CFD prediction of dense gas clouds spreading in a mock urban environment

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ABSTRACT: A computational fluid dynamics (CFD) code is used to predict wind driven dense gas cloud movement and surface concentrations with and without the presence of a generic arrangement of block obstacles to represent urban buildings. Thus the characteristics of plume movement around and within building obstacles and simulated street canyons can be compared to isolated plume behavior. .

1 INTRODUCTION

Dispersion of cold or dense gases such as propane, LNG, or ammonia in the event of an accidental spill is a major concern for storage, chemical processing or transportation safety planning, hazard response, and facility siting. Transportation of such fluids by truck, rail or ship may lead to releases within the urban environment.

Field experiments with actual hazardous gases or safer simulants (CO_2, liquid N_2) have been supported by such groups as the U.S. Dept. of Energy, U.S. Dept. of Transportation (Coast Guard), Gas Research Institute, and the UK Health and Safety Laboratory (Luketa-Hanlin, 2006). Laboratory simulations in environmental wind tunnels have been prepared by the WEFL at Colorado State, the CHRC at Univ. of Arkansas, Meteorology Institute at Univ. of Hamburg, etc.(Meroney, 1984a, 1984b, 1988). Recently, computational models have been developed focused on the dispersion of dense gases such as DEGADIS at Univ. of Arkansas, FEM-3 at LLNL and FLUENT-LNG supported by DOE-NETL (Luketa-Hanlin et al., 2007). Only the latter two models (or similar finite volume models) are really suitable for modeling dispersion in situations complicated by the presence of buildings, tanks or other arrays of obstacles (Cormier et al., 2009). Both FEM-3 and FLUENT-LNG have recently been validated against wind tunnel and field experiments including arrays of building obstacles (Gavelli et al., 2008; Eggenspieler et al., 2006; Riddle et al., 2004; Huber et al., 2002; Tang and Huber, 2006). FLUENT has now been tested against a number of field experiments performed in cities such as Salt Lake City, New York City (Manhattan), and Washington D.C. (Allwine and Flaherty, 2007; Hanna et al., 2002, 2006; Huber et al., 2004; Huber, 2009).

Despite extensive sets of field data, and laboratory experiments and numerical validation exercises, there is relatively little descriptive lore of how different size transient releases of dense gas will behave over arrays of simple buildings. In an effort to study the intrusion of clouds of heavy gas into urban street canyons, this paper reports the results of numerical experiments of dense gas clouds passing among simple block obstacle arrays. FLUENT 6.3© was used to predict plume transport over a building matrix array using different size sources as calculated by various turbulence models (k-epsilon, realizable k-epsilon, and LES algorithms).

1.1 *Cloud/Plume Behavior Among Building Arrays: Neutrally Buoyant Gases*

Concern about pollutants released from power plants and other industrial structures have led to many studies of neutrally buoyant gas clouds/plumes dispersing about isolated buildings (Li and

Meroney, 1983a, 1983b; Meroney, 1982). Such data have been integrated into predictive programs such as the U.S. EPA AERMOD model protocol (Turner and Schulze, 2007). Isolated structures tend to augment the growth of gas clouds locally.

- When the gas cloud dimensions are large compared to the isolated structure, the cloud/plume engulfs the objects, and very little to modest cloud impact is produced by the building.
- When the gas cloud dimensions are small compared to those of the structure, the cloud is usually mixed across the building wake cavity, resulting in an immediate increase in plume width and height and an associated drop in surface concentrations.
- If the plume or cloud is initially above the building height, but the plume centerline is less than 1 ½ building heights in elevation, flow deviations produced by the building may entrain the plume, reduce the effective plume height and result in larger surface concentrations than in the absence of the structure.

Additional field and model scale tests have been made around more complex arrays of structures as concern has focused on petrochemical complexes and transportation pollutants in urban centers (Britter and Hanna, 2003; Chang and Meroney, 2000, 2003; Cheng et al., 2007; Davidson et al., 2006, 2007; Duijim and Weber, 1994; Hall et al., 1997, 1999, 2003; Hanna and Steinberg, 2001; Hanna et al., 2002; Yee and Biltoft, 2004). These data have now been used to validate CFD models for use in urban building configurations. Neutrally buoyant gases released upwind or within structured arrays of obstacles display special transport features.

