3.4 EXAMINING VARIOUS SPATIAL SCALES OF A HYPOTHETICAL CHLORINE RELEASE ON A COLLEGE CAMPUS

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1. INTRODUCTION

1.1 Motivation

The release of a hazardous airborne material into a densely populated area could affect large numbers of people in a short period of time. Because hazardous materials are often stored near highly populated regions, a thorough assessment of the potential hazard is a critical task for community preparedness. In order to properly protect a population, safety measures such as rapid response plans and evacuation procedures must be developed before an event occurs.

This study focuses on one step in developing a rapid response plan: assessing exposure levels that could result from the release of a potentially harmful contaminant. A complete plan might also consider what response is most appropriate, such as sheltering-in-place, sheltering-on-the-run, or evacuation. Because we consider a densely populated area, a crowd behavior model would aid in determining the best evacuation plan.

Here we study the atmospheric transport and dispersion (AT&D) of a chlorine release on a hypothetical college campus. We use state-of-the-science modeling capabilities to assess an extreme-release scenario. Two different approaches are used for near source and regional dispersion predictions. The first approach uses a Computational Fluid Dynamics (CFD) model to resolve explicitly much of the detail of the near source micrometeorology providing a realization of the dispersion event. The CFD flow solver, AcuSolve™, will be described in more detail below. The second approach uses the Hazard Prediction and Assessment Capability (HPAC) system that includes both an Urban Dispersion Model (UDM), suitable for near source AT&D, and Second-Order Closure Integrated Puff Model (SCIPUFF) for regional scale AT&D. HPAC is a probabilistic model that yields a prediction for the ensemble mean plume, useful because the meteorology and source term information is unlikely to be known accurately.

Models like HPAC are practical for making rapid response decisions because run-times are on the order of seconds for near-source predictions to several hours for regional dispersion predictions that are forced by fine-scale mesoscale Numerical Weather Prediction (NWP) output. The corresponding run-time for a practical application of a CFD model for near-source dispersion only may be on the order of hours to days.

1.2 Background

Several railcar accidents in recent years have brought much attention to the study of chlorine dispersion. Buckley et al. (2007) review the real-time response to such an accident as well as conduct a post-analysis of the incident. In January 2005, a freight train collision in Graniteville, SC released nearly 70 tons of pressurized liquid chlorine into the atmosphere. The chlorine vaporized upon contact with the air and a dense cloud formed quickly and spread to the surroundings. The event resulted in nine deaths and more than 500 injuries. In this case, the emergency managers used a Puff/Plume and Lagrangian Particle Dispersion Model to aid in their decision making and used HPAC later in their post-analysis. Buckley et al. stresses the importance of rapid response models that are easy to interpret and provide information quickly enough to pass along to emergency managers.

Hanna et al. (2007) conducted a comprehensive analysis of six commonly used dense-gas dispersion models to study how each model assessed the effects of three recent railcar accidents. They studied the release of 21,792 kg of chlorine in Festus, MO in 2002, the release of 54,480 kg of chlorine in Macdona, TX in 2004, as well as the Graniteville release. While Hanna et al. found generally good agreement for concentration fields among the six models, they point out that an accurate source term is critical to the computation of reliable results. They also recognize the need to incorporate chemical reactions, photolysis, and deposition into existing models.

The chemistry of chlorine itself can greatly complicate the atmospheric transport and dispersion of a release. Chlorine is a greenish-yellow highly reactive gas with a strong, offensive odor (National Research Council, 2004). The chlorine vapor is approximately 2.5 times heavier than air so a cloud will form very near the release and the transport is likely to stay near the ground, which causes accurate prediction to become complicated by the presence of buildings and other structures. Pressurized liquid chlorine presents an additional challenge because a small hole in a chlorine tank creates a jet that expels much of the chlorine in an extremely short period of time (Fauke & Epstein, 1988). Following this initial release, there is a slow release of the remaining liquid and vapor phase chlorine often referred to as off gassing (Buckley et al., 2007). The dual phase nature of chlorine spills makes determining the actual amount of chlorine released extremely difficult.

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The health effects associated with chlorine are extremely dependent upon the duration of exposure and the fitness of the individual. We make no attempt to analyze or assess the various guidelines currently in place. The following refers to the acute effects guidelines of the Environmental Protection Agency (2007). Irritation of the eyes, nose, and throat has been noted at exposure levels less than 1 ppm. The odor threshold for chlorine is 0.3 ppm and the smell of a chlorinated swimming pool is typically associated with a concentration value of 1 ppm. At higher levels of chlorine (30 ppm) chest pain, coughing, shortness of breath and vomiting has been reported. Toxic pneumonitis and pulmonary edema have been reported from 46 – 60 ppm.

1.3 Study Objectives

The objectives of this study are to provide a high quality modeling study for a worst-case scenario, to assess the relative accuracy of the rapid response tools, and to provide an analysis of the maximum possible impact of the release on the nearby population. To this end we use both a rapid response AT&D approach (HPAC) and a CFD modeling approach to illustrate different modeling aspects in an effort to aid development of emergency response preparedness for a worst-case scenario. We seek to provide the results of the physical modeling of the atmospheric transport and dispersion as a case study for situational awareness and preparedness planning. We also assess the similarities and differences in the two different modeling approaches, including an analysis of the differences between the ensemble average approach of HPAC and the specific realization produced by the CFD model.

