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THE PREDICTION OF TOXIC GAS INFILTRATION FOR A BUILDING IN AN URBAN AREA

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1. INTRODUCTION

Buildings in urban areas are exposed to pollutants daily and could possibly be exposed to hazardous toxic gas released into the environment. Most buildings in urban areas have their own heat and cooling units that intake and exhaust the ambient air. This paper addresses how the existence of Heating, Ventilation and Air Conditioning (HVAC) systems affects the gas dispersions in urban environments and how much pollutants penetrate into a specific building.

The study has evaluated near source ambient air concentrations resulting from the street level pollutant emission and toxic gas released nearby. Our evaluation is based upon high-resolution Computational Fluid Dynamics (CFD) modeling which takes into account emissions and the local wind and turbulence fields in order to estimate the contaminant concentrations at pedestrian level and at selected receptor locations situated near a tall building.

The model we have used is CFD-Urban. CFD-Urban is a suite of Computational Fluid Dynamics modeling software that is being used to simulate the wind, turbulence and dispersion fields in urban areas [Coirier et al., 2003.a, 2005.a]. CFD-Urban has been developed under a program sponsored by the Defense Threat Reduction Agency [Coirier, et al., 2003.b], and has been built using parts of a commercially available software suite, CFD-ACE+ [ACE+ 2003]. It solves the Reynolds-Averaged Navier-Stokes equations using a collocated, Finite-Volume method implemented upon structured, unstructured and adaptively-refined grids using a pressure-based approach based upon the SIMPLE algorithm [Jiang, 1994, Jiang, 1999]. Turbulence closure is found by solving a variant of the standard $k-\epsilon$ model [Launder, 1974]. Buildings are modeled either explicitly, by resolving the buildings themselves, or implicitly, by drag modeling the effects of the buildings upon the flow by the introduction of source terms in the momentum and turbulence model equations [Coirier 2003.b]. Turbulence is incorporated into the momentum equations by solution of the steady-state or unsteady Reynolds Averaged Navier-Stokes (RANS) equations, as well as by using a Large Eddy Simulation (LES) approach. The RANS approach resolves the mean flow and models the effect of turbulent eddies. The LES approach uses a finer grid resolution than the RANS approach, so that the larger eddies are resolved and only the smaller eddies are modeled.

Since CFD-Urban solves the governing mass and momentum conservation laws at scales smaller than the buildings themselves, important urban aerodynamic features are naturally accounted for, including effects such as channeling, enhanced vertical mixing, downwash and street level flow energization.

We have performed a series of high-resolution CFD flow and transport and dispersion calculations. The series of simulations include:

- One toxic gas source (puff gas) on pedestrian level, in an attempt to estimate prevailing conditions and source strengths derived from a worse case scenario.
- Four street moving pollutant sources that are generated by heavy traffic in an urban area

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The sections below describe the overall modeling approach, and present the results from our study.

2. MODELING APPROACH

The approach taken here has been to:

- Construct a CFD Volume Mesh including the drag models of buildings using a Manhattan Building Database.
- Clip out ventilations from buildings using an in-house software.
- Perform the flow field calculations.
- Perform unsteady release calculations using both a puff and continuous sources with the existing flow field.

2.1 Construct CFD Volume Mesh

A CFD computational mesh was constructed using an adaptive Octree/Prismatic mesh approach that has a high spatial resolution in the vicinity of the buildings of interest. Buildings are modeled either explicitly, by resolving the buildings themselves, or implicitly, by drag modeling the effects of the buildings upon the flow by the introduction of source terms in the momentum and turbulence model equations. The total computational domain is 3000 m by 2400 m by 1000 m and the internal domain of size 1550 m by 1550 m has a relatively coarse grid. The grid size near the buildings of interest is $\Delta x = 11.67$ m and $\Delta y = 9.24$ m and the first cell from the ground is $\Delta z = 1.0$ m. The total number of cells used in the computation is 519068.

