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DEVELOPMENT AND APPLICATIONS OF CFD SIMULATIONS SUPPORTING URBAN AIR QUALITY AND HOMELAND SECURITY

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1. INTRODUCTION

Prior to September 11, 2001 developments of Computational Fluid Dynamics (CFD) were begun to support air quality applications. There is a need to properly develop the application of CFD methods in support of air quality studies involving pollution sources near buildings at industrial sites. CFD models are emerging as a promising technology for such assessments, in part due to the advancing power of computational hardware and software. CFD simulations have the potential to yield more accurate solutions than existing regulatory air quality models because CFD mechanistically is a solution of the fundamental physics equations and include the effects of detailed threedimensional geometry and local environmental conditions. This presentation reviews CFD developments and applications to help understand the dust cloud on September 11, 2001 and transport of potential emissions from "ground zero" over the following weeks at the New York World Trade Center (WTC) area. Much has been learned and developed over the past few years through research and development. Also, these developments are now being extended to support the US Department of Homeland Security's New York City Urban Dispersion Program (UDP). Developments and applications supporting the UDP will be presented in its program reports. Herein developments and applications supporting US Environmental Protection Agency 's (EPA) WTC

* Corresponding author address: Alan H Huber, NOAA/ARL/ASMD, Mail-Code E243-03, US EPA NERL, RTP, NC 27711 Email: huber.alan@epa.com program to understand the transport of potential contaminants are summarized to illustrate what has been done and to characterize remaining challenges. Additional background information on the CFD methods being developed is presented by Huber et al. (2005). There are three major reports being prepared to fully report the work:

- 1. CFD developments and lessons learned during support of EPA's WTC program.
- 2. Model simulations of air dispersion from the collapsing World Trade Center Towers within lower Manhattan during September 11, 2001.
- 3. Model simulations of air dispersion from the World Trade Center within Lower Manhattan during the weeks following the events on September 11, 2001.

Originally the plans were to develop CFD applications under a more modest progression of urban complexity. Rising to the need to study lower Manhattan, which is likely the most complex urban building environment on earth, presented great challenges. By learning to overcome many of these challenges, future more common modeling of air quality in urban building environments should be easier. Overall, the results of CFD simulations can both be directly used to better understand specific case studies as well as be used to support the development of better-simplified algorithms that may be generally applied. The simulations supporting the WTC program will be used for both purposes. CFD simulations are able to include specific details of building structures as well as a range of physical processes that affect atmospheric turbulent boundary layers. Plume dispersion in the absence of buildings is

generally comparable with standard plume dispersion models for point and line source pollutant emissions. The development of CFD methods and applications in urban building environments is critical when it is important to accurately estimate potential human exposures to local sources of a toxic contaminant. In the absence of being able to measure everything we need to know in the field, finely resolved numerical models are necessary to fully understand relationships between local pollutant sources and air concentrations along their pathways to exposure. CFD simulations have great potential for supporting both urban air quality and homeland security studies.

2. CFD SOFTWARE

Our CFD simulations use FLUENT (2005) which is a general purpose computational fluid dynamics code that solves the governing equations for the conservation of mass, momentum, energy, and scalars such as a The code includes multiphase pollutant. models, moving domain models, combustion models, and turbulence models. All these models are important for the WTC related simulations. The US Environmental Protection Agency has a cooperative research and development agreement with Fluent Inc. to evaluate and find best methods for application of CFD to general air quality modeling. These developments are ongoing and have been helpful in providing developments supporting the WTC studies.

Fluent Inc software includes a supporting meshing program GAMBIT to help build and mesh models. FLUENT also works with much 3rd party meshing software. Computational Engineering International (CEI) mesh and Visualization software is also being used to support the WTC studies. The study domain is divided into discrete control volume cells using a computational grid mesh. For this study all mesh interfacing with the buildings and its surrounding volume were resolved to 2 m. Mesh at this resolution is believed sufficient to resolve the important flow and transport processes through the urban street canyons. FLUENT supports unstructured mesh to provide better computational efficiencies by being able to concentrate the grid mesh in volumes where finer mesh are most critical in resolving complex flows. Setting up a CFD model of an urban area

requires a building database. The derived building data can be expected to have some imperfections, which must be eliminated to support domain meshing for the CFD model. Buildings for the New York City studies presented in this paper were developed from a database licensed with Vexcel Corporation. Developing quality mesh for the complex array of buildings found in lower Manhattan has been particularly challenging. Fluent Inc.'s GAMBIT and TGRID meshing software, along with CEI's HARPOON mesher software that works directly with the FLUENT CFD code are being used. The process is much smoother for idealized building shapes where the model may be developed directing though the GAMBIT code using measured dimensions. The mesh and surface/building boundaries are input into the CFD simulation software solver.

