J4.6 EVENT RECONSTRUCTION FOR ATMOSPHERIC RELEASES EMPLOYING URBAN PUFF MODEL UDM WITH STOCHASTIC INVERSION METHODOLOGY

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ABSTRACT

The rapid identification of contaminant plume sources and their characteristics in urban environments can greatly enhance emergency response efforts. Source identification based on downwind concentration measurements is complicated by the presence of building obstacles that can cause flow diversion and entrainment. While high-resolution computational fluid dynamics (CFD) simulations are available for predicting plume evolution in complex urban geometries, such simulations require large computational effort. We make use of an urban puff model, the Defence Science Technology Laboratory's (Dstl) Urban Dispersion Model (UDM), which employs empirically based puff splitting techniques. UDM enables rapid urban dispersion simulations by combining traditional Gaussian puff modeling with empirically deduced mixing and entrainment approximations. Here we demonstrate the preliminary reconstruction of an atmospheric release event using stochastic sampling algorithms and Bayesian inference together with the rapid UDM urban puff model based on point measurements of concentration. We consider source inversions for both a prototype isolated building and for observations and flow conditions taken during the Joint URBAN 2003 field campaign at Oklahoma City.

The Markov Chain Monte Carlo (MCMC) stochastic sampling method is used to determine likely source term parameters and considers both measurement and forward model errors. It should be noted that the stochastic methodology is general and can be used for time-varying release rates and flow conditions as well as nonlinear dispersion problems. The results of inversion indicate the probability of a source being at a particular location with a particular release rate. Uncertainty in observed data, or lack of sufficient data, is inherently reflected in the shape and size of the probability distribution of source term parameters. Although developed and used independently, source inversion with both UDM and a finite-element CFD code can be complementary in determining proper emergency response to an urban release. Ideally, the urban puff model is used to approximate the source location and strength. The more accurate CFD model can then be used to refine the solution.

1. INTRODUCTION AND BACKGROUND

In the event of an atmospheric release, effective consequence management depends on how much is known about the release event and how quickly the problem can be analyzed to an operationally required degree of certainty. Accurate quantification of specific details of a release can greatly assist relief efforts and subsequent forensic analysis. Such quantification, rarely a straightforward task, becomes particularly complicated when the release occurs in the presence of building obstacles that can cause flow and dispersion complications. To assist the rapid analysis of atmospheric releases, the 'event reconstruction' (ER) methodology was developed to provide answers to the questions surrounding a release event: (1) what was released, (2) how much was released, and (3) when and where it occurred (Aines et al. 2002; Kosovic et al. 2005). The ER approach developed at Lawrence Livermore National Laboratory is a Bayesian inference methodology combining observed data with forward predictive models to determine unknown source characteristics. This capability can leverage from a large computational framework that supports multiple stochastic algorithms, forward models, and runs on a wide range of computational platforms. To analyze urban dispersion rapidly, the ER methodology was linked to the rapid urban puff splitting model, the UDM Version 2.2, developed by Dstl, a United Kingdom Ministry of Defence Lab located in Porton Down. For this study, the stochastic algorithm used in the Bayesian inference scheme is a Markov Chain Monte Carlo (MCMC) algorithm. All UDM and ER runs were processed for this effort using a single processor on an MS Windows operating system.

The Urban Dispersion Model (UDM) is an empirical puff model that estimates atmospheric dispersion in an urban environment by differentiating three different puff splitting regimes (open, urban, and long-range) based on empirical evidence. Different dispersion modeling procedures are applied for each regime in such a way to account for the effect of single building, building clusters, or an entire urban environment on the dispersion of Gaussian puffs (Hall et al. 2003).