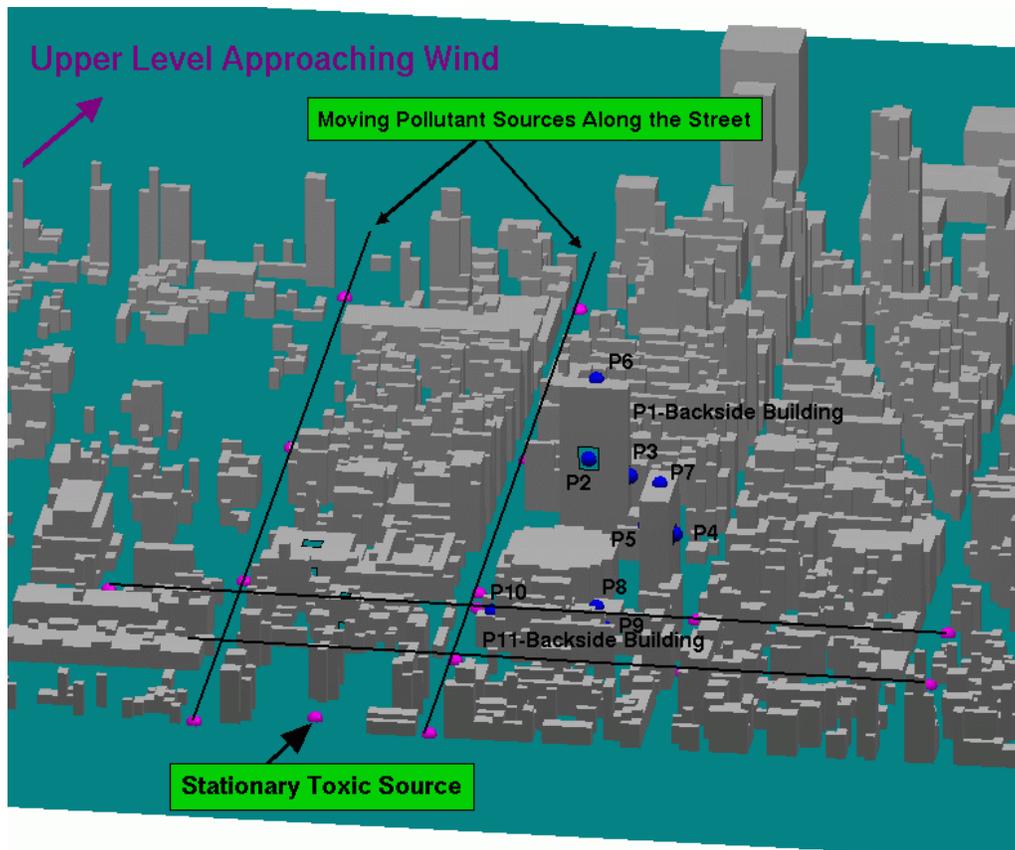


Figure 1. Modeled Geometry, including pollutant source locations and monitoring ventilations.

Figure 1 above shows the geometry to be studied. HVAC ventilation systems of buildings are processed after the computational domain is generated. The figure also shows the contaminant source locations for the both stationary and moving sources. The computational boundaries are located sufficiently far away to insure fully developed urban canopy layer flow and turbulence fields, and are generated in such a way to

allow the imposition of boundary conditions at the buildings of interest intake/outflow vents in order to replicate the emissions from the building vents.

2.2 Defining Heating, Ventilation and Air Conditioning (HVAC) systems at a building

In this study, we arbitrarily select several buildings and clip out some portions of the building walls. We assume that the clipped walls of the side of building are intakes and the clipped walls of the top of building are exhaust. It is assumed that the intakes admit the surrounding air at the rate of 3m/s and the exhausts emit air to the surrounding at the rate of 4m/s. These intakes and exhausts are identified from figure 1 described as P1 to P11.