Algebraic equations for discrete dependent variables such as velocities and pollutants are derived from the governing differential equations and solved within FLUENT. There are options for both a coupled equation solver using either an implicit and explicit discretization, or a segregated equation solver having implicit discretization. For atmospheric flows the segregated solver using implicit discretization is appropriate and is being used for our studies. The momentum equations are solved, and then a pressure-correction is applied to update the pressure field to support calculation of mass fluxes to ensure conservation of mass. The solutions at each iteration for energy, turbulence and other scalar equations (i.e., pollutants) follow separately. In the implicit discretization for a given variable the unknown value in each cell represented at the cell center is calculated using both existing and unknown values from neighboring cells. Overall the software uses an algebraic multigrid method to solve the resultant system of equations for the dependant variable in each cell. The calculations continue and update all the cell properties until selected criteria for a converged solution is reached. Second order calculations are used for the WTC studies. There are options for obtaining volume face values by applying first-order, secondorder. power-law, and for quadrilateral/ hexahedral grid mesh the QUICK (Quadratic Upstream Interpolation for Convective Kinematics) scheme. There are specific options for pressure interpolation including linear, body-force-weighted, second-order, and PRESTO (PREssure Staggering Option). For

pressure-velocity coupling the options are SIMPLE (Semi-Implicit Method for Pressure-Linked Equations), SIMPLEC, and PISO (Pressure-Implicit with Splitting of Operators). We have not noticed a significant effect among these different choices for our studies to date. For this study PRESTO was used as the default.

The software has options for either steady or unsteady (time-varying) solutions. There are options for a first order and higher order implicit schemes for temporal discretization of the time derivative. To date only steady flow solutions are being evaluated. We have been evaluating solutions for the Reynolds-Averaged Navier-Stokes (RANS) governing equations for momentum. Solutions require a selection of boundary conditions and a model for turbulence. The software has options for the wall (ground surface) boundary conditions and several turbulence models. The law of the wall is presently being applied. For this study the realizable $k - \varepsilon$ (turbulent kinetic energy: k; turbulent energy dissipation rate: ε) turbulence modeling option was used. There are several other $k-\varepsilon$ options that are being evaluated for future application. In the future higher order turbulence closure models including Reynolds Stress Models (RSM) and Large Eddy Simulation (LES) within the framework of unsteady solutions will be applied.

3. ATMOSPHERIC BOUNDARY LAYER

Simulation of the atmospheric boundary layer is critical to modeling plume dispersion. Boundary layer turbulence can be simulated as characterized surface roughness by (characterized by z_0 and surface stress u_*) and surface heat flux (characterized by the Obukhov length L). The "law of the wall" is applied to an atmospheric boundary layer develop oncoming as boundary conditions to the study zone with buildings. Some additional evaluations and refinements are ongoing to improve performance, especially, with heated No work has yet been started to surfaces. evaluate strongly stable stratified flow. Having a model for stably stratified flows may not be critical for many urban areas because of the strong turbulent mixing induced by the buildings and the capacity of urban areas to retain heat. Additional information about these ongoing developments is covered by Huber et al. (2004) and Tang et al. (2005). Near thermally neutral boundary layers are assumed for the WTC cases studied to date and discussed herein.

4. CFD APPLICATIONS SUPPORTING EPA'S WTC PROGRAM

Following the collapse of the New York World Trade Center (WTC) towers on September 11, 2001, New York State and Federal agencies initiated numerous air monitoring activities to better understand the ongoing impacts of emissions from the disaster. The collapse of the WTC towers and associated fires that lasted for several weeks resulted at times in a noticeable plume of material that was dispersed around the Metropolitan New York City (NYC) area. А study of the estimated pathway, which a plume of WTC material would have likely followed was completed (Gilliam et al. 2005: Part I and Part II) support EPA's 2002 initial exposure to assessments. In this study, the CALMET-CALPUFF model was applied to examine the general spatial and temporal dispersion patterns over the NYC metropolitan area. This approach not able to resolve the near-source is concentration distribution accurately in lower Manhattan. The 3-km area surrounding the World Trade Center site is an extremely nonhomogeneous surface so similarity relations do not apply well. A complex urban canopy flow is the dominant factor in pollution dispersion within the city and can only be modeled with a suitable model that can explicitly resolve the building influences.

