10.3 TOWARD UNDERSTANDING THE SENSITIVITY OF THE QUIC DISPERSION MODELING SYSTEM TO REAL INPUT DATA

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1. INTRODUCTION

There is a growing need to rapidly and accurately predict the dispersion of toxic agents in the case of an accidental chemical spill or intentional biological attack. In order to use a tool such as the QUIC (Quick Urban and Industrial Complex) Dispersion Modeling System to simulate such a scenario, the basic input parameters used must accurately representative and be fully understood. The study presented here consists of validating the QUIC model using data obtained from the JU2003 (Joint Urban 2003) field experiment.

QUIC is composed of three components: QUIC-URB, QUIC-Plume and QUIC-GUI (Pardyjak and Brown 2001; Williams et al. 2002; Nelson et al. 2006). QUIC-URB is an empirical- diagnostic wind-modeling tool which computes 3-D flow fields around buildings. The algorithms used in QUIC-URB to produce a mass consistent flow field are based on the work of Rockle (1990) as well as a number of additional modifications (e.g. Bagal et al. 2004a; Bagal et al. 2004b; Pol et al. 2006). QUIC-Plume models particle dispersion using a stochastic Lagrangian "urbanized" random walk model. In order to be consistent with the input parameters from QUIC-URB, special turbulence parameterization must to be considered. QUIC-GUI is a graphical user interface designed to allow the user to easily input flow field and dispersion parameters and visualize the computed results.

The JU2003 field experiment was an atmospheric dispersion study conducted from June 28 to July 31 of 2003 in Oklahoma City (Allwine and Flaherty 2006; Brown et al. 2004). The study consisted of tracer gas SF_6 (Sulfur hexafluoride) releases over ten IOP's (intensive operation periods) that were each 8 hours in duration. The tracer gas was released at various locations within the CBD (central building district) and concentrations were sampled at many locations throughout the downtown area and as far as 4 km from the release location. Data were acquired for the experiment using meteorological and tracer instrumentation. Examples of the instrumentation deployed included: SODARs, LIDARs, RADARs, sonic anemometers, etc. Many organizations took part in the experiment from government laboratories and universities to private companies of both foreign and domestic origin.

This sensitivity analysis focuses on three 30-minute continuous, point releases during IOP3. These daytime release times started in the late morning and went into the afternoon. During all of IOP3 the skies were mostly clear with winds ranging from 8-11 m s^{-1} from a southerly to south-easterly direction measured at 100 m above ground level (Clawson et al. 2005). The releases took place near the Myriad Botanical Gardens and consisted of release rates of 4.94, 3.02 and 3.02 g s^{-1} at 1600, 1800 and 2000 UTC respectively. Wind data and concentration data for these times are compared here to simulated values obtained from QUIC. Analyzing the simulated data and modifying the inflow profile to best suit the experimental data has proved to be an iterative process. The aim is to reduce the error in dispersion modeling by understanding and appropriately applying various input parameters. In this work the input parameters that investigated are: wind inflow, source location uncertainty and concentration sensor location uncertainty.

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2. VALIDATION METHODOLOGY

The methodology used here to reduce the error associated with modeling consists of two main areas: wind flow analysis and sensor and source location uncertainty. Wind flow analysis consists of reducing the experimental data and creating inflow parameters which are simplified from the measured data to accurately represent the inflow profile. The second aspect of the methodology is the sensor and source location uncertainty which are related to the amount of error associated with point by point comparisons of velocity and concentration.

2.1 Wind Inflow Analysis

In order to specify the most appropriate inflow conditions for the QUIC model, the JU2003 data were first analyzed and averaged. The sensors that were considered to construct a velocity inflow profile are shown in Fig 1. To avoid wake effects associated with the urban area, only the sensors located upstream of the CBD were considered as candidate sensors. The candidate sensors that were selected included: the profile from the PNNL SODAR (Pacific Northwest National Laboratory), ARL (Air Resources Laboratory) sonic anemometers, IU (Indiana University) sonic anemometers and select Dugway Proving Ground PWIDs (portable weather information display system). These sensors were selected as candidates because they were upwind of the CBD and were not influenced by buildings. For example, the ARL towers 2, 4 and 5 were not used because of their proximity to buildings. The mean wind data from all of the candidate sensors are shown in Figs 2-4. Of the candidate sites, PWID15 was heavily weighted because of its location directly upstream of the release sites and its height of 50m above ground level (approximately equal to the average building height in the CBD). Additionally, because SODARs have greater reliability at greater heights above the ground, the PNNL profile was used as a reference for the shape of the profile at heights above approximately 100 meters.