In the open regime, the overall proportion of the surface covered by obstacles is less than five percent. The puffs arising in this regime travel across a largely open terrain over which single obstacles or groups of obstacles are distributed. Interaction with these obstacles changes the size and rate of travel of the puff. If the obstacle is of sufficient size in comparison to the puff, the puff will split: a portion of the material will become entrained in the wake of the building while the remainder proceeds largely unaffected. The fraction of the puff that is entrained will spread uniformly across the entrainment region and be delayed by a characteristic wake residence time. After interaction with the obstacle, puff spreading of both the unentrained puff and the entrained puff is increased due to turbulence in the recovery region.

In the urban regime, the plan area density of the obstacles is greater than five percent. The single obstacle interactions utilized in the open regime are no longer valid due to interference with multiple entrainment regions from densely distributed obstacles. Puffs quickly become large

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enough to encompass obstacles resulting in a lateral dispersion that is effectively higher than the value given by traditional puff models due to puff interaction with surface obstacles. Atmospheric stratification is assumed neutral in this regime for UDM 2.2, a reasonable assumption as mechanically generated turbulence in the urban environment is likely to dominate dispersion near the ground. For the long-range regime the puff is large compared to any surface obstacles, and puffs are treated with conventional Gaussian dispersion modeling techniques.

The UDM was implemented into the existing ER framework to provide rapid results taking urban obstacles into consideration. The UDM implementation complements efforts employing the FEM3MP CFD model (see Chan et al. (2001); Chow et al. (2006)). The UDM is computationally expedient enough to run on a single processor, as a typical forward simulation with over 100 buildings requires less than a minute to complete for the most complicated case (a similar CFD run requires on the order of 100 CPU hours). Other advantages of using the UDM for rapid analysis are its relative ease-of-use with customizable buildings, source strength and location, and easily described sensor locations. Disadvantages of using a simple empirical model with ER include the fact that empirically based building-wake entrainment and detrainment methods inherent to such a model create inversion difficulties due to discontinuities. Also, the simple wind field and puff splitting techniques which allow for rapid dispersion calculations tend to lead to reduced accuracy in comparison to CFD modeling. As an example of lost detail, the UDM does not directly model channeling effects between buildings, a phenomenon typically observed in urban experiments, including the URBAN 2003 field campaign (Allwine 2004). However, depending on source location relative to important building obstacles, puff entrainment and detrainment can provide some compensation for the lack of channeling effects (Figure 1). The Oklahoma City example discussed below demonstrates the problems that this can cause in the final source characterization.

Two example ER scenarios using the UDM are discussed below. The first scenario is for simple flow around a cubic building; the second scenario is a release in downtown Oklahoma City for observations and flow conditions during the Joint URBAN 2003 field campaign. In both simulations, the event reconstruction code simultaneously samples both source location and source strength. In the UDM 2.2, source strength is represented by total mass released, and results of probable source strength are presented in this way.

2. RECONSTRUCTION METHODOLOGY

The ER framework for this study performs stochastic inversion using MCMC techniques (see, for example, Gelman et al. (2003)). The procedure is as follows: 1. estimates of source location and source strength are obtained from a defined prior distribution or proposal distribution of source term parameters; 2. the forward model (UDM) is run using these input values; 3. the output sensor data from the forward model is compared to the observed data using Bayes theorem; 4. the sampled source term configuration is either accepted or rejected following a Metropolis-Hastings algorithm; 5a. if accepted, the likelihood function is updated and the values used in the next iteration are sampled from the proposal distribution centered on the accepted value; 5b. if rejected, the next point is selected based on the last accepted value; 6. this process is repeated for a large number of iterations until the convergence to a posterior probability distribution of source term parameters (representing the solution to the inverse problem) is achieved. Effective reconstruction using Bayesian inference via stochastic sampling requires model and data error quantification. A single log-normal standard deviation distribution characterized by a single input parameter is used to represent both uncertainty in the sensor measurements and uncertainty in the forward model. The higher the input value of error, the broader the resulting probability distribution will be. More details on this methodology can be found in Johannesson et al. (2004) and in proceedings paper **J4.4** (Chow et al. 2006).