CFD applications have been under development to reconstruct the dust/smoke plume following the events at the New York City World Trade Center on September 11, 2001. The scope of the reconstruction has 3 stages:

a) the plume following airplane impact but prior to the collapse of the towers

b) during and immediately following the tower collapse

c) the days following September 11 when emissions from "ground zero" could be significant.

Working CFD simulations have been developed for each topic and are undergoing evaluation before final production simulations are completed. Preliminary studies are being done over a limited area surrounding "ground zero". While the preliminary studies are for a limited area they do provide best solutions for the critical neighborhood surrounding "ground zero". These developments can be run using computing resources at the EPA. Final production will include the whole area South of Canal Street (400+ buildings). These computations will require resources exceeding the capacity at EPA. Cooperation has been developed allowing access to larger computing systems at the Argonne National Laboratory and the Army Major Shared Resources Center in order to complete this work.

A summary of the preliminary studies is presented and evaluated in the following sections. The goal of the final full production is to extend these developments to simulate transport and dispersion of potential pollutants through lower Manhattan to where interfacing with the Metropolitan scale models could be applied.

The zone of buildings for the preliminary studies extends from the Hudson River eastward including Broadway. The zone extends northward and southward for several blocks surrounding the WTC site to support the development of simulations with oncoming wind the northwest through southwest. from Buildings from the licensed Vexcel Corporation database were prepared for application with the CFD software. The computational mesh for the CFD model domain was developed with 2 m resolution surrounding the buildings and progressively courser resolution away from buildings. Figure 1 presents an example of both surface and volume mesh from the lower Manhattan studies.

4.1 Prior to the tower collapse

After the airplanes hit the towers extensive fire and smoke developed inside the towers. The smoke escaped through open areas on the sides of the building and rose upward along the outside of the towers. Photographs of the burning towers were examined to identity the location and size of these building openings. An initial ambient plume temperature of 500 K was assumed, and a range of settings for the volumetric flow rate has been examined. NNW winds were observed during this period. Figure 2 shows an example of the CFD simulation winds on a plane through the North Tower. Figure 3 shows the simulated plume characterizing the smoke escaping the North Tower. The simulated plume is comparable with what can be observed in photographs taken on September 11, 2001. Further work on simulating this stage will follow after completion of the more critical stages during and following the collapse of the towers.



Figure 1. This example shows one vertical profile of the interior mesh and all of the face mesh.



Figure 2. Example profile of CFD simulated wind vectors on a plane through the North Tower. The blue color shading identifies areas of lower speed.



Figure 3. Example isosurface of the smoke plume from the North Tower.

4.2 During the tower collapse

The airflow around the WTC towers during the collapse is determined by three factors

- the wind around the buildings
- the motion of the tower
- air and smoke that squeezed out of the building as individual floors were collapsing and discharged into the surrounding air.

To simulate the collapse (the motion) of the tower FLUENT's Moving Deforming Mesh capability (MDM) is being used. The MDM capability allows defining arbitrary motions for surfaces and zones. Only the deformation of the outer shape of the tower needs to be included. Interior deformations can be neglected in this analysis. As such, the collapsing tower is represented by a piston approaching the ground surface. 90 to 95 % of the volume of the WTC was air and smoke; the remaining volume contained solid material. At the same time, solid glass particles, dust from concrete and other material, and larger structural components were generated and discharged with the air and smoke.

Solid particles can be tracked through the domain based on a Lagrangian description of the equations of motion and the energy equation solved by FLUENT. Particles can be released from any point in the domain with a specific initial mass flow, size, velocity, direction and temperature. A combination of different particles

can be used to represent all the suspended solid material.

Metropolitan scale winds for September 11, 2001 were modeled by Gilliam et al (2005, Part I) and applied as the inlet boundary condition for the CFD model domain. The winds were from the NNW during the period of the collapsing towers.

