LA-UR- 10-05730

Approved for public release; distribution is unlimited.

Title: Dispersal and Fallout Simulations for Urban Consequences Management (U)

Author(s): F.F. Grinstein, G.Patnaik, A.J. Wachtor, M. Nelson, M. Brown, and R. Bos

Intended for: Proceedings of DLES8 Workshop, Eindhoven, The Netherlands, July 7-9, 2010

Los Alamos
NATIONAL LABORATORY
EST. 1943

WORKSHOP
Direct and Large-Eddy Simulation 8
July 7-9, Eindhoven, The Netherlands

DISPERSAL AND FALLOUT SIMULATIONS FOR URBAN CONSEQUENCES MANAGEMENT

Fernando F. Grinstein (1), Gopal Patnaik (2), Adam J. Wachtor (1), Matt Nelson (3), Michael Brown (3), and Randy Bos (1)
(1) XCP-4, Los Alamos National Laboratory, Los Alamos, NM 87545, USA; (2) US Naval Research Laboratory, Washington DC 20375, USA; (3) D-3, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

INTRODUCTION

Hazardous chemical, biological, or radioactive releases in urban environments may occur (intentionally or accidentally) during urban warfare or as part of terrorist attacks on military bases or other facilities. The associated contaminant dispersion is complex and semi-chaotic. Urban predictive simulation capabilities can have direct impact in many threat-reduction areas of interest, including, urban sensor placement and threat analysis, contaminant transport (CT) effects on surrounding civilian population (dosages, evacuation, shelter-in-place), education and training of rescue teams and services. Detailed simulations for the various processes involved are in principle possible, but generally not fast. Predicting urban airflow accompanied by CT presents extremely challenging requirements [1-3].

Because of the configurations with very complex geometries and unsteady buoyant flow physics involved, the widely varying temporal and spatial scales quickly exhaust current modeling capabilities. Crucial technical issues include, turbulent fluid and particulate transport, initial and boundary condition modeling incorporating a consistent stratified urban boundary layer with realistic wind fluctuations, and post-processing of the simulation results for practical consequences management.

Relevant fluid dynamic processes to be simulated include, detailed energetic and contaminant sources, complex building vortex shedding and flows in recirculation zones, and modeling of multi-group particle distributions, including particulate fallout, as well as deposition, re-suspension and evaporation. Other crucial issues include, modeling building damage effects due to eventual blasts, addressing appropriate regional and atmospheric data reduction, and, feeding practical output of the complex combined simulation process into "urbanized" fast-response models.

In this paper we report progress in developing a simulation framework [3] for dispersal predictions in urban and regional settings (Figures 1-2) based on effective linkage of strong motion (and other) codes capable of simulating detailed energetic and contaminant sources associated with the effects of a conventional or nuclear explosion, an implicit large-eddy simulation (ILES) [4] model (FAST3D-CT [2]) capable of emulating CT due to wind and turbulence fields in the built-up areas, and a fast-response high-fidelity analytical model tool (QUIC) [5] .

SIMULATION APPROACH

The advantages of the computational fluid dynamics (CFD) representation to simulate CT transport and dispersion, 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. Solving for urban flow and dispersion is a problem for time-dependent aerodynamic CFD methods. Unavoidable trade-offs demand choosing between fast (but inaccurate) and much slower (but accurate) models. Relevant time domains can be identified which require appropriate corresponding time-accurate (full physics) simulation codes, involving physical processes that occur in microseconds-to-milliseconds, and seconds-to-one-hour ranges. Target (strong-motion and ILES) codes for these domains are integrated with appropriate mesoscale / atmospheric reduced data. Linking codes between the various time domains allows the results of one code to be used as the initial conditions for the next. The suite of full-physics simulations is used to develop source term, buoyant rise, and flow field parameterizations in urban environments for later use with fast-response high-fidelity analytical model tools [5,6].

The CASH strong motion code [8] includes appropriate methods for accurately modeling explosions, including state-of-the-art models for high explosive (HE) performance, and for the deformation and failure of other materials. It can model shock wave propagation in the atmosphere and the ground. CASH utilizes a lagrangian hydrodynamic solution method and also contains an arbitrary lagrangian-eulerian solver. While CASH can model many aspects of solid deformation and failure, the detailed generation of rubble and dust during fragmentation of building materials due to blasts remains poorly understood. Consequently, we are also investigating the use of codes based on particle and discrete element methods to understand and capture the phenomenology of this latter process (e.g., CartaBlanca [9]). Regardless of which code is being employed, we envision that the calculation at this stage would be run until shock strength and deformation effects are small enough to map to the dispersal code for the remainder of the simulation.

