A FRAMEWORK FOR FINE-SCALE COMPUTATIONAL FLUID DYNAMICS AIR QUALITY MODELING AND ANALYSIS

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1. INTRODUCTION

High-fidelity fine-scale Computational Fluid Dynamics (CFD) simulation of pollutant concentrations within roadway and building microenvironments is feasible using high performance computing. Unlike currently used regulatory air quality models, fine-scale CFD simulations are able to account rigorously for topographical details such as terrain variations and building structures in urban areas as well as their local aerodynamics and turbulence. Thermal heat fluxes may be added to terrain and building surfaces to simulate the thermal atmospheric boundary layer and their influences on pollution transport and dispersion. The results of these 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 for adoption into other modeling systems.

This paper discusses a framework for fine-scale CFD modeling that may be developed to complement the present Community Multi-scale Air Quality (CMAQ) modeling system which itself is a computational fluid dynamics model. A goal of this presentation is to stimulate discussions on what is "Computational Fluid Dynamics" modeling and how can it evolve to support the critical needs for modeling human exposures to air pollutants. Related mathematical equations and their solutions cannot begin to be covered herein and thus no equations are presented.

2. BACKGROUND

Modern day CFD has evolved much since Sir Isaac Newton's physical equations and the evolution of the Navier-Stokes equation for fluid flow due to advancing computational hardware and software.. The Navier-Stokes equation is the general basis for all CFD applications, for example, from weather prediction to vehicular aerodynamics design. The Navier-stokes equation is non-linear and any solution will depend on initial boundary conditions. Practical CFD solutions require both simplifying assumptions and numerical approximations. In practice, solutions for specific fluid flow problems result from calculations of a system of fluid flow and conservation equations generally cast as the Navier-Stokes equations.

While reasonable models can be developed for most physical processes in the atmosphere, their application in a numerical model is limited by the grid scale. The Navier-Stokes equations are a deterministic system. Practical solutions require a sub-grid scale model for turbulence. As computer capacities advance the scale where turbulence is modeled can be reduced and the application of higher order numerical methods can presumably support more accurate turbulence models. Understanding turbulence remains one of the greatest challenges in physics. It is very important not to confuse turbulence with randomness that may be produced by numerical solutions due to numerical errors or other model inadequacies.

3. AIR QUALITY MODELING AND HUMAN EXPOSURE.

3.1 Challenge to Relate to Human Exposure Assessment

Air Quality in the ambient environment is strongly influenced by emissions, the physical environment, and the state of the atmosphere influencing transport and dispersion. Pollution concentrations potentially contributing to human exposure may be considered composed of a regional background concentration due to long range transport, regional scale mixing, and specific local microenvironmental concentrations as depicted in Figure 1. Often it is the concentrations within a few microenvironments that dominate a profile of total human exposure. A human is only exposured to what can possibly contact his body.

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Figure 1. Depiction of local microenvironments plus regional background air concentrations.

The science of human exposure assessment in support of health risk assessment to pollution requires concentrations that are both temporally and spatially resolved to estimate direct contact with the human body. Ott (1995) identified four questions that exposure science should address in support of human health risk analysis: a) how many people are exposed? b) what is the level of each person's exposure? c) what are the causes of exposure? d) how can exposures be altered efficiently? Additional overviews on issues linking environmental concentrations to profiles of human exposure may be found, for example, in Özkaynak (1999) and McCurdy (2000). There are challenges for the air quality modeling community for linking concentration to temporal and spatial scales associated with profiles of human exposure relevant to supporting health risk assessments.

3.2 The Present CMAQ Modeling System

The CMAQ model has been designed to approach air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues (Byun and Schere; 2006, 2004). CMAQ was designed to have multi-scale multi-pollutant capabilities so that separate models are not needed for urban and regional air quality modeling. Various chemical and physical processes thought to be important for understanding atmospheric trace gas transformations and distributions are modeled. The CMAQ modeling system links models for meteorology, emissions, and air quality on a common temporal and spatial scale. It produces air quality concentrations resolved at its applied grid resolution. Regional air quality applications are normally applied at grid resolutions larger than 10 km. Urban applications are applied at smaller grid scales but there is a meaningful limit due to the sub-grid scale process models. The present framework of the CMAQ modeling system well supports environmental issues where its grid-averaged concentration is applicable. For example, regional emission control strategies are especially applicable while specific profiles of human exposure concentrations are not. The system may presently be useful for estimating profiles of human exposure for pollutants having course temporal and spatial distributions at or above the grid scale.