The acceleration of the collapsing floors is being assumed constant at near freefall, 9.8 m/s², based on reported times. The collapsing rooftop reaches a velocity exceeding 40 m/s, which results in comparable wind speeds near the base of the tower. This supports observations of winds sufficient to turn over parked emergency vehicles near the collapsed tower. The final height of the compressed tower is assumed to be 19 m based on the observed rubble pile. Figure 4 is an example picture of the collapsing tower with the depicted smoke outlining the building material plume squeezed from the tower while it is collapsing. The tower collapse is initiated at Time (T) = 0. In the CFD simulation smoke is a fluid representing crushed building materials that remain suspended in the air squeezed out of the building. A range of fluid density for smoke is being evaluated. Final model parameters for simulating the collapsing tower are being based on examinations of photographs and videos.



Figure 4. Example display of a North Tower collapse simulation (Time = 8 s).

A large amount of momentum and kinetic energy is generated by the collapsing tower. The flow impingement and ground reflections create vortex structures. These vortex structures are responsible for further dispersion of gaseous constituents and particulate matter. Smoke and particles are suspended into the flow as material is discharged from the collapsing tower. Large pieces of material naturally fall and remain near the collapsed tower. It is the small particles that remain suspended and are transported away from the collapsed tower. Studies are ongoing to refine parameters of the CFD set up to best match reported observations before final production.

4.3 Following the tower collapse

There are two periods of interest following the collapse. Immediately following the collapse of the towers material was transported and dispersed throughout lower Manhattan. For weeks following September 11, 2001 there were potential emissions of pollutants from the rubble pile at "ground zero" as material was removed and as fires flared up. During these periods any pollutant emitted from this area was carried away by the winds passing through the complex urban street canyons. During some periods winds are very light near the ground and any emissions can become elevated due to vertical motions created by the "chimney effect", especially if there is some added solar heating. The wind patterns through lower Manhattan street canyons are very complex and do not follow the usual straight line pathways of the There is no simple model prevailing winds. which can provide reliable information on the wind patterns which carry pollutants through these complex urban environments. Once potential emissions from "ground zero" pass through lower Manhattan they should generally follow along the pathway of the prevailing winds.

4.3.1 Immediately after tower collapse

A large amount of momentum and kinetic energy is generated by the collapsing tower. During the collapse potential energy is being converted to kinetic energy. The flow impingement created by a collapsing tower creates vortex structures which transport gaseous constituents and particulate matter radially outward from the base of the towers. These materials were dispersed though lower Manhattan into the surrounding Metropolitan area. Nearby the collapsed towers the material was transported radially in all directions. However, this radial impulse created by the collapsed tower is short lived and soon the material is caught by the prevailing winds. Understanding the material transport during this period is of critical interest to supporting assessments regarding which areas of Metropolitan New York City may have been potentially impacted during September 11, 2001.

Figure 5 presents an example pattern of particle transport at the end of the collapse (Time-12 s) for three different sizes, each having equal numbers released from each tower floor.

Red: 10 cm Yellow: 1 cm Blue: 0.01 cm

Note that some of the smaller (lighter) particles remain suspended following the collapse while most of the larger (heavier) particles fall to the ground. The image of the tower remains visible as a column of smoke, as observed in photographs taken immediately following the tower collapse. Near the ground even the heavier particles are transported out from the base of the building due to the short-lived near 30-40 m/s winds immediately following the collapse. The CFD simulations appear to be matching observations. Performance for a wide range of particle sizes and densities are being evaluated. Being able to simulate such tragic events provides some ability to understand without ever having to test - since repeating these types of events is not an option.



Figure 5. Example display of three sizes of particles with equal number released from each floor of the collapsing of the North Tower (Color Scale: meters).

Figure 6 presents a time sequence of the smoke and small particle plume following the collapse of the North Tower. The suspended particles are concentrated in the central core of the plume since they disperse less rapidly relative to the smoke as outlined by the grey shading. Particles released near the ground or that otherwise have time to come into contact with the ground or building surface are modeled to lose 90 percent of their momentum. A close look at some of the surfaces near the collapsed tower will find deposited particles. A range of values for momentum reflection at surfaces is being evaluated including the assumption that all particles will stick once making contact with a surface. Performance for a wide range of particle sizes and densities is being evaluated. The goal is to complete simulations for the full period following the collapse that are necessary to simulate the patterns of particles (dust) observed to have deposited before the cleanup began.