Figure 1: Given a highly complex domain, with buildings of various shapes and sizes, and concentration measurements at a few locations, is it possible to find the source of a contaminant plume with a fast urban puff model?

3. ISOLATED BUILDING

The first test of integrating UDM with the ER methodology is a simple cubic building, 10m to a side and is a follow-on study to the ‘Isolated Building’ of paper **J4.4** in these proceedings (Chow et al. 2006). Figure 2 shows a forward simulation using the UDM. The entrainment region is clearly visible in the figure. Also, the intentional slight asymmetry of the source location can be seen in the resulting plume. The ER was performed in comparison to synthetic data generated by the UDM for an ‘actual’ source location.

The resulting Markov chains for the source inversion are shown in Figure 3. The asterisks mark the initial location of each of the four chains. The diamonds represent the four sensors, and the actual source is shown as a magenta square. After some exploration of the domain space, the chains quickly converge to the area immediately surrounding the actual source location. Note that two of the Markov chains explored the entrainment re-

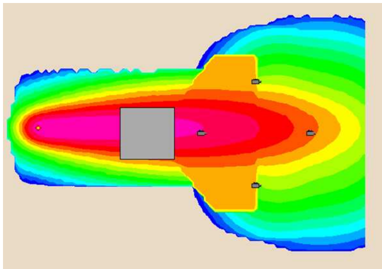

Figure 2: Horizontal concentration contours at the first vertical level generated by a UDM forward simulation for flow around an isolated cubic building. Four sensors are placed in the lee of the building.

gion. This result reflects how puffs arising in a building entrainment region are automatically fully entrained and how the detrainment process simulates a source. However, the resulting probability distribution, Figure 4, shows that the number of samples that the Markov chains sampled from the entrainment region is negligible compared to the number of samples in the vicinity of the actual source. Note the peak of the probability distribution is close to the actual source location.

In addition to the source location, release strength was stochastically sampled during this simulation. The resulting release strengths are displayed in a histogram in Figure 5. The distribution of total mass has a single, significant peak in very good agreement with the actual value, shown as a solid vertical line. When model predictions are compared to synthetic data, as in this example, the source inversion calculation is very accurate. However, to conduct source inversion for actual events, the model must be able to predict source characteristics using real data. Due to random and systematic differences between sensor measurements and model predictions, we expect that event reconstruction will be less accurate in this case.

4. OKLAHOMA CITY - JOINT URBAN 2003 IOP3

Given a highly complex domain, with buildings of various shapes and sizes, and concentration measurements at a few locations, the possibility of locating the source of a contaminant plume and determining its characteristics using a fast Gaussian puff model is of great interest (Figure 1). Event reconstruction with the UDM was applied to Oklahoma City in order to compare the model output to observations from the Joint URBAN 2003 field campaign. A standard shape file of downtown Oklahoma City was used to construct the buildings. Actual source and sensor locations were used to recreate the field experiment. An event reconstruction calculation was conducted using concentration measurements from the Intensive Observational Period 3 (IOP3) from the Joint Urban 2003 tracer field experiment in Oklahoma City with a southerly wind input. A UDM 3D puff simulation and the downtown of Oklahoma City is illustrated in Figure 6. During our simulations, one large building in the south of the modeled domain was found to play a key role. The entrainment region of this building will be shown to adjust for some deficiencies of the forward model, specifically the lack of