We use a case study of a hypothetical chlorine release on a college campus to accomplish these objectives. We use the enhanced fidelity of CFD to local geometry and meteorology to model in detail the near-source dispersing plume. That data then provides a means to assess how well HPAC is able to model short-term, near-source behavior. The CFD source is a hypothetical chlorine release inside a college natatorium vented via a fan into the separated flow on the lee side of the structure and then transported through a cluster of campus buildings toward a major football stadium. The HPAC release specifies the same release rate; however, it does not guarantee the same dispersion path between the natatorium and the stadium. Here, we also address the interpretation of both CFD and HPAC model data and how to make well informed decisions based on those data.

The paper is organized as follows: we first lay out the modeling approach, discussing the common features in section 2, the CFD methodology in section 3, and the HPAC approach in section 4. Results appear in section 5. Section 6 summarizes and discusses implications and areas of future work.

2. GENERAL MODELING APPROACH

2.1 Modeling Scenario

Typical college campuses have natatoriums and a dense student population, which makes this an interesting case to study. We choose a worst-case scenario and we model the transport and dispersion of an artificially large amount of chlorine contained in a natatorium on the day of a major sporting event with light winds transporting the material towards a stadium. We expect to produce a scenario that can subsequently be used as a starting point for planning appropriate response measures.

2.2 Source Term

Natatoriums typically store several canisters of chlorine. Assuming a worst-case event, we model the release of the entire mass of chlorine from 24 canisters at one time. This results in an artificially large release of 1650 kg of chlorine. We assume that all the chlorine is expelled from a hole in the canister over a 60 minute period, resulting in an emission rate of 0.46 kg/s. Note that we assume no measure is taken to mitigate the leak before that time.

We model the release of chlorine as emerging from an idealized leak from a single canister. We assume no liquid pooling near the source as a result of a jet. Therefore we model a vapor phase release only. Chlorine removal via dry deposition and chemical reactions are not considered, therefore concentration values are likely to be conservative or even inflated.

2.3 Weather Conditions

The initial runs assume a fixed wind direction and wind speed throughout the entire domain. In this scenario, the wind direction that is most likely to impact the stadium and, therefore, the greatest population is deliberately chosen, thus creating a worst-case scenario. In this case, 205° will be most effective at transporting the material towards the stadium. High winds cause rapid advection of the material out of the area so a light wind speed of 4 ms^{-1} is used. We assume scattered clouds, no precipitation, and normal soil moisture. Later, we examine the release on a regional scale using temporally and spatially varying wind fields from actual weather data.

3. CFD METHODOLOGY

3.1 Numerical Method

The near source flow conditions and the resulting concentration patterns are most accurately computed using CFD. CFD allows for the simulation of fine structure detail of fluid flow and the resulting transport and dispersion of a contaminant. While computationally prohibitive for rapid response planning, CFD is an excellent tool for examining localized flow interacting with building structures. The proprietary flow solver, AcuSolve™, is used in this study because it is capable of modeling a passive scalar, allows for an unstructured mesh, and has a fan model (AcuSim™, 2005). It is a commercial finite element flow solver based on the Galerkin/Least squares finite element formulation and was developed by the AcuSim™ Corporation of Mountain View, CA. The simulation was run on 8 nodes at 240,000 grid-points per node for 200 hours to create the 6 minute release.

3.2 Domain and Boundary Conditions

The computational domain consists of both a large outer area representing a portion of a typical college campus, comprised of a mix of building types, Figure 1. This outer area has coupled to it a single interior room, located at the rear of the natatorium building, from which the chlorine is released. The outer area is approximately 1 km by 2 km in the horizontal and 300 m in height with a constant inflow velocity of 4 ms^{-1}. We use an unstructured mesh comprising wedge, pyramid, and tetrahedral elements. Building geometry is resolved using quadrilateral surface elements with 1 m spacing. The ground mesh is formed from nearly isotropic triangular elements ranging in size from 1 m resolution near buildings to 200 m at the far field. The nominal resolution in the spaces between buildings is about 20 m. Mesh spacing normal to all solid surfaces is 1 m. This resolution does not allow the turbulent boundary layer to be modeled explicitly. Instead, approximate boundary conditions (wall functions) are used. The implementation in AcuSolve™ steers the running average of the near surface flow toward flat-plate boundary layer statistics with an accommodation of pressure gradient effects. Details of the computational grid, comprising about 1.9 million grid points, are shown in Figures 2 and 3.

The basement interior room, Figure 2b, represents the site of the chlorine release. It contains an idealized single release location representing an agglomeration of chlorine tanks, a duct to guide the chlorine to the outside and a modeled exhaust fan. In order to satisfy continuity, a door open to the inside of the building allows air to enter the room replacing the exhausted volume. The pressure-drop in the room caused by the exhaust fan precludes flow from the room into the building interior. The exhaust fan is modeled as a 0.3 m by 0.3 m opening with body forces acting as the fan; it expels the chlorine from the storage room at a flow rate of 60 ms^{-1}.