- When the plume or cloud dimensions are large with respect to characteristic building scales, the plume engulfs the objects, and their presence is primarily felt through the augmentation of mixing due to increased turbulence.
- When the plume or cloud dimensions are less than characteristic building and building spacing scales, the plumes tend to initially stagnate against upwind surfaces, wrap around the building sides, and intrude or extrude laterally when side streets are encountered driven by street canyon flows and vortices.
- In the later case the orientation of the street corridors to wind direction may lead to asymmetric plume width growth with respect to plume centerline, but
- As the cloud/plume ages it mixes vertically until vertical and lateral scales are again larger than characteristic building and spacing dimensions, and then it develops more or less independently of the underlying building array.

1.2 *Cloud/Plume Behavior Among Building Arrays: Negatively Buoyant Gases*

Initially, it was presumed that dense gases would disperse in a manner similar to neutrally buoyant mixtures; however, accident experience with spills of ammonia, LNG, propane and other heavy gases revealed this was not the case. Dense gas clouds collapse under the effect of gravity, move upwind against low near ground level winds, and spread laterally in a pancake like manner. Hence, in the 1970s research programs were initiated to examine dense cloud/plume behavior both in the field and the laboratory. Initial attention was again focused on simple configurations of isolated releases in the absence of obstructions (Luketa-Hanlin, 2006; Meroney, 1982b, 1984a, 1984b, 1987a, 1987b; Meroney and Lohmeyer, 1984a, 1984b).

But practically, most realistic releases are expected to occur near structures; hence, studies focused next on dense cloud behavior near isolated objects such as buildings, tanks, fences, and even water spray curtains (Kothari and Meroney, 1984; Meroney et al., 1984; Ohba et al., 2004). These tests resulted in the development of CFD codes designed to account for dense gas behavior (Coldrick et al., 2009; Iving et al., 2007; Gavelli et al., 2008; Hankin et al., 2003; Lee and Meroney, 1988)

Measurements of dense gas clouds/plumes in the presence of extended arrays of obstacles might initially be presumed to behave in a similar manner to neutral gas releases as discussed in section 1.1, but with suppressed vertical growth and enhanced lateral movements. It was also initially assumed that such obstacle arrays would primarily act as increased boundary layer roughness, and their effects might be incorporated into existing models by simply increasing effective surface roughness or decreasing near ground wind speeds. Hanna and Steinberg (2001) reported the results of an experimental program by the petroleum industry intended to clarify these points. Roberts and Hall (1994) also replicated some of these measurements. They found that effects of obstacle arrays on dense gas dispersion could be accounted for by surface roughness augmentation in numerical models if the obstacle to cloud heights remains below a critical limit, but when it exceeds a specified value then the initially rapid lateral cloud growth is diminished due to interference with the dense cloud edge gravity fronts, and it gives way to a much slower rate of spread. During these tests the effective full scale roughness height, z_o, did not exceed 0.5 m. For larger obstacles (~3.5 m full scale) channeling between obstacles confines the flow and increases concentrations by factors of 3 to 4, and the size, arrangement and distribution of elements is critical to the resultant dispersion pattern.

Wind tunnel experiments were performed by Harms (2005) for dense gases dispersing among large size obstacles. His array configuration duplicated the Mock Urban Setting Test (MUST) field tests performed in Utah during 2001. 120 shipping containers (12.2 m long x 2.42 m wide x 2.54 m high) were arranged in a 10 x 12 array about 200 m x 200 m in size in a flat desert terrain. Harms tests were performed in a model atmospheric boundary layer in the U. of Hamburg WOTAN boundary-layer wind tunnel at a scale of 1:75. The model tests replicated approach wind profiles, turbulence profiles, and integral scales observed during the field measurements. Plumes of gas were released from comparable locations, but wind conditions were limited to oblique angles that ranged between 20 to 45 degrees to the long dimension of the shipping container objects. Most of the dense plume concentration variations occurred close to the sources and at height below the container height. Wind orientations were found to be important in determining maximum fetch to a given concentration level, and gases below container height were deflected away from the primary wind axis and along simulated street canyons. No time dependent visualizations of the modeled plume behavior were archived.

Prediction of dense gas dispersion in a complex building arrangement was presented by Gavelli et al. (2008). They used the FLUENT code to predict flow and dispersion during the Falcon test series performed in 1978 in Nevada for LNG spills onto a test pond surrounded by barrier fences. The Gavelli predictions replicated most of the plume behavior seen in the field tests. Brambilla et al. (2009) combined a shallow layer model with the flow field predictions of the Los Alamos Laboratory QUIC wind solver to follow the movement of a hypothetical release of heavier-than-air gases within a non-ideal array of buildings with no cross flow. The initially cylindrical gas cloud slumps below building height and, it spreads by channeling along street canyons. There is some gravity head speed up as it travels into narrow streets.