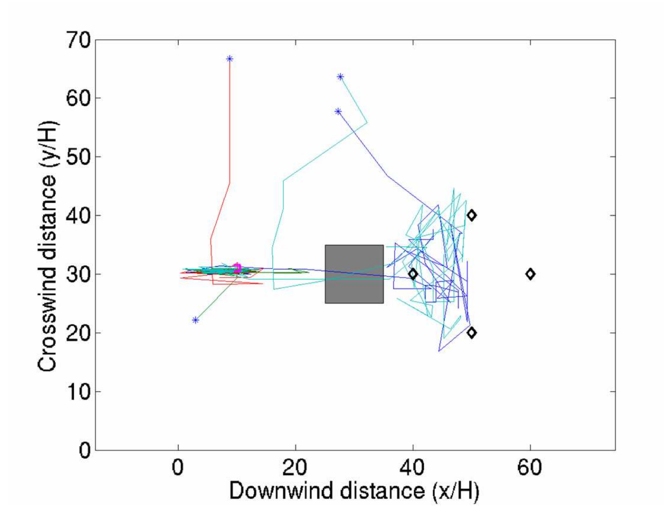

Figure 3: Paths of four Markov chains for flow around an isolated cubic building. Note that the magenta square indicates the source and the black diamonds indicate the four sensors.

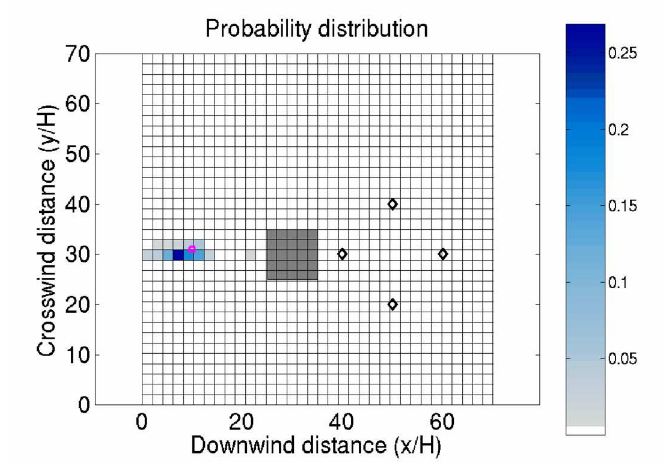

Figure 4: Probability distribution of source location for flow around an isolated cubic building.

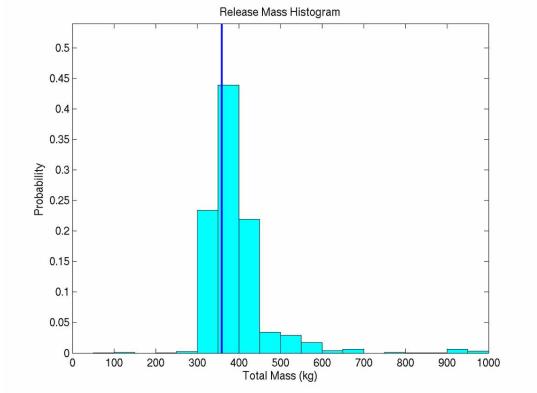

Figure 5: Histogram of source strengths for flow around an isolated cubic building. Vertical blue line indicates actual release rate.

channeling effects.

Puffs and 2D contours of ground-level concentration are displayed in Figures 6 and 7, respectively. Wind speed was 6.5m/s at 50m above ground. The number of iterations is 1700 and each of those iterations involved four Markov chains. The complete calculation took less than 33 hours on a single 857 MHz processor. Scaling linearly, if eight Markov chains are distributed to eight separate 857 MHz processors, the entire calculation, could be completed in approximately one hour.

The resulting Markov chains are illustrated in Figure 8. Note how the chains quickly converge to south of the domain. While there is good mixing by three of the chains, one chain becomes stuck in a local minimum, and remains at the northwest corner of the building. The resulting probability distribution is shown in Figure 9. There are three distinct peaks visible in the distribution. One peak is within 20m of the actual source location, which is shown as a triangle. Another peak is towards the bottom of the domain, and the third near the large building, part way between the other two locations. Three peaks are also noted in the release strength histogram, Figure 10. One peak is a very low value of release mass. The second, smallest, peak corresponds with the actual release mass, shown as a solid vertical line. The final peak is a higher value, between 8 kg and 9 kg of total mass released during the simulation.