3.3 Potential Framework for Interfacing CMAQ CFD with Fine-scale CFD Models

With ever increasing computational capacities the ability of extending or interfacing CMAQ to spatially finer-scales is becoming practical. Finer temporal scales are a greater challenge. Traditionally, fine-scale CFD software uses finite volume numerical method to best accommodate complex geometries and unstructured grids. CMAQ software uses finite difference methods which must use a structured grid. Extending to finer scales is most meaningful where there are significant sub-grid inhomogeneities to the present CMAQ grid scales and where supporting information is available at the finer scales. In principal, the fine-scale finite volume numerical methods can be interfaced with the present CMAQ-type grid system. An extension of CMAQ to already existing fine-scale CFD code with advanced chemistry and physical processes models is envisioned as the complete way to proceed. Further scoping of the related issues is needed and justified to extend CMAQ's capabilities to model human exposure profiles. This challenge is presented now to start the discussions with hope it may lead sooner to a working plan.

An interim alternative to full implementation of an extension of CMAQ to fine-scales would be when needed to run a fine-scale model separate from CMAQ but pass resulting useful information between the two model codes. The larger CMAQ grid scale could be used to form the external boundary conditions for the fine-scale model through driving wind fields and adding background pollutant concentrations for the fine-scale model. Likewise, output from the highly resolved fine-scale model could pass improved local scale winds (and other atmospheric state variables) along with pollutant concentrations generated from internal emissions into the CMAQ model.

Meeting the challenges of extending a CMAQ-like air quality modeling system to fine scales is the natural way to support total human exposure modeling. In rural areas without significant buildings or variation in landuse characteristics, if necessary, more simplifying methods may be applicable. The CMAQ sub-grid may be carefully linked for simple situations with an analytical plume model. For example, applications of EPA's AERMOD (Cimorelli et al., 2005) model on the fine "local" scale may be interfaced with and driven by the wind field from a regional grid model. This should work well where there are only a few significant sources and/or no significant complications due to buildings or other structures influencing pollution transport and dispersion. AERMOD cannot be expected to be applicable within an urban environment. Earlier applications applying adjustments to analytical plume models (for example; Huber; 1988, 1989) found limited success for isolated clusters of simple-shaped buildings.

3.4 Fine-scale CFD Models for Exposure Factors.

Fine-scale CFD models can support the development and application of human exposure factors without interfacing to a CMAQ-type air quality modeling system. This would especially be applicable to the simulation of exposure profiles from sources within the fine-scale model domain. Human exposure models apply human exposure factors principally based on observations of relationships between pollutant concentrations at human contact and concentrations at surrounding points in the ambient environment, often a single neighborhood monitor. The CFD model can be used to develop databases to complement the dearth of exposure measurements and ambient measurements that exist in all urban areas. Measurements from field case studies are more limited than desired to support the development of human exposure profiles. The time has come for field measurements to support the evaluation of fine-scale CFD simulations so there is a reliable model for developing expanded databases to support human exposure assessments.

4. PRESENT EXAMPLES OF FINE-SCALE CFD MODELS AND THEIR APPLICATIONS

The US Environmental Protection Agency (EPA) has a project using FLUENT CFD software to develop applications for urban environments. A goal has been to demonstrate best practices for using CFD as a tool for estimating potential human exposures to local sources of toxic air contaminants in geometrically complex environments. FLUENT (2005) is a general purpose CFD software system with options for developing new and expanded applications through use of user defined functions. Examples of this work can be found, for example, in Huber et al. (2004, 2006) and Tang et al. (2006). To date the project has focused on steady-state solutions to the Reynolds-Averaged Navier-Stokes (RANS) equations with the widely used k-ε turbulence models. Ongoing developments are being extended to include unsteady solutions and higher order turbulence models as well. In any case, the fine-scale RANS models are most appropriate for interfacing with a CMAQ-like air quality model. Much has been learned and we are now ready to begin to determine how best to interface with the framework of a CMAQ-like larger grid modeling system.