2 CFD SIMULATION OF TRANSIENT DENSE GAS CLOUD DISPERSION

The commercial software selected for these calculations, FLUENT 6.3 ©, solves the three-dimensional Reynolds averaged equations of motion discretized using a control volume approach for flow, pressure, turbulence, and concentration distributions. The Reynolds stress terms were modeled by one of several turbulence models: standard k-epsilon (k-ε), realizable k-epsilon (rk-ε), or large eddy simulation (LES). Since in this study the unsteady behavior of dense cloud drift is predicted for flow separating and recirculating around obstacles, all these methods are considered. Ground and wall surfaces were specified as rigid planes with zero roughness. Inlet (upwind) velocity and turbulence profiles were selected to reproduce field observations. Lateral boundaries were specified as symmetry boundaries with slip velocity conditions, and the top boundary was set to a moving wall fitted to the inlet velocity profile. The inlet power-law profile coefficient was p = 0.14, the velocity was set to U = 0.5 m/s at z = 0.5, with a lower surface roughness of z_o = 0.002 m. For the LES cases a spectral synthesizer inlet option was used to randomize the inlet eddy sizes.

A simple rectangular domain was selected (20 m long x 10 m wide x 5 m high), a limited array of 9 rectangular blocks (1 m x 1 m x 0.5 m) were arranged in a three row staggered rectangular array. Street canyon dimensions were set to a ratio of H:D = 0.5:1. The initial dimensions of the source volumes were rectangular (1m x 1m x 0.5m or a 0.5m cube) and placed 5 m upwind of the center of the obstacle array. Source gas was carbon dioxide (CO_2) with an initial specific gravity relative to air of 1.52. The grid system created within the computational domain used hexagonal cells (0.1 m cubes) for depths below 1 m, and tetrahedral and pyramid cells ranging from 0.1 to 1 m at the top of the domain (Fig. 1). For comparison to the cloud over array behavior simulations were also performed for cloud behavior over an unobstructed ground surface and for flow and behavior about a single centrally-located block obstacle. Table 1 summarizes the test matrix and dimensionless parameters considered.[1]

Case	Turbulence Model	Empty Domain Test	Single Building Test	9 x 9 Building Array	H_{cloud}/H	Froude No. = $\rho U_{ref}^2/(g\Delta\rho H_{cloud})$	Ri_* No. = $g' V_i^{1/3}/u_*^2$
1	std k-e	Yes	No	Yes	1	0.049	3126
2	real k-e	Yes	Yes	Yes	1	0.049	3126
3	LES	Yes	Yes	Yes	1	0.049	3126
4	real k-e	Yes	Yes	Yes	0.5	0.098	1969
5	LES	Yes	Yes	Yes	0.5	0.098	1969

Table 1: Test Matrix for CFD Simulation of Unsteady Dense Cloud Behavior

3 RESULTS OF NUMERICAL COMPUTATION

The primary results from these calculations are the visualizations of cloud behavior for unobstructed dispersal, dispersal around a single building obstacle, and dispersal about the simple 9-building array. Video clips (*.avi format) have been archived on a Colorado State web site under the category of Recent Research Presentations, where they can be downloaded on demand. (http://www.engr.colostate.edu/~meroney/index.html) The behavior of the various test cases are summarized below in prose statements that describe the primary behavior of the transient movement of the dense cloud released..

[1]Note: Ri_* values for instantaneous releases are comparable to field experiments at Porton Downs (40 m^3 spills, No. 29 & 33) and at Thorney Island (1000 m^3 spills, No. 11 & 18) as noted in Meroney, 1987a.

- When the clouds are released in an unobstructed domain, it is found that the cloud movements and growth are basically similar for all turbulence models and initial cloud dimensions. The cloud volume initially collapses and moves radially outward in all directions. Subsequently, the cloud is swept downstream, spreading until it strikes the lateral symmetry boundaries. For the RANS models an isoconcentration surface remains smooth and pancake like (Figs 2 & 5) ; however, for the LES models the upper surface and edges eventually becomes more ragged and display distortions due to individual eddies and stretching by longitudinal boundary layer vortices (Fig. 6).