Effective use of ILES strategies has been reported for large scale urban flow and dispersal simulations for consequences management [2,3]. ILES is capable of simulating key unsteady flow features that cannot be handled with the industrial-standard gaussian plume methods [7], while providing higher accuracy than Reynolds-Averaged Navier-Stokes approaches. In ILES, the large energy containing structures are resolved whereas the smaller, presumably more isotropic, structures are filtered out and unresolved SGS are emulated with physics capturing finite-volume numerics [4]. The ILES urban CT model FAST3D-CT (see [2] and references therein for more details), involves a scalable, low dissipation, 4th order phase-accurate FCT convection algorithm, implementing direction-split convection, 2nd-order predictor-corrector temporal integration, and time-step splitting techniques. In typical urban scenarios, particulate and gaseous contaminants behave similarly insofar as transport and dispersion are concerned, so that the contaminant spread can be effectively simulated based on tracers with suitable advection velocities, sources and sinks. The fallout simulation relies on unsteady buoyant particle advection, parametrized terminal velocities [10], and particle groups selected based on typical relevant available dust particle mass / size distributions [11].

The Quick Urban and Industrial Complex (QUIC) Dispersion Modeling System [5,12] is a fast response urban dispersion model that runs on a laptop. QUIC is comprised of a 3D wind field model, a transport and dispersion model, a pressure solver, and graphical user interface. Chemical, biological, and radiological agent dispersion can be computed on building to neighborhood scales in tens of seconds to tens of minutes. QUIC accounts for the effects of buildings in an approximate way and provides more realism than non-building aware dispersion models. Algorithms for buoyant rise, buoyancy-generated turbulence, fresh-air entrainment, and gravitational settling of particles are included using an integral approach [13].

DISPERSAL MODEL VALIDATION ISSUES

Establishing the credibility of the solutions is one of the stumbling blocks of urban 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. A primary difficulty is the effective calibration and validation of the various 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. Validation studies with experiments require well-characterized datasets with information content suitable to initiate and evaluate unsteady simulation models as well as the cruder steady-state models. Obtaining full-scale (field) datasets for the inherently complex flows in question is costly and difficult; alternate validation approaches at present ([2], chapter 17 in [4]) involve code-to-code comparisons, comparing urban flow simulations with carefully controlled laboratory-scale wind-tunnel experiments, or carrying out detailed comparisons with actual urban field experimental databases as they become available.

Simulations of flow and dispersal over an urban model with the ILES FAST3D-CT code involved simulating flow over cube arrangements in wind tunnels [2] (Fig.3). The available datasets from the laboratory experiments consisted of high quality, spatially dense (but not time-resolved) single-point statistical data. Relevant insights followed from these studies, when comparing predicted and measured volume fractions of a tracer scalar in the first few urban model canyons using various different grid resolutions and inflow condition models (Figs.4-5). The resolutions considered were on the fairly coarse side, e.g., if simulations of flow over a single (surface-mounted) such cube were to be performed. On the other hand, these are resolutions representative of what we can afford to resolve practically in urban simulations relative to typical building dimensions. A comparison of the average tracer concentration profiles from simulations and experiments is shown at selected stations located in the first three canyons. In all cases, the agreement is within a factor of two or better, 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 [2]. This also reflects on the simulated and measured mean velocity and fluctuations agreeing better as we move downstream.

Prescribing some reasonable inflow turbulence as opposed to prescribing steady inflow, was found to be critical (Fig. 5). On the other hand, the fluid dynamics within the cube arrangement, i.e., beyond the first canyon, becomes somewhat insulated from flow events in the boundaries, i.e., it is less dependent on the precise details of the modeled inflow turbulence and largely driven by the urban geometry specifics within the urban arrangement.