Figure 4 depicts the boundary conditions used in this analysis. Flow enters the domain by a specified inflow boundary condition at a constant 4 ms^{-1}. Symmetry boundaries are used on the walls parallel to the flow as well as at the top of the mesh. An exit-type boundary condition is applied to the exit of the domain as well as the open door in the chlorine room. This is a characteristic-type boundary that can allow flow in any direction. Thus, it provides for outflow at the northern boundary and inflow from the open door to the basement chlorine tank storage room of the natatorium. Solid-wall no-slip conditions are employed on all solid walls, including those of the interior walls.

The computational model uses detached-eddy simulation (DES), a hybrid approach that blends Reynolds Averaged Navier Stokes (RANS) modeling near walls and in the far field with Large Eddy Simulation (LES) within building wakes. The transition between the RANS and LES regions is controlled by local grid resolution. The grid is constructed to maintain LES in the region containing the chlorine plume. This method provides fine-scale time varying features of the flow field without sacrificing much of the computational economy of RANS. The initial guess for the DES solution was a converged RANS solution for the geometry with the same boundary conditions. This initialization sets up the dominant shear layers. Once the vortices, channeling, and separation behind buildings are fully developed in the flow, the chlorine is released and the simulation is allowed to transition to DES.

4. HPAC/SCIPUFF METHODOLOGY

4.1 HPAC/SCIPUFF Model

The second model used is the HPAC transport and dispersion package developed by the Department of Defense to provide rapid response modeling of the transport and dispersion of a harmful contaminant (HPAC User's Guide, 2001).

Part of the appeal of HPAC for this application, is its ability to model dense gases, such as chlorine, and its Urban Dispersion Model (UDM) which accounts for building interactions and wakes. The UDM option of HPAC requires a database of building locations and geometries. The preprocessor, Urban Wind Model (UWM) alters the wind field to assure continuity. An advantage of UDM is that it provides rapid calculation of an urban flow in the spirit of CFD models. Unlike CFD, UDM does not account for channeling effects (Neuman, 2006). UDM has three different puff splitting parameterizations depending on whether the puff interacts with one building, a group of buildings, or an entire urban setting. In an urban environment puffs become larger than the structures in their path resulting in greater lateral dispersion than a model without UDM.

At a distance farther from the source, HPAC transitions to using the SCIPUFF AT&D model. SCIPUFF is a sophisticated puff-based transport model used in HPAC that accounts for turbulence, terrain, and weather effects in its calculations (Sykes, 2004). SCIPUFF uses sophisticated methods to track the puffs, evolve the dispersion coefficients, split the puffs, and incorporate advanced methods to assess turbulence levels.

HPAC allows for the setup of various source scenarios and uses high-resolution meteorology to calculate the amount of material released into the environment. HPAC runs with UDM take as a little as 5 minutes to complete on a single processor for this setup.

4.2 HPAC Domain

Since UDM works with the building aware UWM to model shunt the flow around the buildings, it is necessary to provide a database of building configurations. Such a database was provided for the college campus and environs. The near source domain illustrated in Figure 5 is approximately 1 km by 2 km in size and includes traditional college buildings ranging from 3 to 10 stories in height. The dormitory buildings, academic buildings, stadium, event center, and natatorium coupled with open areas create inhomogeneous terrain.

We also use HPAC to explore the regional transport of the chlorine over a much larger domain. That larger domain is defined in conjunction with the weather data, including detailed terrain data.

4.3 Complex Weather Conditions

For the regional transport analysis meteorological data from a 24 hour long, 4 km grid resolution run of the NCAR/Penn State MM5 mesoscale model are used. The scenario chosen emphasized light winds from the southwest (to transport the contaminant toward the stadium) on a warm sunny data that would include a high level of atmospheric turbulence. The data are converted into MEDOC (Multiscale Environmental Dispersion Over Complex terrain file) format that is compatible with SCIPUFF. MEDOC data provides time-dependent wind, temperature, humidity ratio, terrain elevation, boundary layer height, and surface heat flux, at a number of x, y, z grid points on the 4 km grid (Sykes, 2004). Incorporating MEDOC data into the calculation increases the computation time significantly, from several minutes using a single wind speed and direction to several hours for the high resolution MEDOC data.

5. RESULTS

The CFD simulation produced a coupled flow between the chlorine room and the external flow field forced by an exhaust fan. Figure 6 illustrates the flow of chlorine throughout the storage room 3.3 minutes after the release. Several streamlines indicate the flow of chlorine leaving the tank, traveling through the room, and exiting via the exhaust. Two cut planes, one in the vertical and the other in the horizontal indicate the chlorine concentration patterns. Higher concentration levels are indicated in red and orange and lower levels are indicated in blue and green. Near the open door, fresh air enters, resulting in lower concentrations in that vicinity. The duct leading to the exhaust fan shows the chlorine being vented from the room and mixing with the fresh air outside.

The external flow field produced by the DES run appears in Figure 7. We note the pervasive horseshoe vortices upwind and around the sides of each building. Such features assure us that the CFD model is producing appropriate vortical structures that are expected to influence the transport and dispersion of the chlorine. The CFD-produced chlorine plume is indicated in Figure 8. It exhibits fine structure in the wakes behind buildings and pockets of higher concentration due to the time dependent vortical structures. There is ample evidence of the influence of the building geometry on both the flow and the dispersion of the chlorine.