- When the clouds are released upwind of a single obstacle they spread as before, but when the cloud front stagnates against the upwind obstacle face, it breaks and wraps around the block into a horse-shoe shape. Immediately downwind of the obstacle the gases mix laterally into the obstacle wake cavity, but lower velocities slow the downwind cloud motion producing a kidney-shape when viewed from above (Fig. 3). Again the isoconcentration surfaces for the RANS models remain smooth and the profiles are laterally symmetric; however, for the LES models the upper surfaces and edges are again distorted and ragged, and the building wake is present but may not be laterally symmetric.

- When the clouds are released upwind of the 9-building arrays, the cloud motions are a composite of the first two situations. The clouds initiate as pancake shaped surfaces, but they are deflected around the building complex, some fluid “squirts” between the buildings along street canyons, filling laterally into the building wakes where they slow downwind movement (Figs 4 - 7). However, the portions of the cloud which are deflected around the first row of buildings transport more rapidly downwind that those portions inhibited by the drag of the building array resulting in a comb-like distribution of surface contact downwind when combined with the flow down windward oriented streets.

- For the LES simulations the cloud displays a gravity-head or “nose” along the forward edge of the cloud (Figs 6 & 7). The cloud also seems to spread faster laterally for the LES turbulence model cases than for the RANS case simulations.

There are several distinctive differences between the large (1 x 1 x 0.5 m rectangle) spills and the smaller releases (0.5 m cube). The most obvious is that the RANS simulations do not reach the lateral boundaries of the domain until downwind of the building array. The more rapidly spreading LES simulations still contact the lateral domain sides. There is also a tendency for the smaller clouds to induce lower surface concentrations in the street canyons and wakes of the building array. However, if one compares isoconcentration surfaces of 0.01 for the larger spills to the 0.001 surfaces for the smaller spills the geometric surfaces are almost identical, suggesting that once the cloud is diluted and spreads the subsequent mixing is dominated by the boundary shear and the building wakes (Figs 4 vs 5 and 6 vs 7).

4 SUMMARY

This study of dense gas cloud transport and dispersion confirms earlier experience that given density differences between the cloud and ambient air, the clouds initially collapse toward the ground and spread rapidly radially. However, once spread into a pancake like shape, the ambient winds convect the gases downwind. If the stratification produced by the density differences are undisturbed, then the cloud may retain its pancake like or slab like appearance for considerable distance downwind.

But if the cloud is significantly disturbed by stagnation against and intrusion into obstacle wakes, then the stratification seems to diminish, vertical motions are permitted, and the clouds eventually disperse in a manner similar to neutrally buoyant gas clouds. Within the wake of single obstacles and building arrays high concentrations may persist and arrival times will be delayed due to the lower inter-building velocities.

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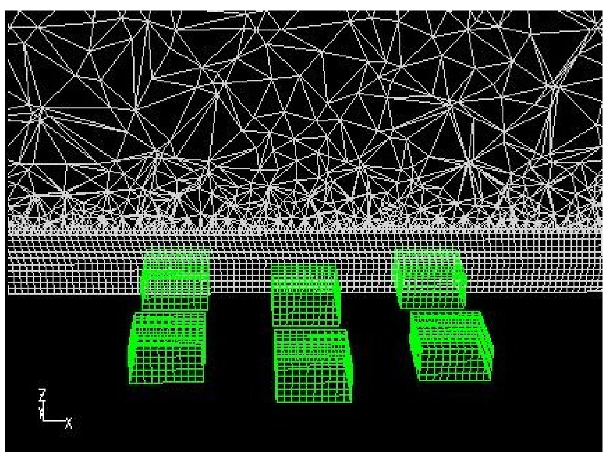

Figure 1. Grid discretization with trapezoidal cells (0.1m cubes) below z = 1 m and tetrahedral and prismatic cells (0.1 to 1 m) above z = 1 m. Building dimensions are X:Y:Z = 1:1:0.5 m spaced in a staggered array 1 m apart.