RESULTS

Detailed urban dispersal studies in typical urban settings based on effective linkage of strong motion CASH AND FAST3D-CT are first described in what follows. As noted, in the type of simulations represented by the dispersal of contaminants due to an energetic release of energy in an urban environment, no one code can adequately simulate the full range of physics involved, nor should a user want that to be the case. Codes such as CASH and FAST3D-CT have been specifically developed to simulate very precise ranges of the relevant physics. CASH has the ability to simulate the strong motion regime where shocks are present due to an energetic source (such as a high explosive) but is not able to do the dispersal of contaminants in the atmosphere over a the size of a typical urban setting. On the other hand FAST3D-CT is not able to handle shocks or solid material descriptions,

The solution we have proposed is to use results of a strong motion code (e.g., CASH) as detailed initial-condition energetic and contaminant sources to the dispersal code (e.g., FAST3D-CT) at a time when shocks are no longer present or reduced to neglible levels. The calculations then proceed as in a regular dispersal simulation. We have been able to establish such a link using FAST3D-CT to simulate flow over a flat terrain. Figure 6 shows results using a FAST3D-CT restart file with a neutral ambient logarithmic atmospheric boundary layer (ABL) profile (U 3m / sec at 10m height), we overwrite a cylindrical sub-volume with the results from a 2D axially-symmetric simulation of the detonation of a high explosive (HE) source above ground level at a time when the physics of the CASH simulation is at levels appropriate for FAST3D-CT to use (Fig. 5). Ongoing CASH / FAST3D-CT linkage studies including actual urban geometries will be reported separately.

The urban dispersal studies described in what follows used "energy-pill" HE releases modeled in terms of initial cubic volumes having 15m side length at a 550 deg-K and 1316 deg-K (approximately equivalent to, 0.25-ton and 1-ton HE yields, respectively). Dispersal is found to be very sensitive to release characteristics, e.g., hot vs. release, as well as release height (cf. Figs. 7).

Particle tracer results with FAST3D-CT shown in Figures 8-9 are associated with particle sizes ranging between 7- 200 microns, and a HE energy-pill release occurring at 6m height (red dots). Figure 8 shows 100-micron particulate distributions 4.5 after initial release, whereas Figs. 9 show time series of particle concentration and velocity magnitude at selected locations at 15 m height above street level. Terminal velocities are modeled in terms of particulate size and mass [10], and prototypical dust particle sizes were selected [11]. Local concentrations and velocity magnitude are found to be very sensitive to urban geometry and significantly more variability is observed at plume edges, where the presence of less coherent vortical structures is suggested by the velocity magnitude time series.

Finally, comparison of predictions with FAST3D-CT and QUIC codes, are examined, and effects of particle group specifics (e.g., sizes) are addressed in this context. (Figures 10 and 11). Both simulations were initialized with similar mean flow field and same energy pill (approximately equivalent to 1-ton HE), except for QUIC not accounting for the turbulent impact of the urban geometry on the ABL profiles. Figure 10 shows that both codes give surprisingly similar plume rise results (based on height of peak particle concentration evolution), but actual concentration distributions are qualitatively fairly different (Fig.11). The comparisons have suggested improvements on the QUIC modeling, specifically, changing the constant temperature assumption in buoyant cloud model.

ACKNOWLEDGEMENTS

Los Alamos National Laboratory is operated by the Los Alamos National Security, LLC for the U.S. Department of Energy NNSA under Contract No. DE-AC52-06NA25396.

REFERENCES

1. Britter, R.E., and Hanna, S.R., 2003, Flow and Dispersion in Urban Areas, *Ann. Rev. Fluid Mech.*, **35**, 469–496, .

2. Patnaik, G., Boris, J.P., Young, T.R., Grinstein, F.F., 2007, Large Scale Urban Contaminant Transport Simulations With MILES, *J. Fluids Eng.*, **129**, 1524–1532.

3. F.F. Grinstein, R. Bos, and T. Dey, 2009, "LES based Urban Dispersal Predictions for Consequence Management", by invitation, *ERCOFTAC Bulletin*, **78**, 11–14.

4. Grinstein, F.F, Margolin, L.G., Rider, 2007, W.J., Editors, *Implicit Large Eddy Simulation: Computing Turbulent Fluid Dynamics*, Cambridge University Press.

5. Brown, M., Urban Dispersion Challenges for Fast Response Modeling, 2004, in *Fifth AMS Symposium on the Urban Environment*, LA-UR-04-5129, LANL, Los Alamos, NM,.

6. Boris, J.P., 2002, The Threat of Chemical and Biological Terrorism: Preparing a Response, *Comp. Science and Eng.*, **4**, 22–32.

7. Pullen, J., Boris, J.P., Young, T.R., Patnaik, G., and Iselin, J.P., A Comparison of Contaminant Plume Statistics from a Gaussian Puff and Urban CFD Model for Two Large Cities, *Atmos. Environment*, **39**, 1049–1068, 2005.