2.3 Flow field

We have established a wind library and we generate the flow fields from the stored files in the wind library [Coirier, et al 2006]. The wind library concept works as follows: (1) we construct all possible combination of the wind and turbulence fields for the urban area under consideration and store these fields in a library. Each entry of the wind field library stores the velocity and turbulence fields at all points in the CFD mesh corresponding to a particular set of prevailing conditions that have been applied as boundary conditions, (2) when we compute gas dispersions in the urban area, we estimate the prevailing wind speed and direction during the time period of gas dispersion. If the measured data are available, we use these measured data as a scheduler, (3) then, we can get the transient wind flow fields by simply interpolating the flow fields stored in the library.

For the cases shown here we use a logarithmic profile for the prevailing wind speed, which uses the following equilibrium relations:

$$U = \frac{u_*}{\kappa} \log\left(\frac{z}{z_0}\right) \quad (1)$$

$$k = \frac{u_*^2}{\sqrt{C_\mu}} \quad (2)$$

$$\varepsilon = \frac{u_*^3}{\kappa z} \quad (3)$$

Since we vary the friction velocity, u_* , and the wind direction θ , we can view any quantity taken from the wind library as a function of the two parameter space (u_*, θ) . We established two flow fields. One is without HVAC systems and another is with HVAC system as described in section 2.2. Both flow fields use $u_* = 3.5\text{m/s}$ and $\theta = 135$ degrees for the prevailing wind conditions and these flow fields are remaining steady during the period of the gas release.

2.4 Gas Dispersion

One puff source and four moving sources are assigned in the area. One puff source releases 1 g/s mass for 15 minutes and four moving sources those move along the streets at the rate of 5 m/s, assuming pollutants from cars, release 1.e-03 g/s of mass along the streets.

Figure 2 presents the gas dispersion as a function of time. The red iso-surface indicates that the gas came from the puff source (toxic gas) and the entire space within the red iso-surface has 1 part per billion by volume (PPBV) or greater species concentrations. Iso-surface colors other than red indicate that the gas came from the moving sources (pollutants) and the space within the colors has 1 part per trillion by volume (PPTV) or greater species concentrations. We learned from these iso-surface plots that some dispersed gases are locally trapped and reside in the area for a long time.