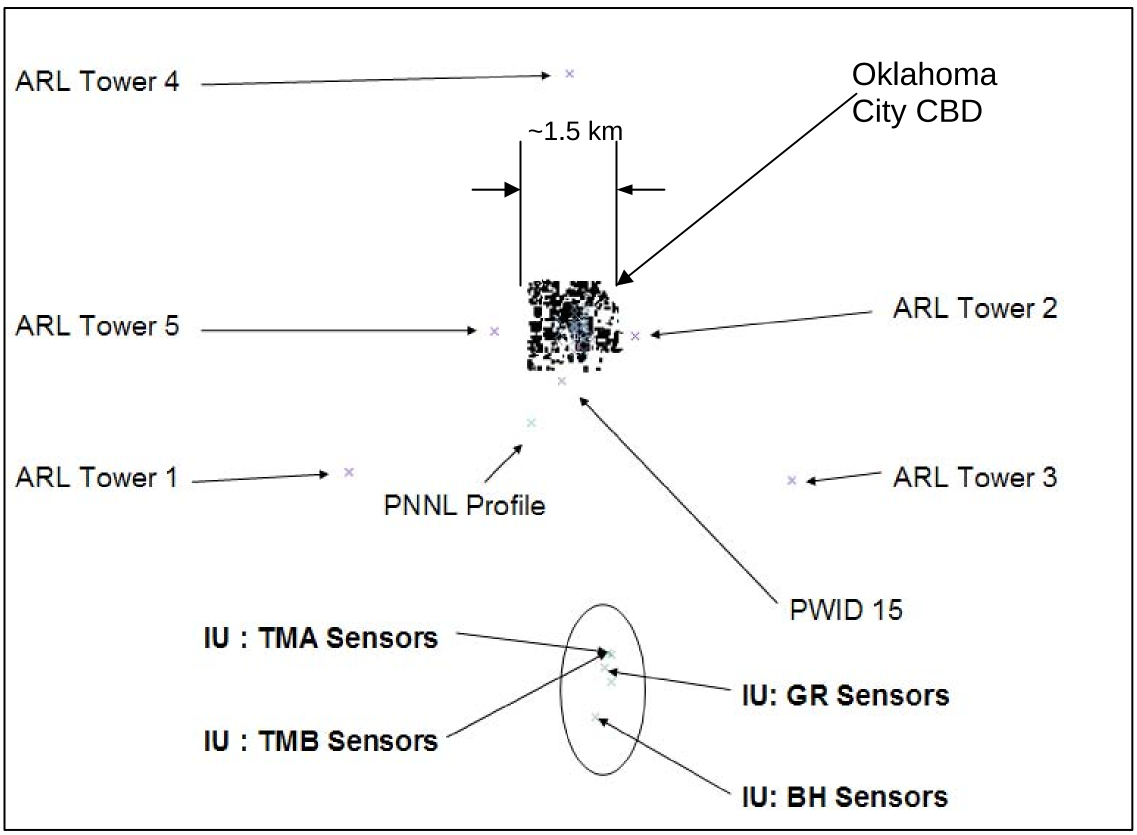

Figure 1: Plan view showing the locations of the various wind sensor considered for constructing an inflow profile with respect to the Oklahoma City CBD.

The wind speed data used to fit logarithmic profiles are shown in Figs 2, 3, and 4 for 1600-1630, 1800-1830 and 2000-2030 UTC respectively.