Figure 7 presents the near surface (H= 5 m above ground) wind field at three modeled time steps. Immediately following the completion of the collapse (T= 15 s) an impulse radiating out from the tower base is shown. As stated above there are computed velocities in the 30-40 m/s range but they are short lived. The generated vortices cannot be depicted in these figures. It is the 3-dimenisonal vortices that carried the smoke and particles outward into the streets of lower Manhattan. The main features of these vortices are being captured by the CFD simulation. In Figure 7 the flow field at T=115 s is very close to the steady-state simulation and not being affected by the collapse. For the intermediate time (T=40 s) effects from the collapse are noticeable in the block surrounding the collapsed tower. The wind field affected by the collapse is critical to the initial transport of the smoke and particles. The plume moving upwind farther than the wind field would suggest is due to its being heavier than air. Test runs are ongoing to find the setup that best replicates the visual observations that were photographed and video recorded.

4.3.2 Weeks after tower collapse

After the initial minutes following the collapse of the towers the smoke and particles are transported by the prevailing winds through lower Manhattan. A CFD model has been set up for this period and is being evaluated in

comparison with measurements from EPA's wind tunnel model study (Perry et al. 2004). When possible the first step for evaluating a new CFD model should be comparison to wind tunnel model measurements since the wind tunnel is a controllable environment. The wind tunnel model domain includes all the buildings in lower Manhattan South of Canal Street. The building geometry for the wind tunnel physical model was constructed to match the same Vexcel building database used to construct the CFD model. The present CFD model domain is the preliminary model domain which is a smaller area than used for the completed wind tunnel model study. Present common area for both models includes the critical area surrounding "ground zero" and includes six of the wind tunnel locations where there were vertical profiles of the wind velocity and turbulence. The areas common to both models are generally viewable as part of Figure 8. The buildings seen through the transparent color map are common. The inlet boundary conditions for mean velocity and turbulent kinetic energy (TKE) for the CFD model were set to match wind tunnel model measurements near the beginning of the study domain.

Figure 8 presents a map of TKE from the CFD model at height z=100 m above the ground surface.

$$TKE = \frac{1}{2} \left(\overline{u'^2} + \overline{v'^2} + \overline{w'^2} \right)$$

where u', v', and w' are the three directional standard deviations in wind speed.

The present CFD simulation uses a $k \cdot \varepsilon$ turbulence model which solves for total TKE assuming turbulent viscosity is isotropic. In the wind tunnel model and in the atmosphere, the generation of TKE due to mean flow gradients may be different depending on which mean flow velocity gradients are being considered. While atmospheric turbulent viscosity is known to be anisotropic applications of $k \cdot \varepsilon$ turbulence models are believed to be sufficient for simulating plume dispersion. This is a first level approach for CFD applications since substantially more computing resources are needed for higher order turbulence models.

The CFD model resolution is 2 to 5 m and through interpolation all solved variables may be estimated at any specific point location. TKE



Figure 6. Example visualization of outer boundary of smoke and of a particle cloud immediately following the building collapse.



Figure 7. Surface winds immediately following the building collapse.



Figure 8. CFD model TKE on a horizontal plane at z=100 m for Westerly winds (Port #'s mark locations for vertical profiles).



a) Port 200





e) Port 206

Figure 9. Comparisons between CFD model and wind tunnel model vertical profiles of horizontal wind. speed and direction, vertical wind speed, and TKE for Westerly winds case.

presented in Figure 8 shows high areas of production on the leading edges of buildings which are transported downstream. There are some areas in the shadow of buildings where TKE is low which is due to the area having very low velocity. Overall, there appears to be a trend of decreasing TKE downstream through the domain. This can be due in part to the choice of CFD boundary conditions and is continuing to be explored. Note that most of the locations where wind tunnel model profiles of winds were measured are in a zone with gradients in TKE and near the outlet end of the CFD model domain. Specific comparisons between CFD and wind tunnel model data may be sensitive to small changes in location.