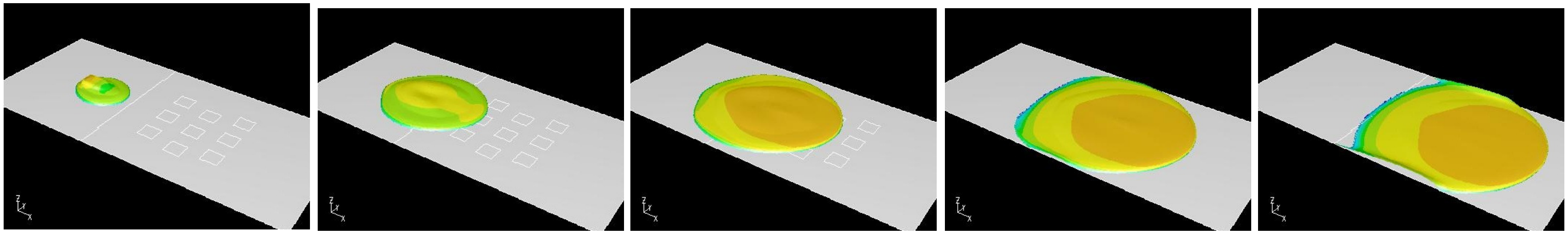

Figure 2. Source (1 x 1 x 0.5 m, SG = 1.52) released at X = 5 m, unobstructed domain. Realizable k-epsilon turbulence model. Times: t = 1, 5, 10, 25 & 20 sec.

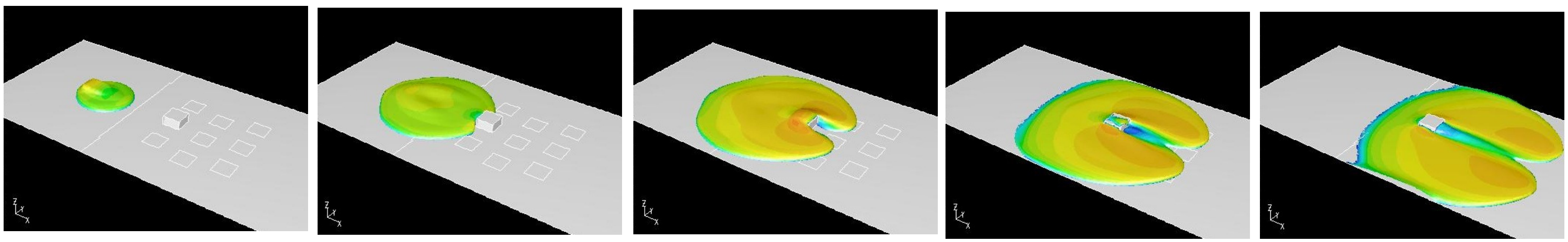

Figure 3. Source (1 x 1 x 0.5 m, SG = 1.52) released 5 m upwind of single building (1m x 1m x 0.5 m). Realizable k-epsilon turbulence model. Times: t = 1, 5, 10, 25 & 20 sec.

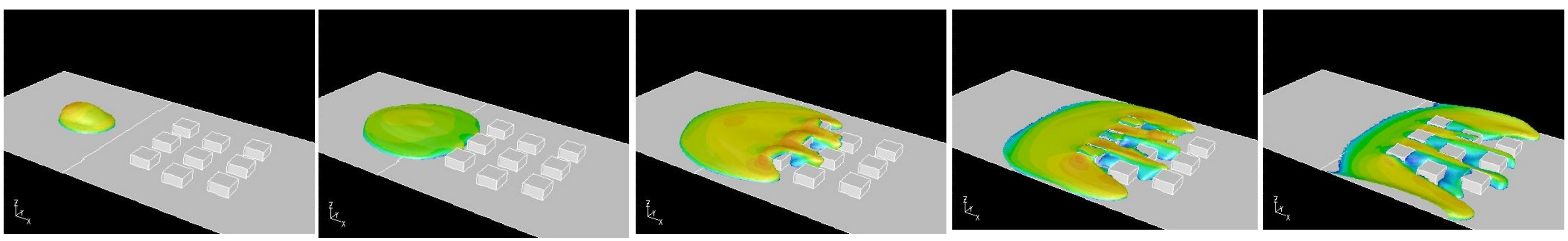

Figure 4. Source (1 x 1 x 0.5 m, SG = 1.52) released 5 m upwind of 9 building staggered array (1m x 1m x 0.5 m), H:D = 0.5:1. Realizable k-epsilon turbulence model. Times: t = 1, 5, 10, 25 & 20 sec.