The comparable chlorine plume produced by HPAC appears in Figure 9 , both two (Figure 9a) and six (Figure 9b) minutes after the release. The irregular shape of the 59.0 and 29.5 mgm^{-3} contours suggests distortion of the plume due to building interactions as computed by UDM. After 6 minutes a very low concentration, 1.45 mgm^{-3} (0.5 ppm), begins to reach the stadium.

It is instructive to compare the HPAC results with the CFD simulation. Six minutes following the release the CFD simulation (Figure 8) keeps the 60 mgm^{-3} contour confined more closely to the natatorium and channels the flow between several of the buildings downwind. While HPAC (Figure 8b) does not capture the channeling effects found in CFD (Figure 8), the two still exhibit favorable agreement in width and lateral extent of the plume as well as concentration levels. The plumes generated by HPAC (Figure 9) are the result of an ensemble of realizations and as such we expect them to appear more Gaussian in nature than the single realization of the CFD simulation.

One advantage of applying HPAC is that it additionally includes a probabilistic model, allowing us to assess the probability of exceeding a specific concentration level. The probability plots in Figure 10 suggest the likelihood that a given region will experience a concentration above 1 ppm (3.9e-6 kgm^{-3}) for 6 (Figure 10a) and 61 (Figure 10b) minutes following the release. Figure 10 suggests that the plume is nearly steady after 6 minutes since it changes very little when compared to the plume after 61 minutes. Also, the probability of exceeding 1 ppm at the stadium is less than 30% 61 minutes following the release. Recall that 1 ppm is the level commensurate with the smell of a typical swimming pool. Probability plots of 10 ppm concentrations (not shown) confine the region of exceedence to within ~400 m of the natatorium. Note that the stadium is approximately 800 m from the natatorium so it is unlikely that the large population in the stadium would experience health effects. Probability plots of 30 ppm and greater (not shown) confine the region of exceedence to the immediate vicinity of the leeside of the natatorium. We would expect that only professionally trained personnel in Hazmat suits would be this close to the release.

The regional transport is displayed in Figure 11, which illustrates the resulting concentration 2 and 6 hours following the release. This HPAC run used the MM5 modeled MEDOC data. Note that when MEDOC data is used, one can no longer include the building geometry, necessitating a separate HPAC run. The concentration values are given in kgm^{-3} and approximately correspond to a range from 3.5e-4 ppm to 3.5e-8 ppm. The long range transport of chlorine becomes more diffuse over time resulting in levels so low that human scent detection would be unlikely.

Caution must be used when assessing health effects due to exposure because severe, acute events can be more harmful than an equivalent amount over a longer period of time (National Research Council, 2004). In the event of an artificially large chlorine release the major portion of the population present at the stadium will experience less than 3 mgm^{-3} (1 ppm) exposure and is unlikely to experience major health effects. In this study the peak concentration values were ~59 mgm^{-3} (20 ppm), which according to the EPA may cause irritation, chest pain, and cough in some individuals. However, those individuals very near the vicinity of the release could suffer harm depending on their health and the amount of chlorine they inhaled. Such individuals would be likely to self-evacuate.

6. DISCUSSION

This work has produced a worst-case scenario case study of an artificially large release of chlorine at a college natatorium. Two separate approaches allow both a validation of the rapid response model and an analysis of the differences that are expected. The rapid response model, HPAC, was used both in the near source mode that invokes the UDM building-aware model and in a regional mode that incorporates gridded mesoscale meteorological model data. The CFD simulation produced using the commercial code, AcuSolve^{TM}, exhibits the fine structure expected of a single realization model. The near source HPAC plume, on the other hand, exhibits a more diffuse plume indicative of an ensemble averaged model. The two models exhibit favorable agreement with similar plume footprints and consistent concentration levels in space and time. Thus, we conclude that HPAC provides excellent guidance for emergency managers in real time while the CFD simulation illustrates a high fidelity level of detail. As expected, the maximum concentrations for the CFD simulation are a bit higher because they have not been averaged over a large ensemble of realizations. For producing a case study, the two approaches complement each other. The CFD model provides a short term picture of what could happen in a worst-case realization. It, however, required 8 nodes and 200 hours to run a 6 minute simulation. In contrast, HPAC produces a reasonably good estimate of the near source concentrations in a matter of seconds on a desk top PC. The regional scale application of SCIPUFF, however, requires several hours using high resolution mesoscale model data.

In the future we expect to address the discrepancy between the ensemble average approach of the HPAC modeling suite with the individual realizations that are inherent to the CFD by creating an ensemble of CFD flow realizations with differing meteorological conditions. This approach is necessary to include the "outer variability" inherent in the changes in wind direction (Peltier et al. 2008). This work may also be extended further to incorporate the infiltration and exfiltration of buildings. In collaboration with other groups, we additionally hope to integrate this work into crowd behavior models.