In order to determine the probable locations that corresponded to each of the three most likely release rates, conditional probability for each was computed. Figure 11 illustrates the conditional probability of source location depending on release mass (low, mid and high) and Figure 12 illustrates the relatively rapid convergence on source location as opposed to source strength. The low peak, less than 1 kg, corresponded to the location very near the actual source location. The resulting probabilities for both location and strength are about 25%, indicating that one of the four chains spent much of its time in that location without being able to further explore the domain. This is confirmed by examining the details of the Markov chains: one chain spends the simulation in that location. The release strength is low because of the close proximity to the sensors.

The conditional probability corresponding to the actual mass, 3.1 kg < q < 4.1 kg, peaks toward the bottom of the domain, almost 200m south of the actual source location. When the source material is released in the model from the actual source location, the puffs are too narrow to hit the sensors channeling northeast of the source. When the source is located at the peak of the middle plot of Figure 11, the increased distance to the sensors and the interaction with the large building sufficiently enlarge the puff to better agree with the actual concentrations. The conditional probability corresponding to the highest release strength, 8.25kg < q < 9.25kg, is shown in the far-right plot of Figure 11. Due to its proximity to the large building, material released from this point is automatically entrained in the building's wake. Here, the entrainment region acts as a source, releasing material from the entrainment region over time. The entrainment creates a large, diffuse puff in the wake of the building, resulting in predicted source strengths for this location that are higher than the actual value.

5. DISCUSSION AND CONCLUSIONS

Event reconstruction calculations using the Urban Dispersion Model, UDM, can be performed very rapidly to provide a valid initial approximation for source location and release strength even in a complex urban environment. As an emergency response tool, event reconstruction with the UDM is more applicable than a CFD equivalent because of the speed at which a complete calculation can be completed. Ideally, results obtained from reconstruction with UDM can be used to significantly decrease the sampling domain needed to perform more accurate CFD calculations. That is, using independent data, posterior distributions obtained using ER with the UDM can be used as a prior distribution for ER with a CFD code. With a smaller domain, those subsequent calculations can be conducted much more expediently.

When conducting a source inversion calculation using the UDM as a forward model, it is important to have all Markov chains exploring the domain space in order to predict accurate source probability distributions. In order to obtain sufficient mixing, input parameters such as step size in x and y, step size in q, and quantified error should be specified carefully with attention to appropriate values relevant to the scale of the problem. Determining the correct input values for these parameters can take some trial and error. As illustrated in the Oklahoma City example, one of the main sources of error in the posterior probability distributions for complicated city examples is the lack of channeling effects in the forward model UDM. The wind field applied by UDM is very simplified and cannot reproduce complex urban flows beyond building entrainment. Channeling effects are somewhat compensated for by building entrainment effects, but the results of the reconstruction consequently may not reflect the actual source location.

The next step in this research is to test the UDM with a larger domain space and with more sensor data. Sensor data for the Oklahoma City example exists up to 4 km from the source. It is anticipated that with an extended domain, the lack of channeling producing error over the short range will have less impact on the results. Also, stochastic sampling of wind direction as well as source location and strength may give better results.