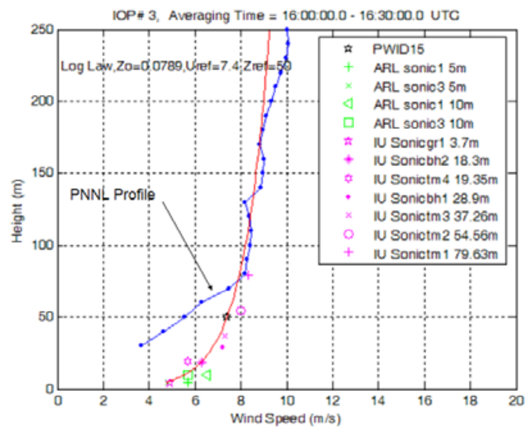

Figure 2: Log law fit for 1600-1630 UTC

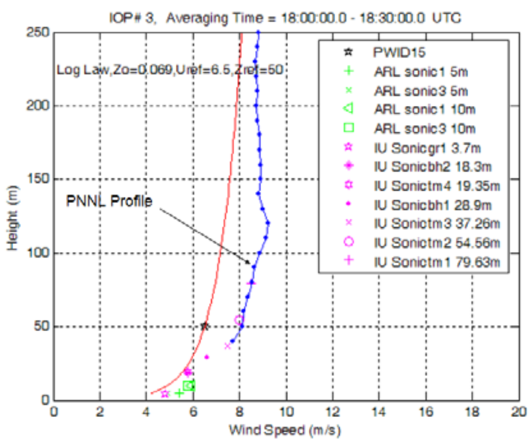

Figure 3: Log law fit for 1800-1830 UTC

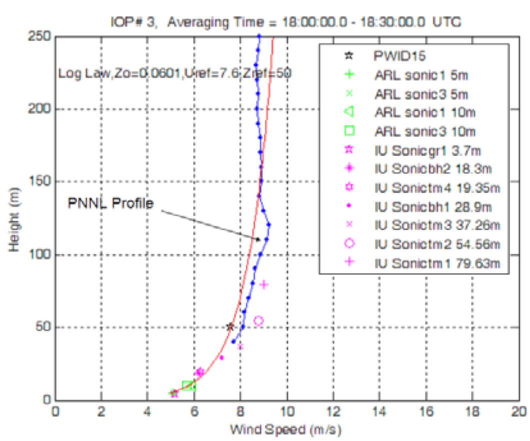

Figure 4: Log law fit for 2000-2030 UTC

Once reasonable profiles were produced using the PNNL sodar for reference above 100 meters and the ARL and IU sonics for reference under 100 meters for the entire 30 minute periods, the PWID15 sensor was averaged into both 30 minute period and six 5 minute periods. The two averaging periods allowed for two sets of simulations to be run in QUIC that account for varying amounts of wind meander. The PWID15 data used for wind direction was assumed to be constant with height. In order to validate the PWID wind direction data, the direction was also estimated by plotting the measured concentrations of the SF_6, as shown in for 1600-1630 UTC in Fig 5. The wind direction was determined by estimating the centroid of concentration values and comparing with the measured PWID value.

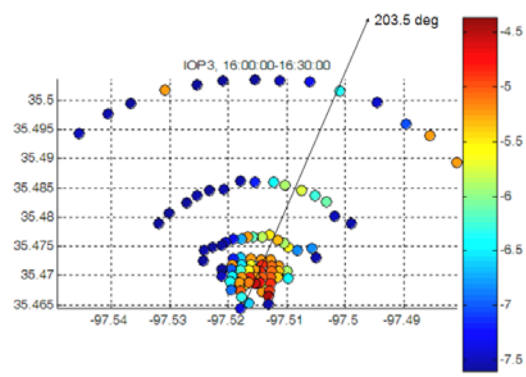

Figure 5: Wind Direction from Concentration Values for 1600-1630 UTC

2.1 Sensor and Source Location Uncertainty

Other parameters affecting the concentration simulation results include the uncertainties in sensor locations and the release source location. All of the instrumentation was set-up and its location recorded from a hand-held GPS (Global Positioning System). The error associated with any GPS can be up to 5 meters due to Ionospheric effects, shifts in satellite orbits, clock errors of the satellite clocks, multipath effects, Tropospheric effects and calculation or rounding error (Enge et al. 1996). To try to understand the importance of this uncertainty, another set of simulations were run using 5-minute wind speed averages and a shifted source location. The analysis below shows a comparison of the results obtained by shifting the source with respect to the original source location. The QUIC domain used for the simulations is shown in Fig 18 in the appendix with the locations of the ARL, LLNL and Volpe sensors along with the source location.

For each simulation run, sensitivity of sensor location was investigated. An analysis was conducted around each sensor were the sensor location was shifted 1 grid cell (5 meters) in any direction. Figure 6 shows the grid structure used for the analysis. The central location represents the location specified by Allwine and Flaherty (2006). Figure 6 also shows the symbols used in the comparison plots that follow to annotate the analyzed points.