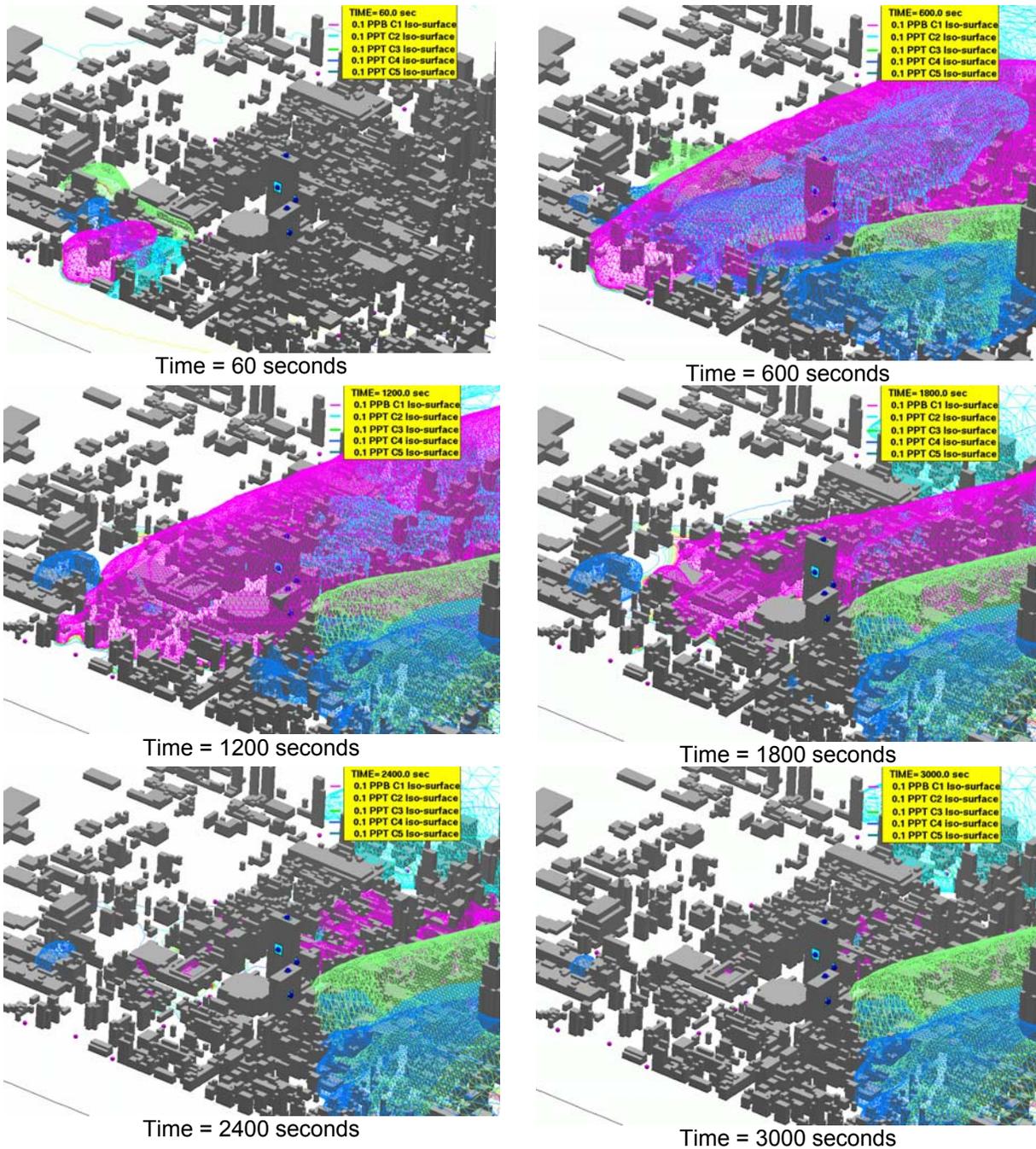
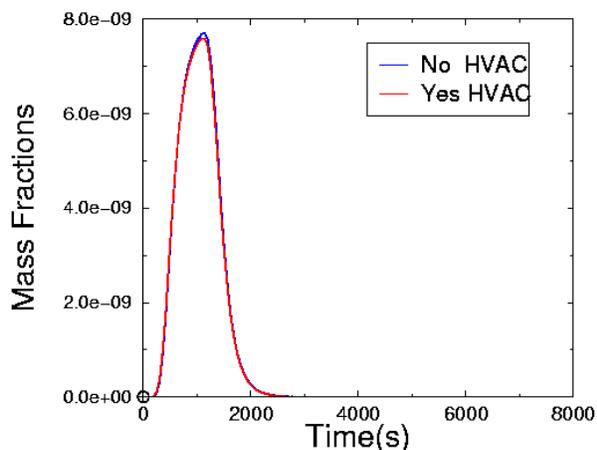


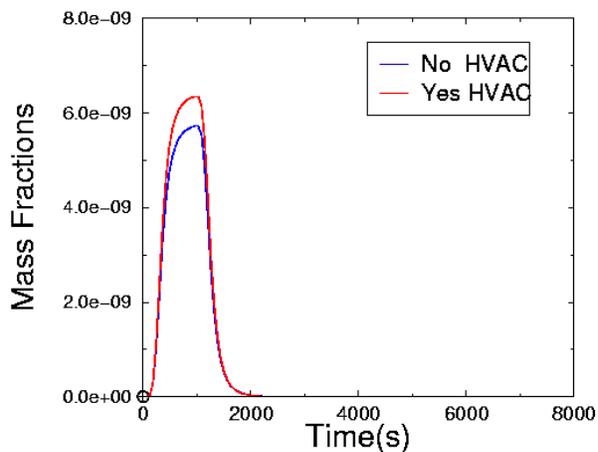
Figure 2. Gas dispersion in urban area.