ACKNOWLEDGEMENTS

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FIGURES

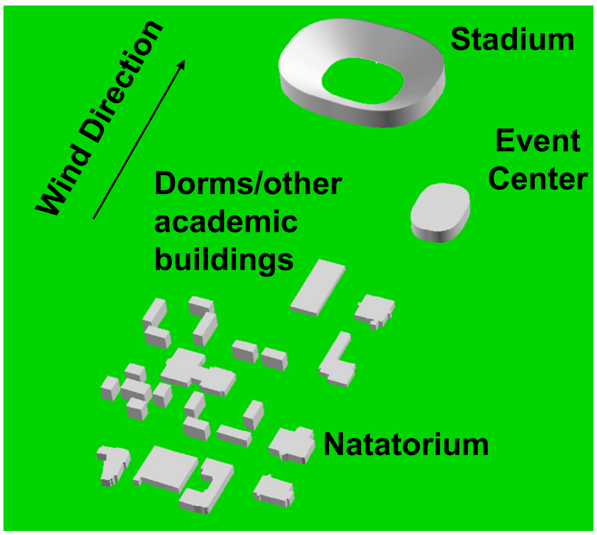


Figure 1. Various building structures typical of a college campus are indicated along with the source of the release (natatorium) and the wind direction that produces the highest impact at the stadium.

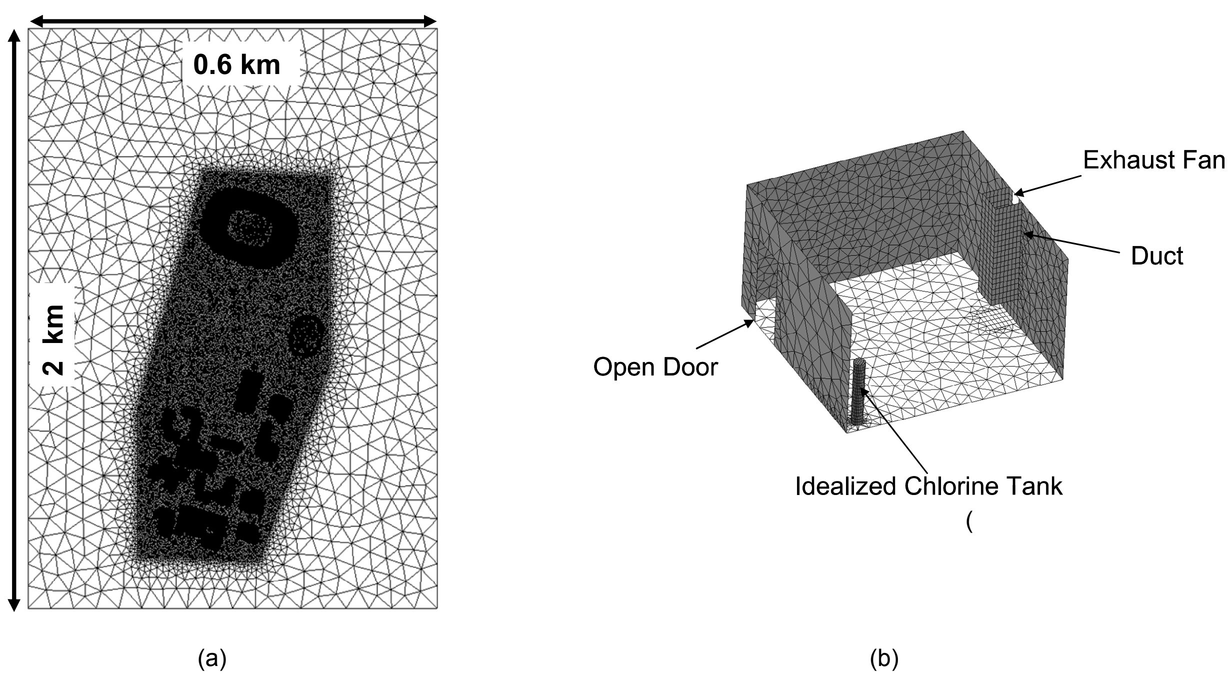


Figure 2. Computational domain and mesh for the chlorine release scenario. The overall domain is shown on the left; a close-up of the chlorine room on the right.

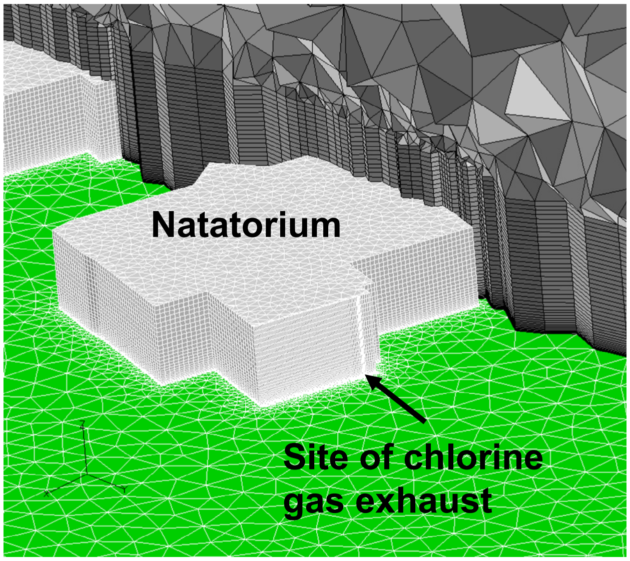


Figure 3. Cross section of the computational mesh in the vicinity of the natatorium. A combination of wedge and tetrahedral elements is used.