8. T.N. Dey and R.J. Bos, "CASH, Version 01(CASH) Code," LANL computer code LA-CC-01-053 (2001) and ECCN 0D999.

9. http://www.lanl.gov/projects/CartaBlanca/.

10. N-S. Cheng, "Comparison of formulas for drag coefficient and settling velocity of spherical particles", *Powder Technology*, **189**, 2009.

11. R.G. Pinnick, G. Fernandez, and B.D. Hinds, "Explosion dust particle size measurements", *Appl. Optics*, **22**, 95–102, 1983.

12. http://www.lanl.gov/projects/quic/.

13. Boughton, B.A. and J. M. DeLaurentis, An Integral Model of Plume Rise from High Explosive Detonations, SAND-86-2553C.

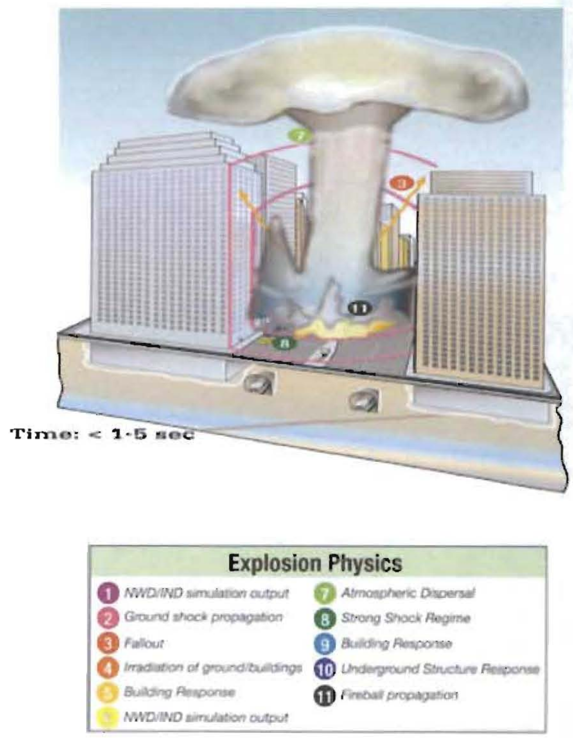

Figure 1: LANL urban consequences management project: early time simulations.

Figure 2: LANL urban consequences management project; later time simulations.

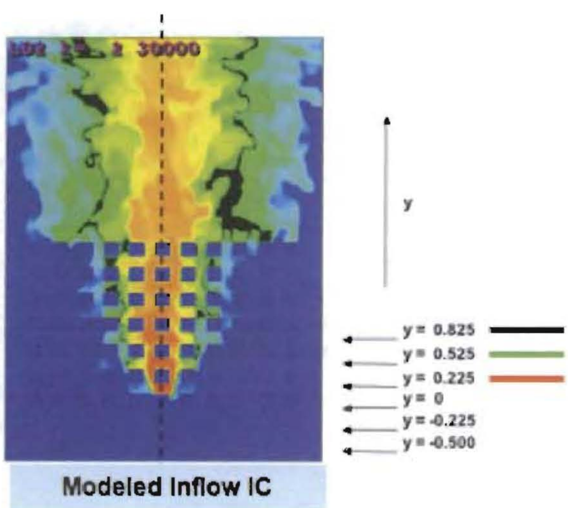

Figure 3: Urban dispersal validation studies; simulation of flow over an urban (cube arrangement) model from Ref. 2.

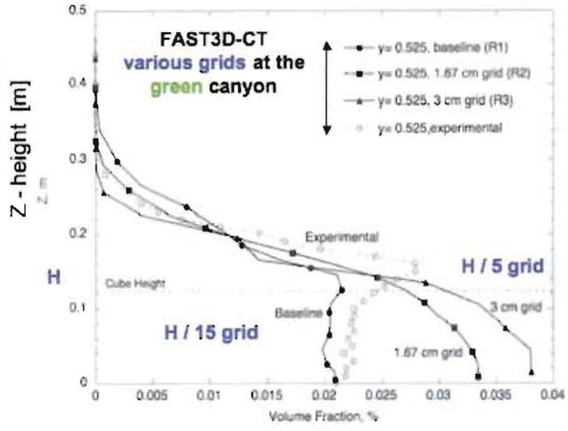

Figure 4: Urban dispersal validation studies from Ref. 2: resolution studies; H denotes the cube height and separation.