Figure 3 presents the gas concentrations of toxic gas at each intake/exhaust window on the monitored buildings (probes 1 to 11 in Figure 1). The red curve represents the results where there are HVAC systems in the buildings, while the blue curve represents the results where there are no HVAC systems. Two concentration curves at each monitoring location reflect that the air in and out from the window of HVAC system of buildings disturbs the local flow field. As shown in Figure 1, the building with probes 10 and 11, that is, the low level building near the gas source is exposed to the high concentrations of toxic gas. The gas residence time for the case of no HVAC systems is much longer than that for the existence of HVAC (see probes 10 and 11). The buildings with probes 4, 5, 8, and 9 are located at the outskirts of the gas cloud and less exposed to the toxic gas. Since probes 6 and 7 are located high level from the ground, less amount of the toxic gas is dispersed.

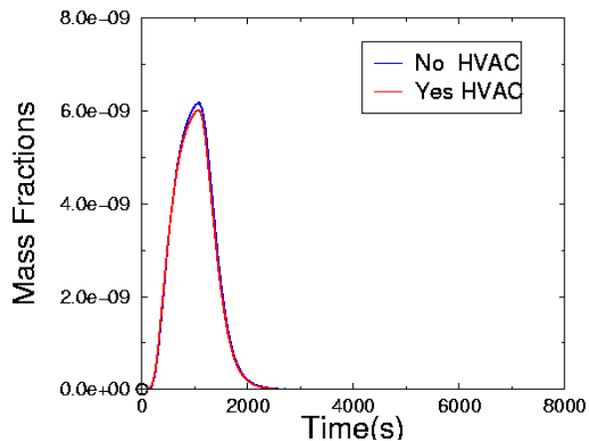
C1 Mass fraction vs. Time at Probe 1