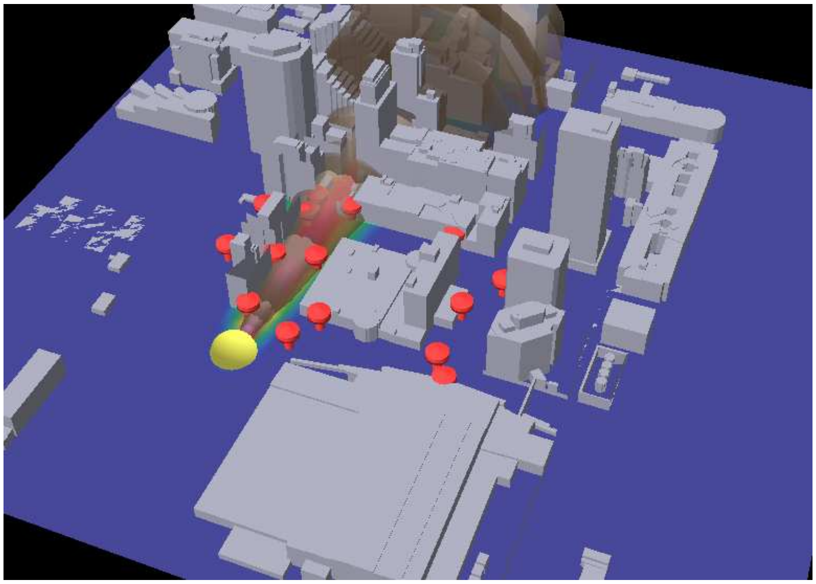

Figure 6: Three-dimensional puffs generated by a forward simulation with the UDM 2.2 for flow in and around the downtown business district of Oklahoma City. Note how the puffs expand and entrain behind the larger buildings.

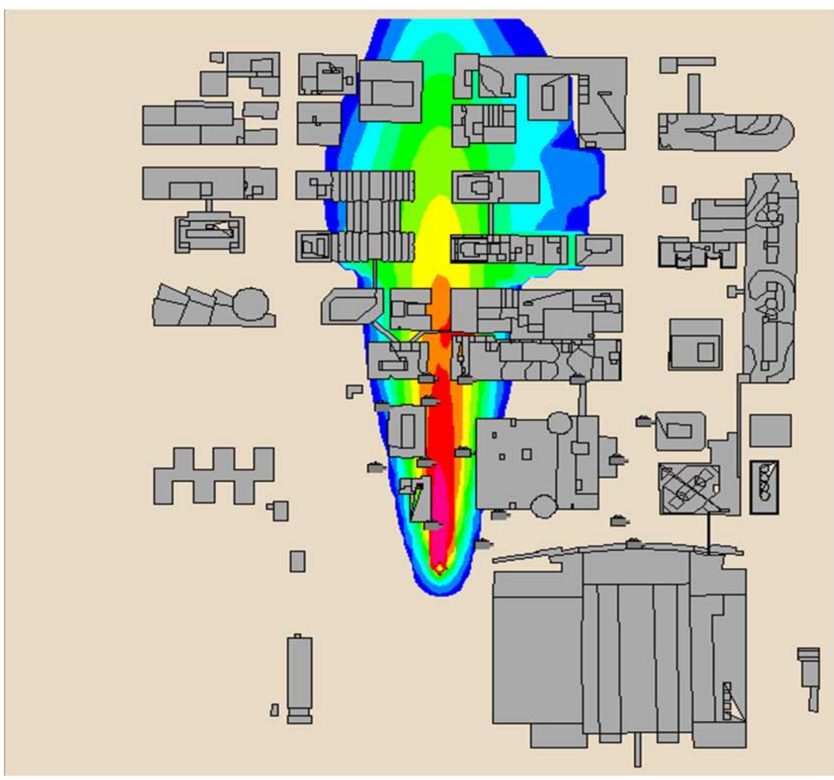

Figure 7: Horizontal concentration contours at the first vertical level generated by a single forward simulation with the UDM 2.2 for flow in and around the downtown business district of Oklahoma City.