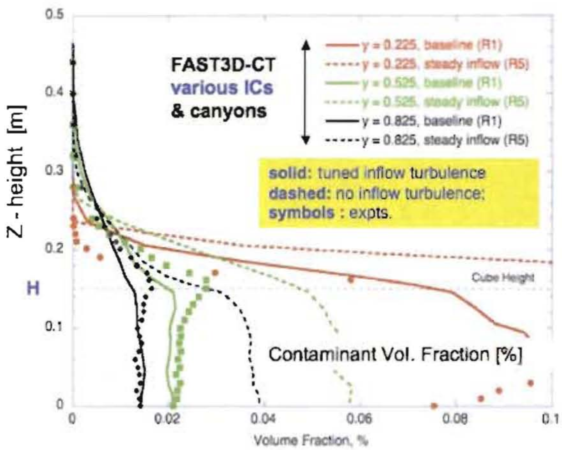

Figure 5: Urban dispersal validation studies from Ref. 2: impact of inflow model; H denotes cube height and separation.

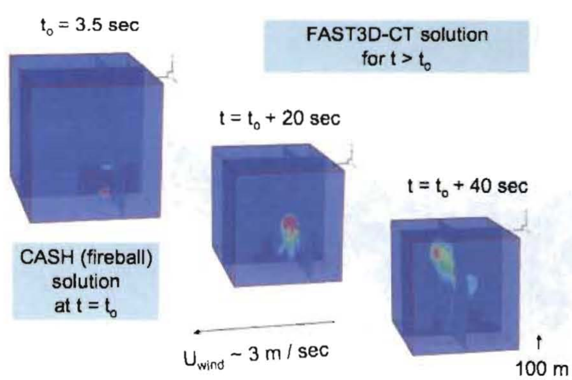

Figure 6: Linking strong motion (fireball) and dispersal simulations for a 1-ton HE, 2m above ground.

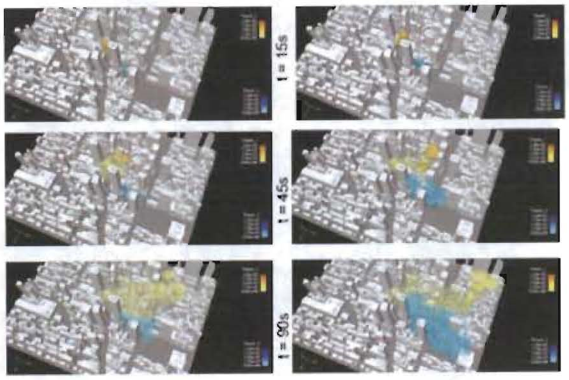

Figure 7: Dispersal studies on a typical urban setting: effects of release characteristics. Simulations of a 0.25-ton uniform HE energy-pill release with FAST3D-CT. Particle concentration distributions; hot (orange) / cold (blue) releases at 15m height

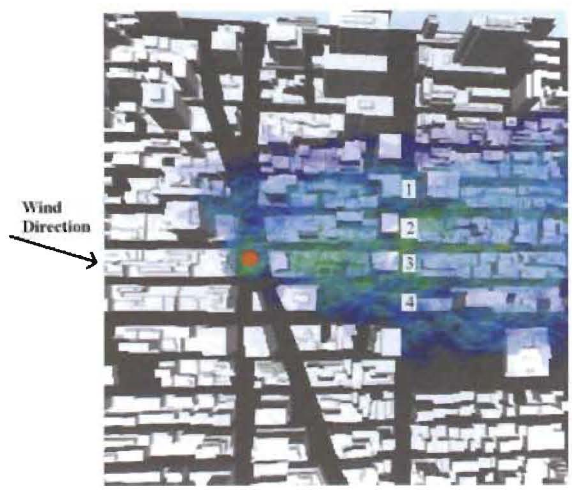

Figure 8: Simulations of a 0.25-ton uniform HE energy-pill release with FAST3D-CT. Distributions of 100-micron particulate distributions 4.5 minutes after initial release (at red circular region).