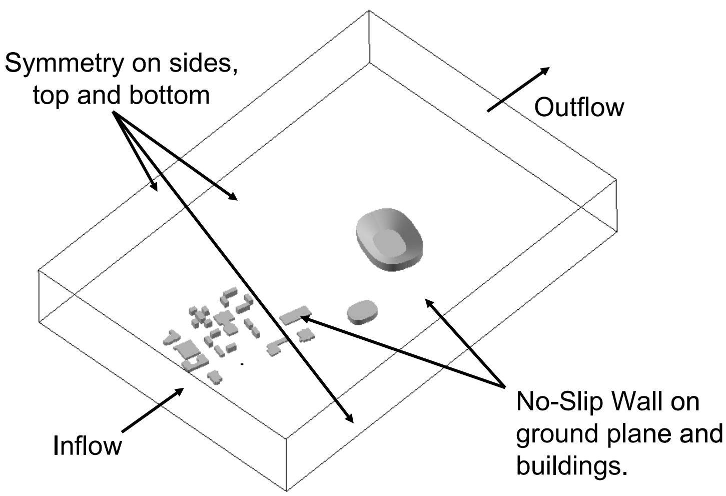


Figure 4. General boundary conditions for the chlorine release scenario computational domain.

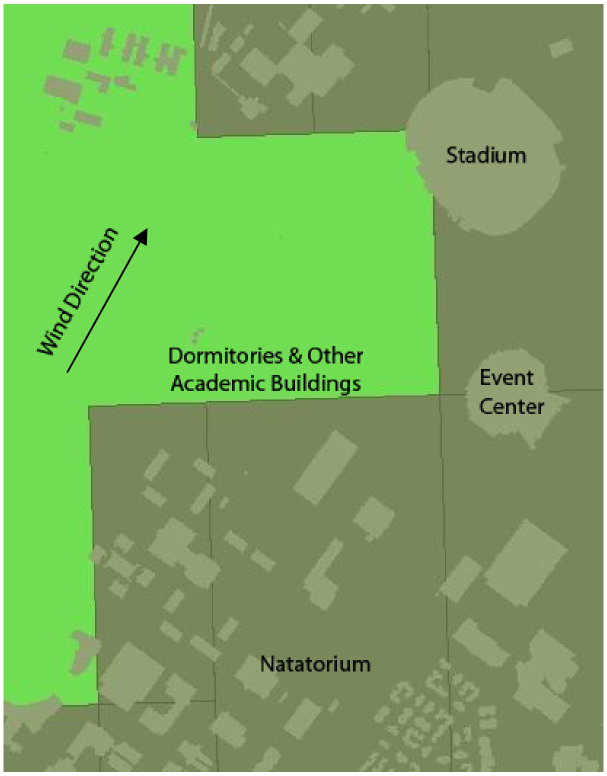


Figure 5. Near Source HPAC domain: The CFD domain is identical to the HPAC domain except the HPAC domain contains more buildings.

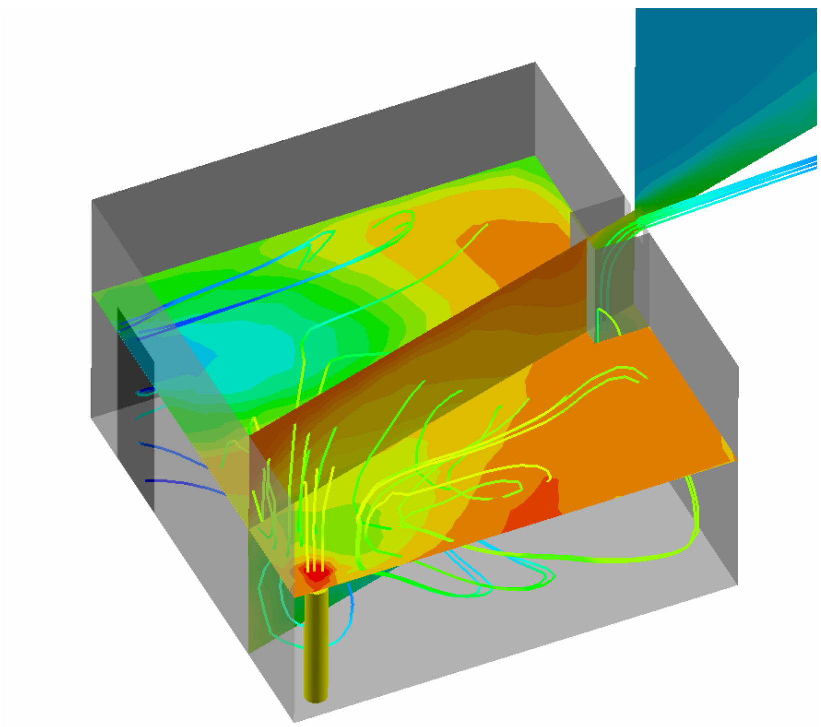


Figure 6: Flow of chlorine through the storage room 3.3 minutes after the initial release. A chlorine cylinder is indicated in the bottom left corner and the exhaust fan is located on the upper right wall.