A few example study cases are presented below to show the high-fidelity that is presently possible. While there is no thermal heating for these cases, methods have been developed for adding heat fluxes to any grid face or volume. These examples show that urban building environments may be specifically modeled within 1-4 km^2 at very fine scales to sufficiently resolve the significant features in the wind field to support simulation of steady-state pollution transport and diffusion distributions. Special source emissions and effects from moving vehicles may be added to these steady-state simulations. There is a growing literature with similar examples. For example, Kondo et al. (2006) demonstrates application of a multi-scale CFD model. Multi-scale CFD for this application is a nested regional meteorological model at 3 grid resolutions and a separate fine-scale CFD air quality model to estimate concentrations in the neighborhood of a major roadway. The state-of-art and science for applying fine-scale CFD models is rapidly growing. Just a taste of what is possible could be provided herein.

Test cases have been developed for Manhattan, NY. The building and terrain geometry was licensed from Vexcel Corporation. Test cases were run with boundary inlet winds set at S(180), SW(225), W(270), NW(315), and N(360). The 20 million cell solution is rich with fine-scale detailed structure in the wind distribution. Figure 3 shows a nearly 4 km^2 building domain and surface grid placed on a larger model domain including terrain.

A 20 million cell unstructured grid was constructed with 1-2 m size near the building surfaces to larger than 10 m far away from the buildings within a 1 km deep atmosphere-like boundary layer. The domain is oriented as depicted by the 3-axes displayed in Figures 3 and 4 (red arrow pointing East, green arrow pointing North). Figure 4 shows vertical velocity on several horizontal slice-planes through a volume study zone (defined as a 1.8 km by 0.8 km horizontal area through the full 1 km vertical domain depth). Vertical velocity is minimal near the top of the 1 km deep domain (not shown). Vertical velocities were observed to be generally largest in the windward half of the study planes or specifically near tall building faces such as shown near the tall Empire State building.

The patterns of horizontal winds near the surface have winds oriented in all directions making it hard for an isolated local bystander to estimate the boundary wind direction or even which way the winds would blow on the neighboring block. Simulations are being examined to determine “bulk” flow parameters. The horizontal wind velocities were area-averaged at z= 5, 10, 25, 60, 85, 110, 160 and 210 m above ground level (AGL) and compared with the inlet boundary conditions. Figure 5a shows the urban canopy effect. At 210 m (most buildings are lower) the wind speed nearly equals the inlet value accept for the N case. The average wind direction is strongly influenced below 25 m. This is very useful information for supporting the development of reliable site-specific urban canopy models.

Figures 6 and 7 show that there are variations in the wind patterns due to influences from specific buildings. There tends to be downward mass flow along windward building faces and upward mass flow along leeward building faces. Pollutants are naturally transported within the wind fields. Figure 7 shows how the shape and direction of a pollution plume may vary within the same wind field. The visualized plume represents the outer boundary from point emissions. Plume differences have been found to be significant for even minor changes in the emission location.

A CFD model of a 1 km^2 urban residential Baltimore, MD neighborhood with building and street geometry has been developed to support a study of human exposure from local street emissions. The digital model has sub-meter accuracy based on analyses of aerial and ground photographs. Methods have been developed to simulate time-averaged roadway turbulence and

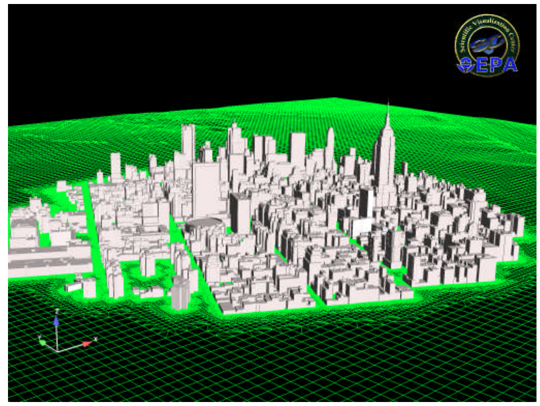


Figure 3. Model domain with surface grid.