(x-1,y+1) V	(x,y+1) ◊	(x+1,y+1) >
(x-1,y) +	(x,y) *	(x+1,y) <
(x-1,y-1) O	(x,y-1) X	(x+1,y-1) □

Figure 6: Sensor locations sensitivity grid; each grid is 5m x 5m.

The general set-up parameters used in QUIC-URB are shown in Table 1 and the parameters used in QUIC-Plume are shown in Table 2. The parameters which varied for each of the simulations are inflow wind averaging times and instrumentation location. Two averaging times for the wind field were simulated and compared for each 30-minute release. The first was a 30-minute average and the second was a 5-minute average. These averages were set as inflow parameters into the QUIC model and the results compared.

Using a 30-minute average will produce similar results but due to the low resolution, flow phenomena such as wind meander are averaged out. Using 5-minute, high resolution averaging captures such flow effects but is more computationally expensive and may include scales of turbulence simulated in QUIC-Plume that should not be resolved.

A plan view of the QUIC generated Oklahoma City domain is shown in Fig 7.

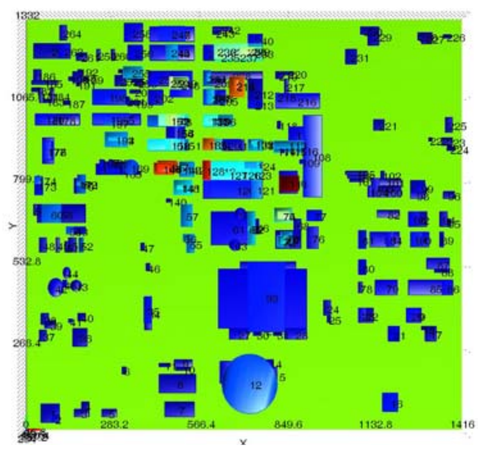

Figure 7: QUIC Domain, Plan View, Courtesy of Matt Nelson, LANL

The buildings are colored by height which can be more easily distinguished in the 3-D view shown in Figure 8.

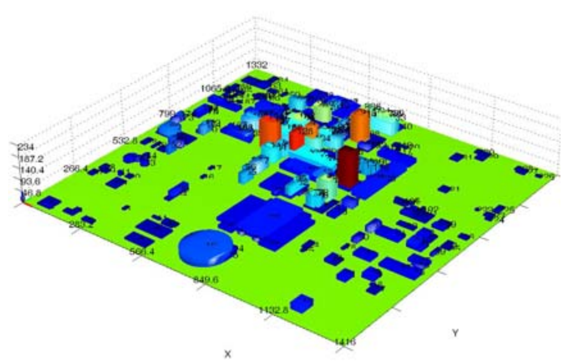

Figure 8: QUIC Domain, 3-D View, Courtesy of Matt Nelson, LANL

3. RESULTS AND DISCUSSION

Three separate sets of simulations were conducted and compared over each 30-minute release to better understand the sensitivity of the specified parameters. The first was a 30-minute average of the winds for the inflow profile and a 30-minute average of the concentration data. The second simulation was composed of six 5-minute averages of the wind data in order to achieve the 30-minute simulation, along with 30-minute average of the concentration data. The final simulation was composed of six 5-minute averages of the winds along with a source location moved approximately 26 meters north and 31 meters west of the original location.

To investigate the source of error in the concentrations, the wind field velocity within the CBD should be understood. Figure 9 is a vector plot of the measured winds and the simulated winds. Some of the values in intersection areas indicate measured winds that are significantly different than those predicted by QUIC.