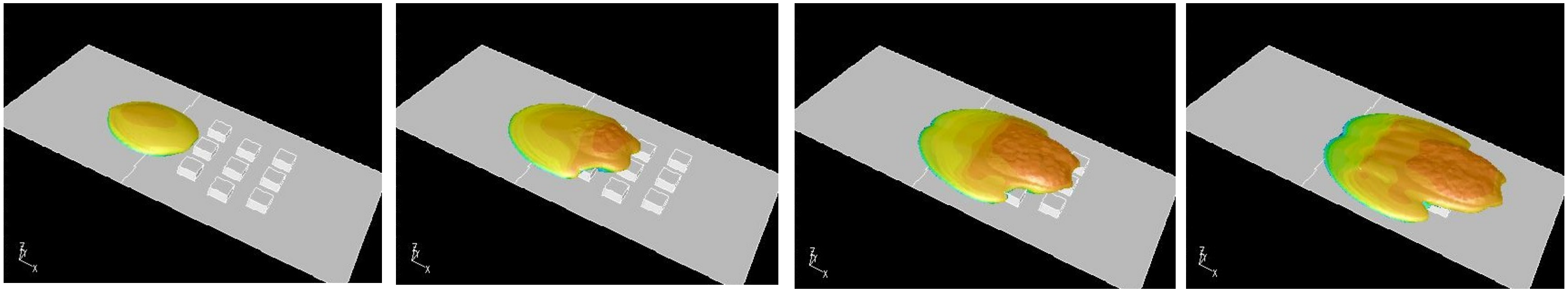

Figure 5. Small source (0.5 m cube, SG = 1.52) released 5 m upwind of 9 building (1 m x 1 m x 0.5 m) staggered array, H:D = 0.5:1. Realizable k-epsilon turbulence model. Times: t = 5, 10, 25 & 20 sec

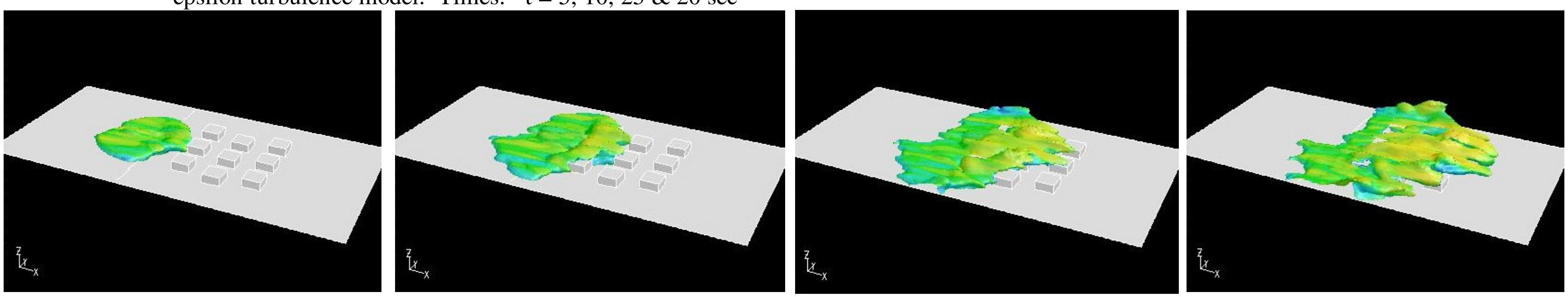

Figure 6. Small source (0.5 m cube, SG = 1.52) released 5 m upwind of 9 building (1 m x 1 m x 0.5 m) staggered array, H:D = 0.5:1, Large eddy simulation turbulence model. Times: t = 5, 10, 25 & 20 sec.

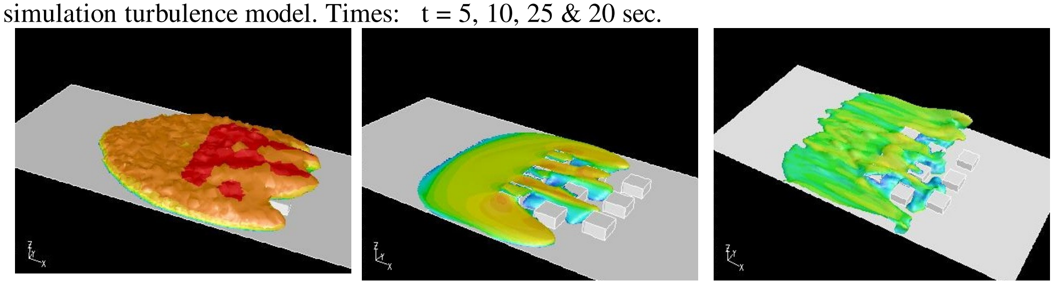

Figure 7. Source (1 x 1 x 0.5m, SG = 1.52) released 5 m upwind of 9 building array, t = 15 sec. Turbulence models ske, rke & LES from right to left.