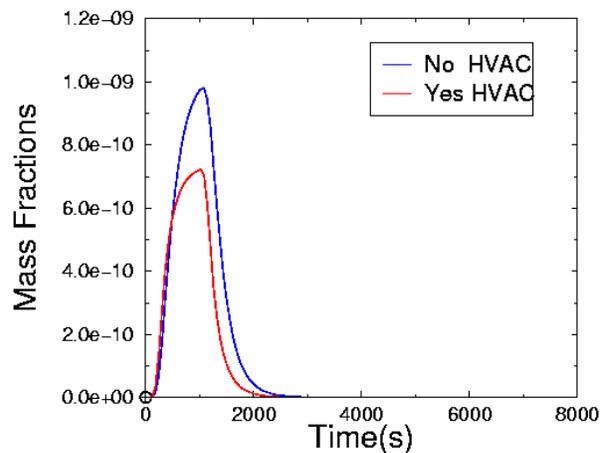
C1 Mass fraction vs. Time at Probe 2



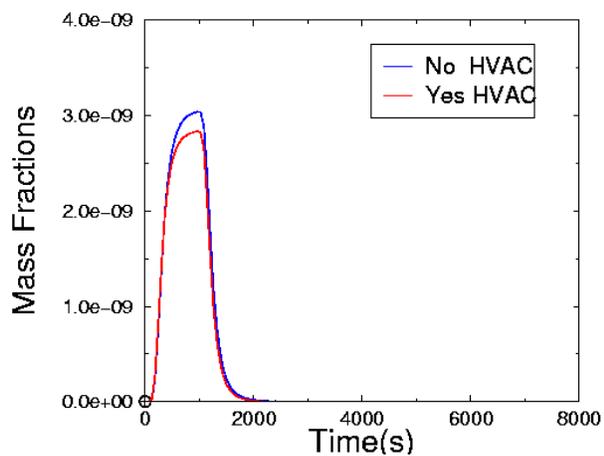
C1 Mass fraction vs. Time at Probe 3



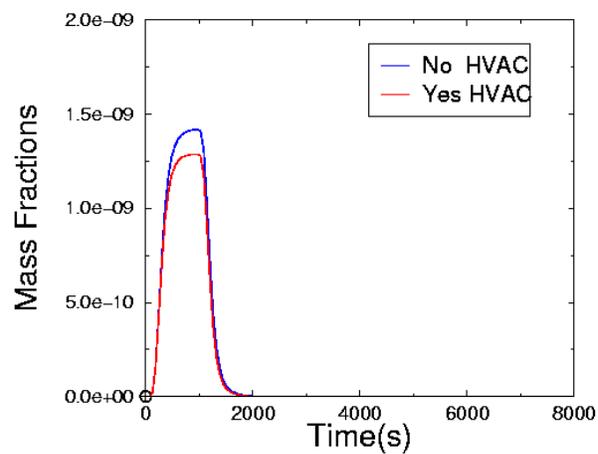
C1 Mass fraction vs. Time at Probe 4



C1 Mass fraction vs. Time at Probe 5



C1 Mass fraction vs. Time at Probe 6



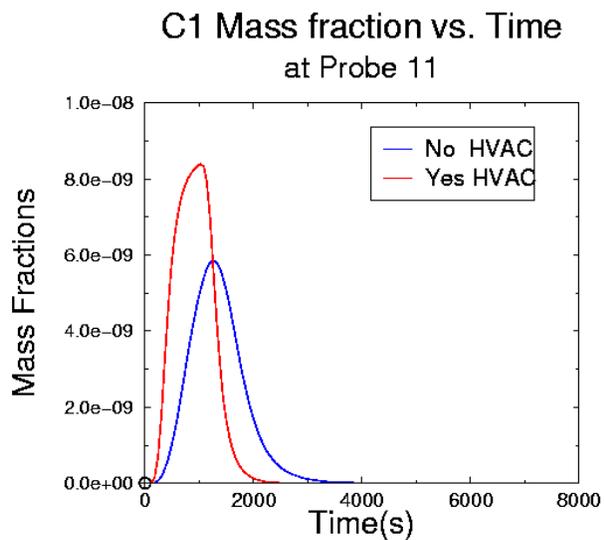
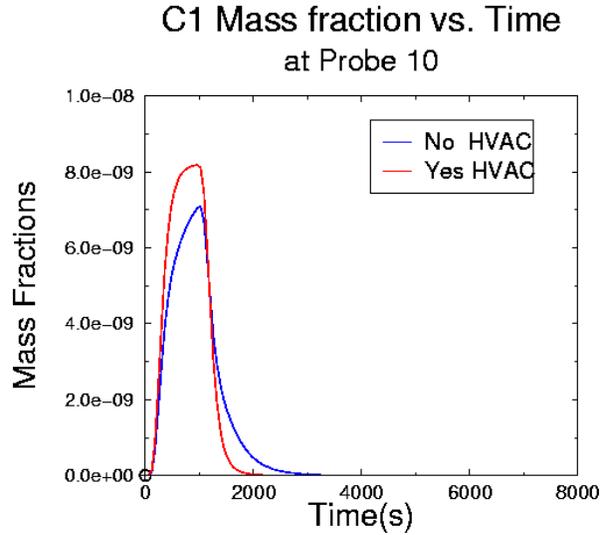
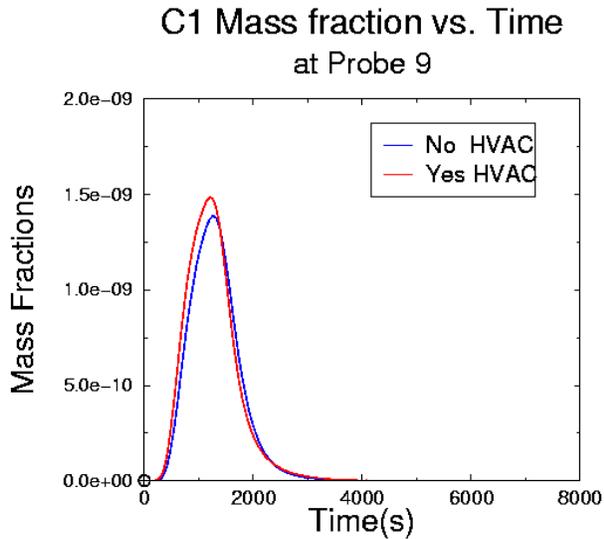
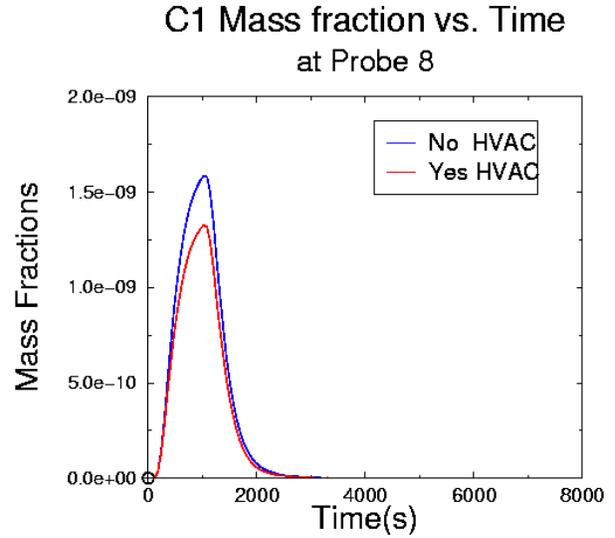
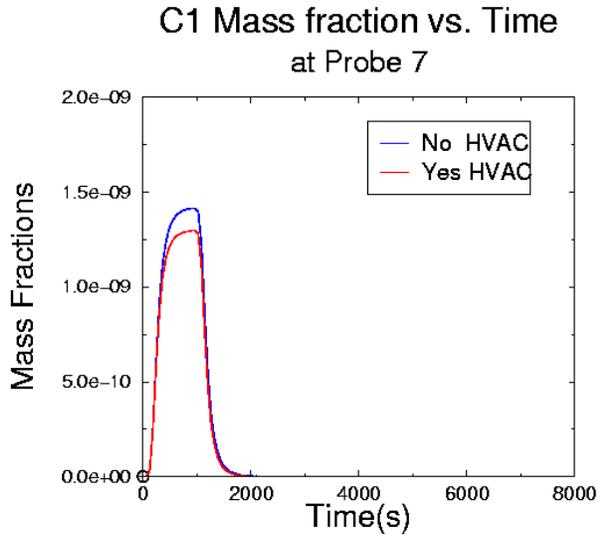


Figure 3. Gas concentrations of toxic gas at each intake/exhaust windows.

It is interesting to note that probe 1, located in the wake zone (see Figure 1), shows 30 percent higher concentrations than the probe 2, located in front of the building. But the residence time of the toxic gas in the wake zone (probe 1) is not necessary longer than that in the area exposed to the flow directly (probe 2).

5. CONCLUSIONS

We have demonstrated a technique that may be used to predict an intake amount of toxic gas at buildings having HVAC systems those are exposed to potentially hazardous environments. The approach is based upon using high-resolution CFD-generated wind fields in conjunction with the wind library.

In this paper we have outlined the steps taken to perform the gas dispersion predictions. We have shown that the existence of HVAC systems may effect the urban area gas dispersions. We are able to predict the amount of gas infiltrated into the buildings. When a building is located near the gas release source, more gas may be infiltrated into the building which has a HVAC system.

When a building is located near the source, the HVAC systems may blow away the dispersed gas. When buildings are located rather far from the source and HVAC systems are located in the wake zone, HVAC systems do not significantly affect building gas infiltration. The gas concentration in the wake zone is higher than the gas concentration in the area of facing wind directly.

7. REFERENCES

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