Comparisons between the initial CFD model and the wind tunnel model are being used to evaluate CFD model performance and guide refinements before final production of CFD simulations of the larger whole domain of lower Manhattan. Figure 9 presents comparisons of horizontal wind speed, horizontal wind direction, vertical wind speed, and TKE at Ports 200. 206. 207, 208, and 209. Note that degree on the wind direction scale represents direction toward which the wind vector points (West winds are reported as 90 degrees). This is for a Westerly winds case. The horizontal wind speed and direction appear to be matching well. There are some zones with strong wind shear and which are well matched. There are significant differences near the ground for Port 208. The vertical wind speed also appears to be well matched. The comparisons for TKE are mixed with a tendency for the CFD model to underestimate (further discussed below).

Matching TKE between the two models is more challenging than matching velocities. The mean velocity is generally matched by matching wind profiles characterizing vertical distribution of mass flow which is conserved in both models. Matching TKE is challenging for two main reasons. First the wind tunnel model uses a technique of spires and surface roughness to rapidly develop an atmosphere-like surface boundary layer. While the mean velocities may have stabilized in the wind tunnel study zone, turbulence is likely still evolving with turbulence production not in balance with turbulence dissipation rate. The CFD model needs initial values for and solves for turbulence dissipation rate which is not something that is easily measured as part of wind tunnel studies. This

issue can be overcome through some trial and error applications of the CFD model. Some work toward this goal has been done but more remains. The second challenge is for the CFD to use a fine enough mesh and turbulence model to fully simulate the physical conditions in the wind tunnel including the boundary layers on the building surfaces. Present CFD applications are using a k- ε turbulence model as discussed above. The goal here is to demonstrate that the present application study using a $k-\varepsilon$ turbulence model and 2 m grid resolution near the building surfaces is sufficient. A complete collaborative study between the CFD modeling group and the wind tunnel modeling group is ongoing and will soon be fully reported. For this presentation a summary of progress on this evaluation to date is provided. Modifications to the present CFD set up are being examined to identify how best to improve the simulations of TKE.

Not reported here is progress on simulating emissions from the "ground zero." There have been some test cases of emissions from the rubble pile and resulting patterns of concentrations appear reasonable. Now specific emissions studies are being set up to match the wind tunnel model studies of emissions. Figure 10 shows the geometry representing the rubble pile at "ground zero." It was constructed from the LIDAR observations reported by the National Geodetic Survey. Some smoothing of sharp spikes in the observational data was necessary to get a working CFD model. This represents how the pile appeared before there was major removal. Naturally, following weeks of removal the pile began to take new shapes. Potential emissions were most significant during the first few weeks so there have been no further refinements of pile geometry.



Figure 10. Surface model geometry of "ground zero" (derived from National Geodetic Survey LIDAR data).

5. CONCLUDING OVERVIEW

While setting up working models of the extremely complex building environment for lower Manhattan has been a challenging exercise there have been many lessons learned that will make it easier to set up similarly complex urban environments in the future. Understanding the pathway of toxic air pollutants from source to human exposure in urban areas finds immediate application for both routine air pollution assessments and in support of Homeland Security. While problem-specific applications of CFD may not be feasible in "realtime" support, it does seem that there is a major role for CFD simulations to be run for developing databases that could be tabularized for supporting real-time applications or reducedorder models. Also, CFD simulations should have a significant role in supporting field studies in urban environments, which should then be used to develop performance verification. Future research and development including CFD simulations should lead to the development of reliable simplified models (or databases) as needed to support emergency responders. In any case, CFD simulations can be used to support necessary post-event analyses presentation.

To date the project has focused on RANS steady-state solutions and the k- ε turbulence models. This is being extended to include unsteady solutions and higher order turbulence models. Detailed technical papers will be prepared as this project reaches final production.

CFD modeling has emerged as a promising technology for simulating wind flow and pollutant dispersion in urban microenvironments. In order to have confidence in such models, thorough evaluation and consideration of their abilities to represent dispersion mechanisms are required. The application of CFD simulations should work hand-in-hand both with wind tunnel model and field measurements. Confidence bounds for the application of CFD simulations need to be developed. All the measurements one can afford should be collected in critical situations for supporting urban air quality and homeland security; however measurements alone will never be sufficient for planning well or understanding what may have happened during an event. There is a need to demonstrate how to reliably and accurately utilize CFD simulations

for urban air quality and homeland security applications.

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