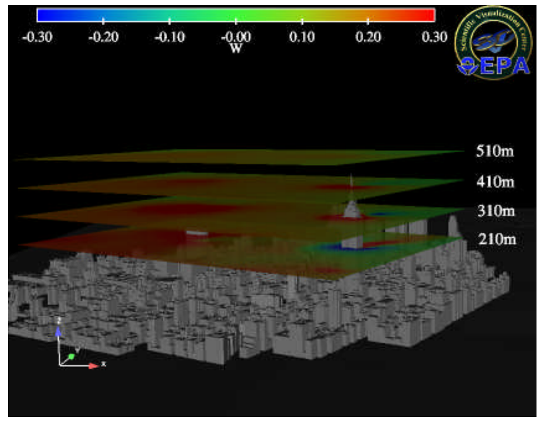
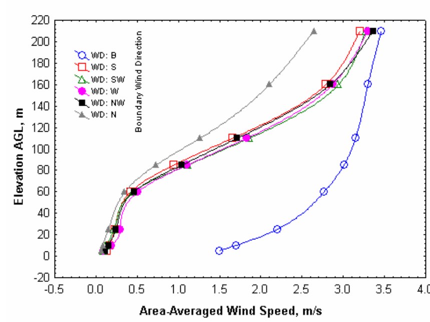


Figure 4. Horizontal planes displaying vertical velocity.

a) Wind speed



b) Wind direction

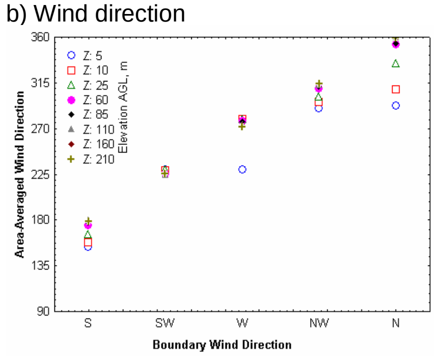


Figure 5. a) Area-averaged wind speed. Blue circles (B) plot the inlet wind profile b) Wind direction.

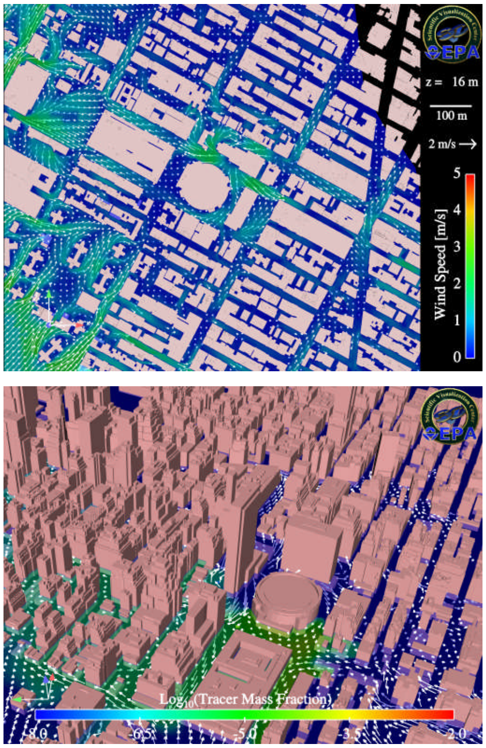


Figure 6. Surface winds (Top) and with concentration from a point source (Bottom) for the SW case.

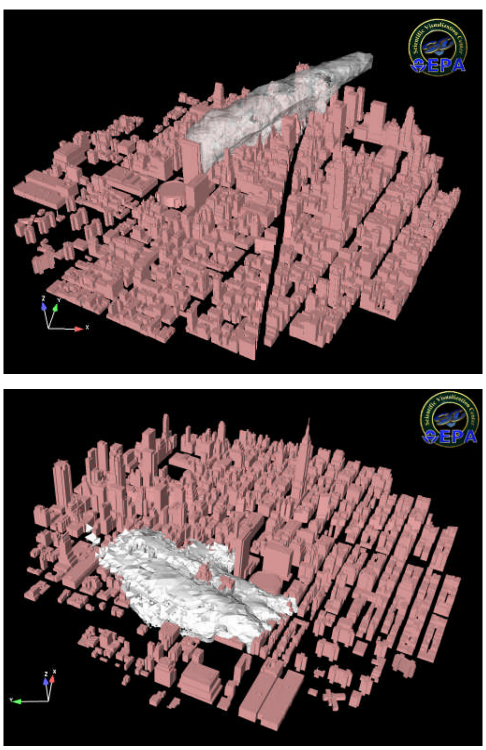
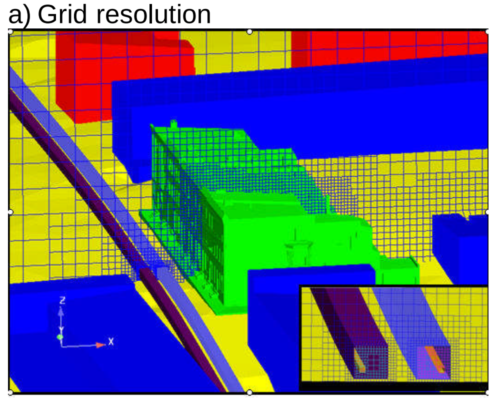


