to be further quantified by comparison with high quality reference data. Judicious choice of test problems for calibrating models and numerical algorithms is essential and sensitivity analysis helps to determine the most important processes requiring improvement.

Despite inherent physical uncertainties and current model trade-offs it is clearly possible to achieve some degree of reliable prediction. Direct comparisons with field data, e.g. from Los Angeles, provide an intuitively more “believable” validation; however, the sparsity of experimental data makes quantitative validation difficult. Wind tunnel comparisons allow more rigorous validation, but typical available data insufficiently characterized the coherent structures that control dispersion.

The FAST3D-CT simulation model can also be used to simulate sensor and system response to postulated threats, to evaluate and optimize new systems, and to conduct sensitivity studies for relevant processes and parameters. Moreover, the simulations constitute a virtual test range for micro- and nano-scale atmospheric fluid dynamics and aerosol physics, to interpret and support field experiments, and to evaluate, calibrate, and support simpler models.

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6 REFERENCES