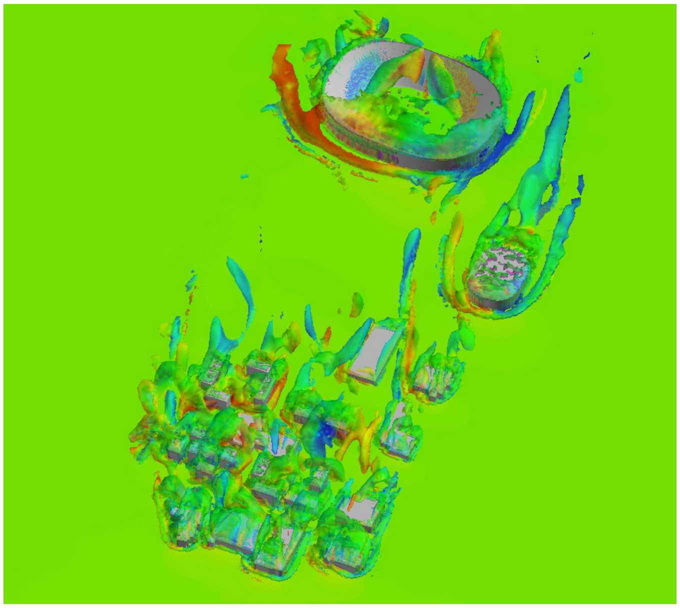


Figure 7: Vorticity (visualized by Q-criterion) colored by rotation (in terms of helicity).

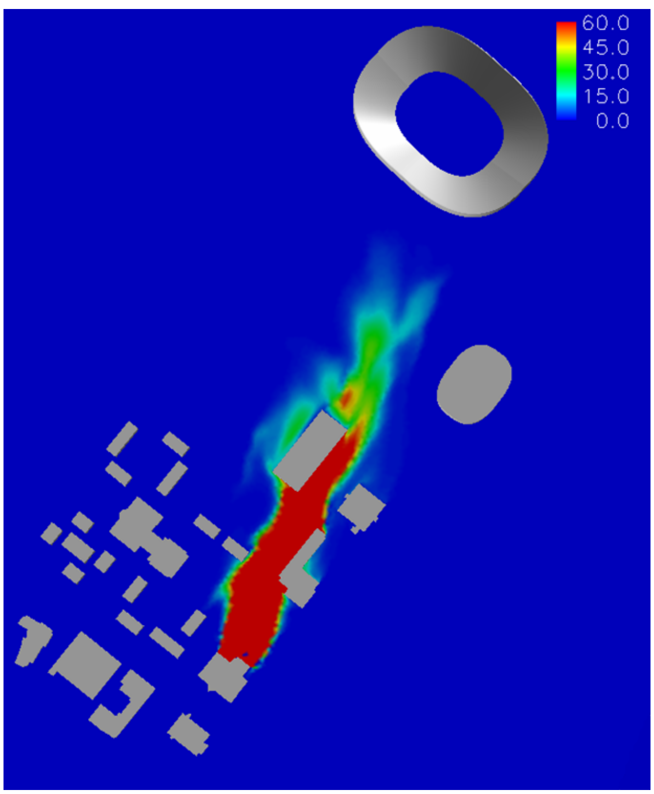
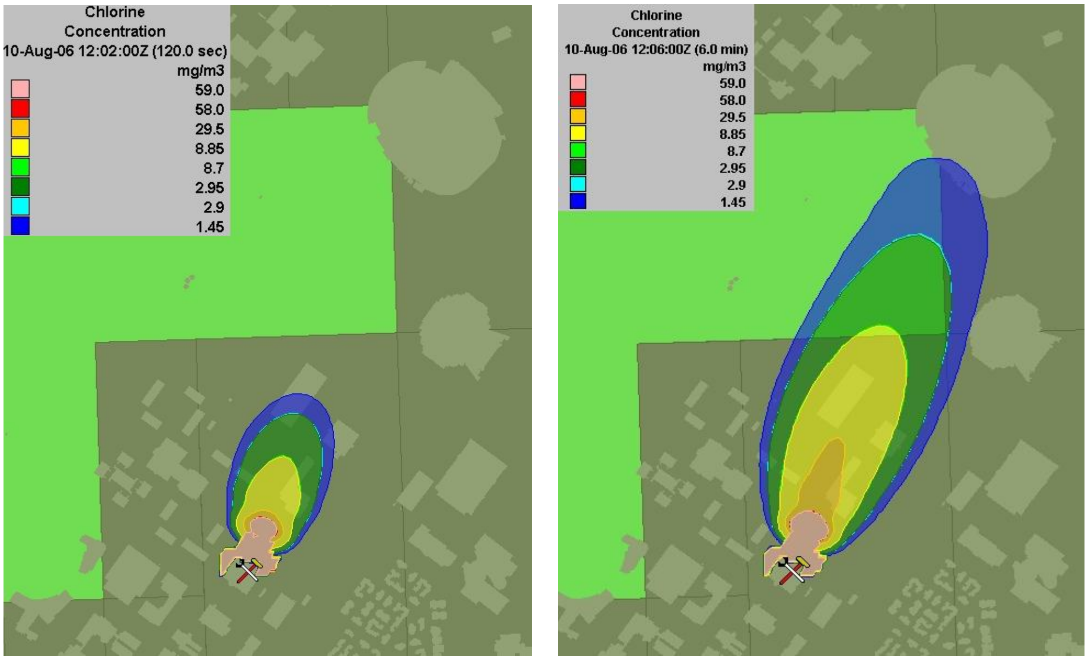
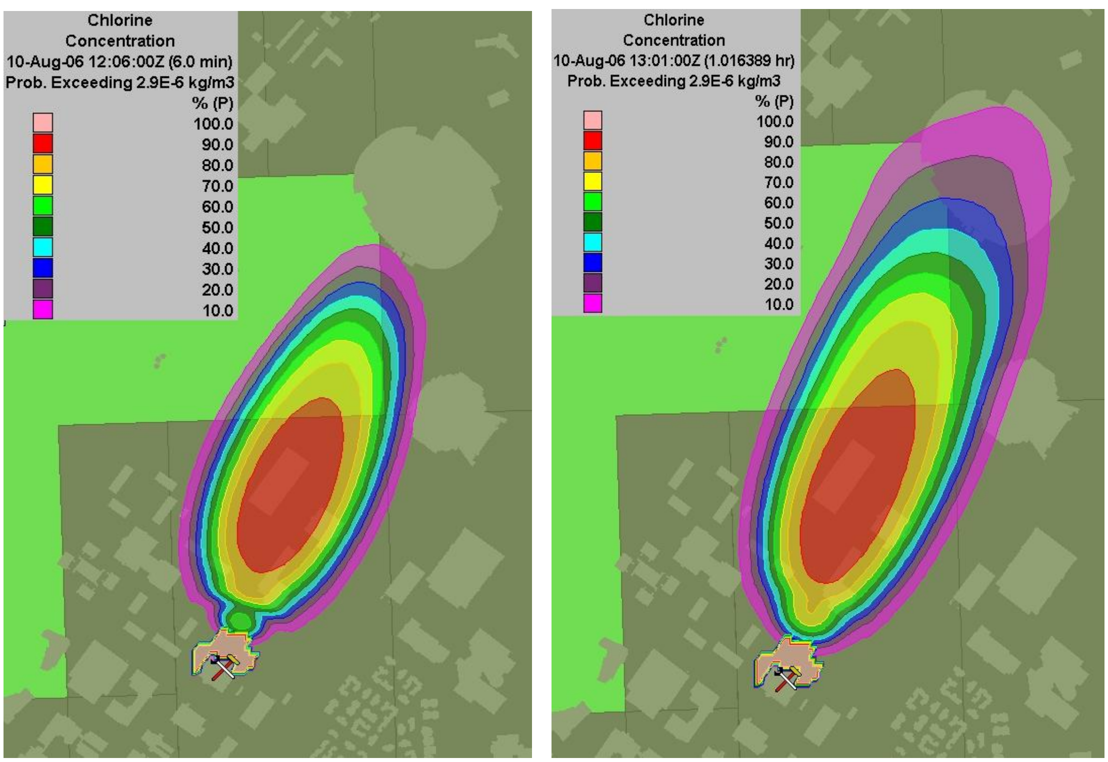