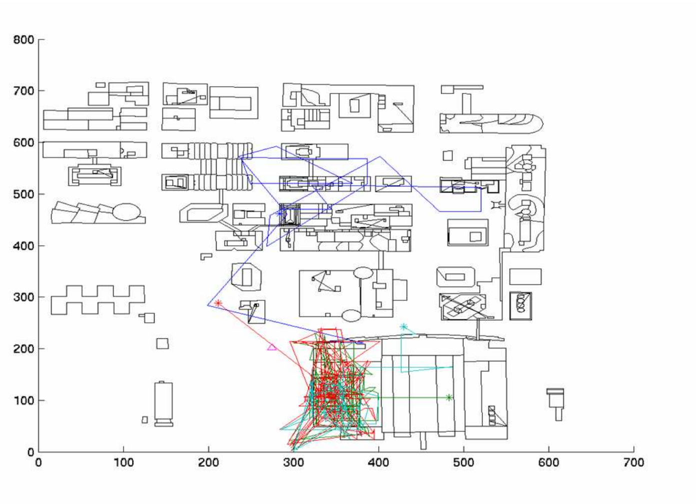

Figure 8: Paths of four Markov chains for flow in and around the downtown business district of Oklahoma City.

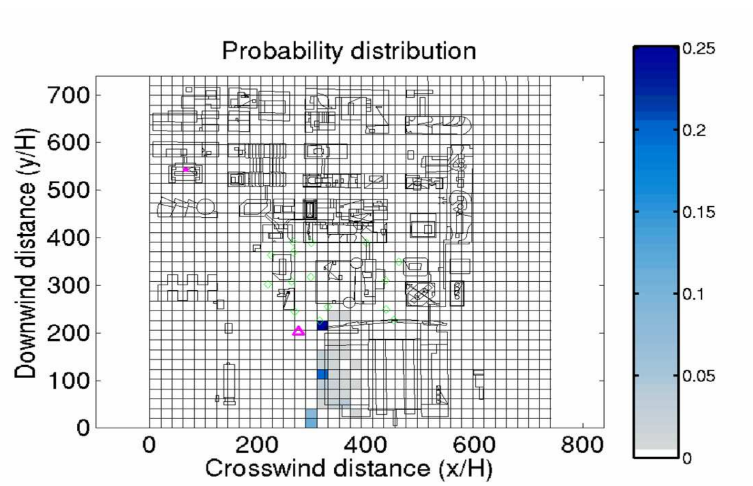

Figure 9: Probability distribution of source location for flow in and around the downtown business district of Oklahoma City. The magenta delta indicates actual release location.

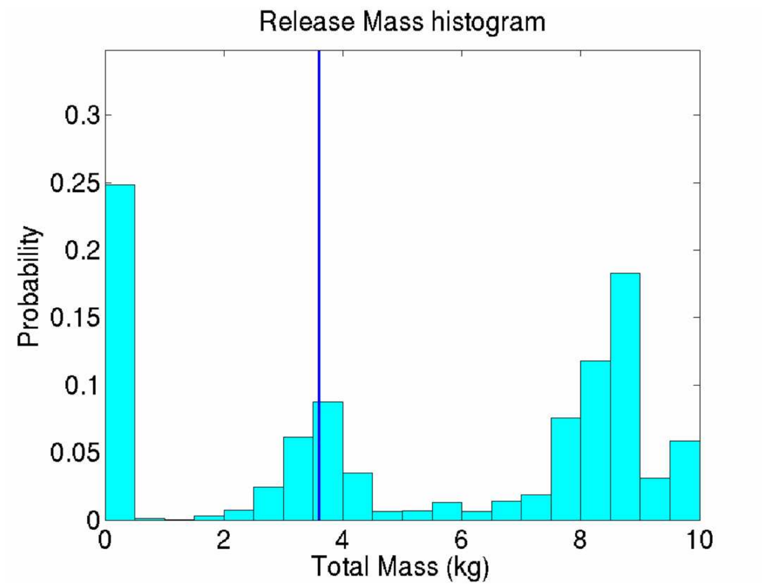

Figure 10: Histogram of source strengths, q, and the conditional probabilities for flow in and around the downtown business district of Oklahoma City. Vertical blue line indicates actual release rate.