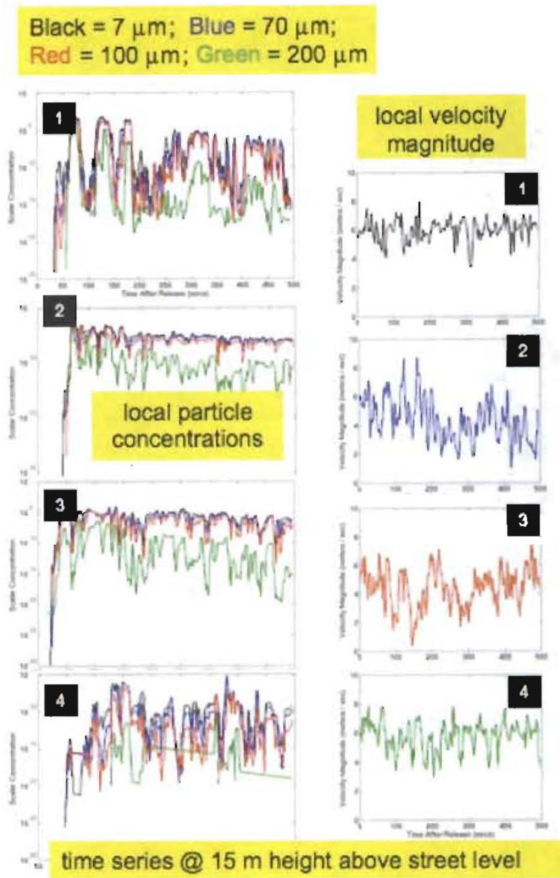

Figure 9: Simulations of a 0.25-ton uniform HE energy-pill release with FAST3D-CT. Time series of local particle concentration and velocity magnitude at locations indicated on Fig. 8 .

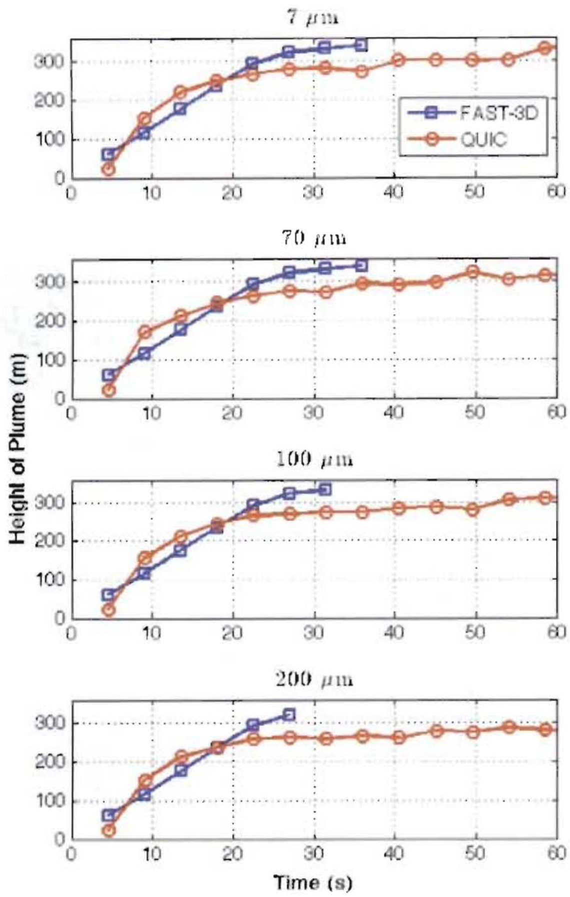

Figure 10: Plume rise predicted by FAST3D-CT and QUIC for various particulate sizes; FAST3D-CT used geometrically stretched grid above 300m: corresponding plotted results do not account for that.

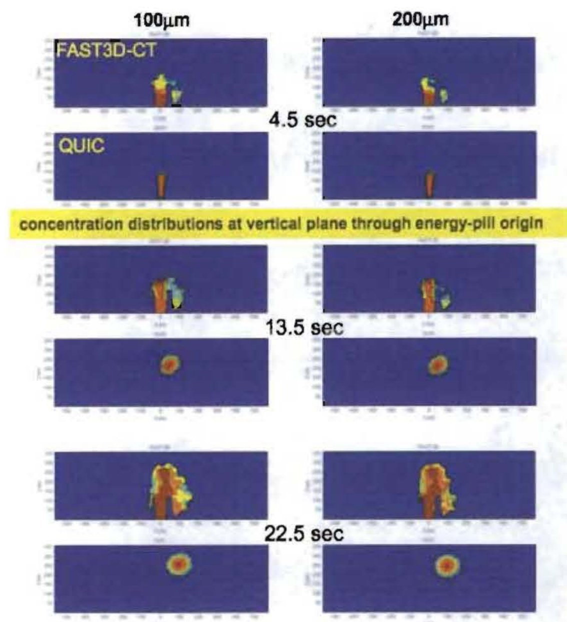

Figure 11: Comparison of FAST3D-CT and QUIC predictions of particle concentration distributions.