Figure 8: CFD concentration values six minutes after the onset of release. Contour levels are indicated in mgm^{-3}.



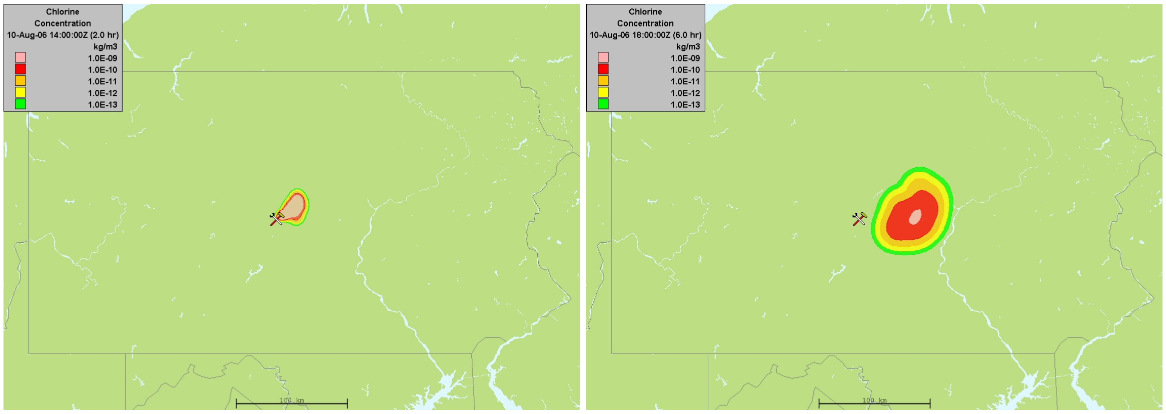
(a) (b)

Figure 9: HPAC concentration values two (a) and six (b) minutes after the onset of release.



(a) (b)

Figure 10: Probability that the concentration of chlorine will exceed 1 ppm (2.9e-6 kgm^{-3}) in a given region for 6 minutes (a) and 61 minutes (b) following the release.



(a) (b)

Figure 11: HPAC dispersion of chlorine on a regional scale two (a) and six (b) hours following the release.