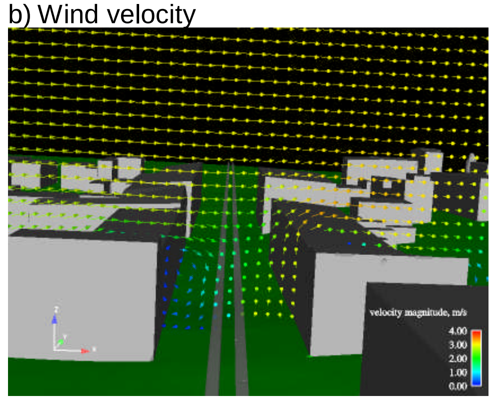
Figure 7. Top and Bottom picture shows a plume initiated from different point locations but within an identical wind field.

mobile source emissions based on Kastner-Klein et al. (2003) and Di Sabatino et al. (2003). Figure 8a below shows a vertical cross section slice of the domain grid with higher resolution near the building faces. This figure also shows the vehicle effects box (source of momentum and TKE within blue and purple boxes and shown expanded in the insert) and the smaller vehicle emissions box (yellow and orange shown in the insert) both running along a street. Ambient winds are from

a) Grid resolution



b) Wind velocity



c) Concentration

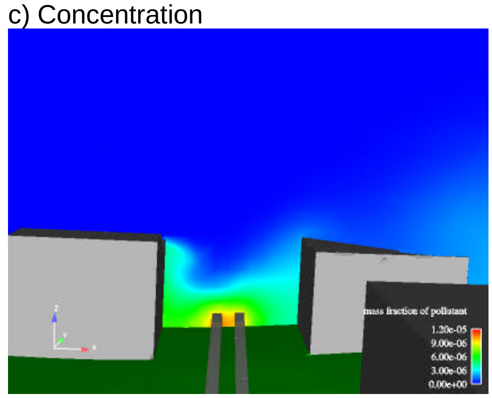


Figure 8. View of modeling a) domain grid resolution including the vehicle effects box along the roadway and vehicle emissions source box within b) wind and c) concentration.

left to right. Vehicle traffic is simulated assuming two lanes of one-way traffic at 20 mph.
There is a recirculation flow induced with the street canyon zone being displayed (Figure 8b) and the resulting concentration pattern (Figure 8c). For example, simulations for a few select wind directions can be used to study mobile source pollutants near the street and inside the adjacent buildings throughout the domain. This project is being completed to demonstrate how CFD simulations may be applied to model human exposure to mobile source emissions within specific neighborhoods.

5. SUMMARY STATEMENT

Fine-scale CFD models can be both interfaced with and applied independent of a larger scale grid model to support the development of human exposure factors and human exposure profiles dominated by local source emissions. Advances in computing hardware and software make it possible and increasingly more practical to consider extending present CMAQ-like air quality models to increasingly finer scales. The methods are all scaleable to larger domains as computing capacities grow. Routine fine-scale CFD modeling of air quality will happen.

Acknowledgements. Dr. Matt Freeman (Lockheed-Martin Operations Support) and Dr. Wei Tang (National Research Council Research Associate at the US EPA and now Lockheed-Martin Operations Support) are acknowledged for their support of the CFD applications and visualizations. Drs. Walter Schwarz, Brian Bell, and Karl Kuhlert (Fluent, Inc) are acknowledged for their support in developing CFD application using FLUENT. Scientific visualization and high performance computing were provided through support from the US EPA's Environmental Modeling and Visualization Laboratory. Additional computing support was provided through collaboration with Michael Lazaro and the Argonne National Laboratory, Laboratory Computing Resource Center.

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