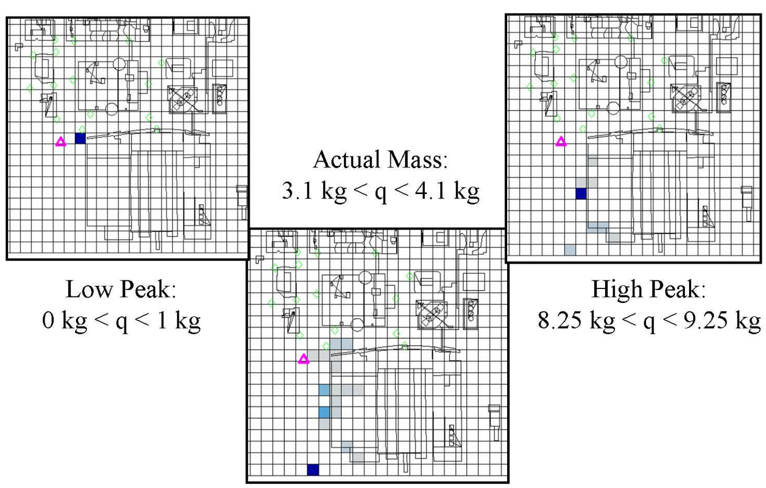

Figure 11: Conditional probability distribution of source location for flow in and around the downtown business district of Oklahoma City. The magenta delta indicates actual release location.

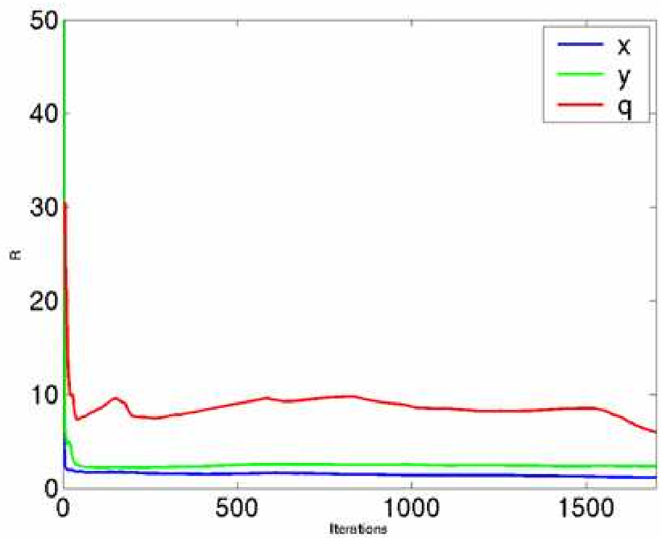

Figure 12: Convergence of x and y location, and slower conversion of strength q for the Oklahoma City example.

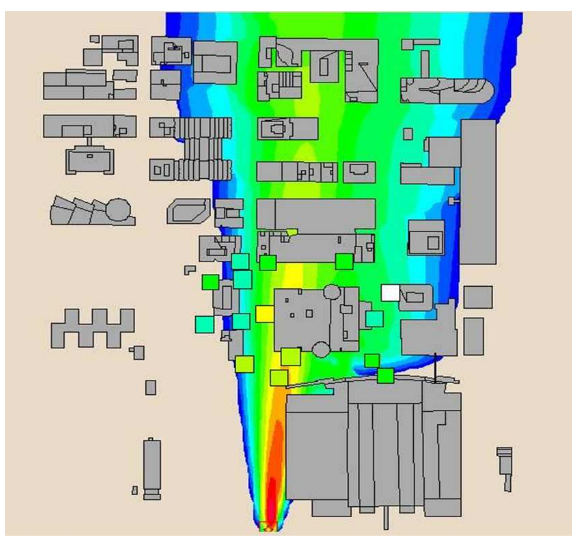

Figure 13: The building wake entrainment acts as a flow channeling effect within the UDM. Horizontal concentration contours at the first vertical level generated by forward simulation with UDM for flow in and around the downtown of Oklahoma City for the location associated with actual source strength.

6. ACKNOWLEDGMENTS

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