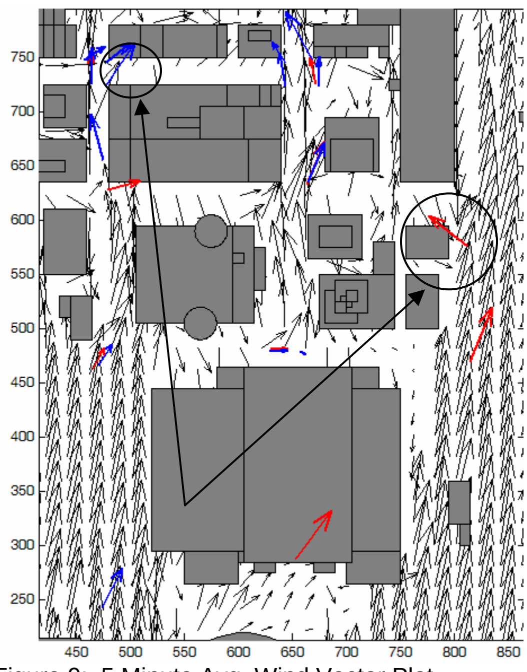

Figure 9: 5 Minute Avg. Wind Vector Plot 1600-1630 UTC

Point comparison plots of wind speed and wind direction shown in Figures 10 and 11 shows that about half of the wind speed and direction points are being under predicted by the model. Figure 11 also shows that for a wide range of observed wind directions, the simulated winds do not vary as much, predominately coming from the south. This may indicate that some aspects of channeling in the crosswind direction as well as recirculation in the building wakes in QUIC need to further be investigated.

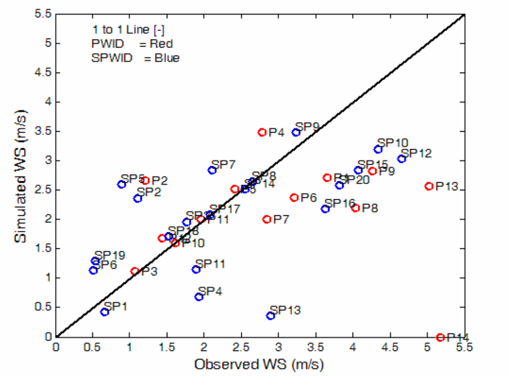

Figure 10: 5-minute average wind speed comparison: 1600-1630 UTC

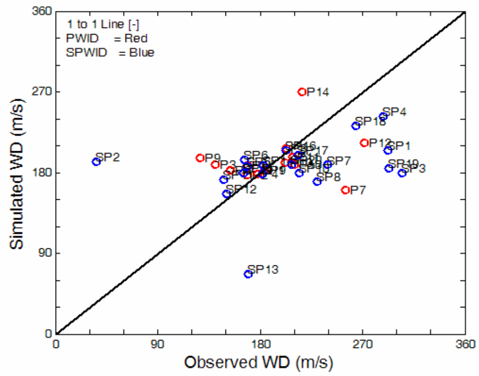

Figure 11: 5-minute average wind direction comparison: 1600-1630 UTC

Now considering the concentration data, in order to quantify the error at each sensor for each simulation, the fractional bias (FB), the normalized absolute difference (NAD) and the bounded normalized mean square error (BNMSE) were calculated using Eqs 1-3 following Warner et al. (2006). The predicted or simulated value is denoted as C_p and the observed or measured value is denoted as C_o.

$$FB = \frac{(\overline{C}_p - \overline{C}_o)}{0.5 \cdot (\overline{C}_p + \overline{C}_o)} \qquad (1)$$

$$NAD = \frac{\sum_{i=1}^{n} \left| C_p^{(i)} - C_o^{(i)} \right|}{\sum_{i=1}^{n} \left[C_p^{(i)} + C_o^{(i)} \right]} \qquad (2)$$

$$BNMSE = \frac{\sum_{i=1}^{n} \left[C_p^{(i)} - C_o^{(i)} \right]^2}{\sum_{i=1}^{n} \left[C_p^{(i)} + C_o^{(i)} \right]^2} \qquad (3)$$

The error values for concentration of all of the sensors in the domain are shown for all of the simulations in Figs 12-14.

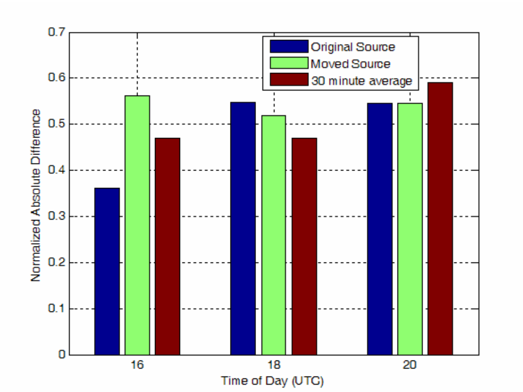

Figure 12: NAD error for simulations.

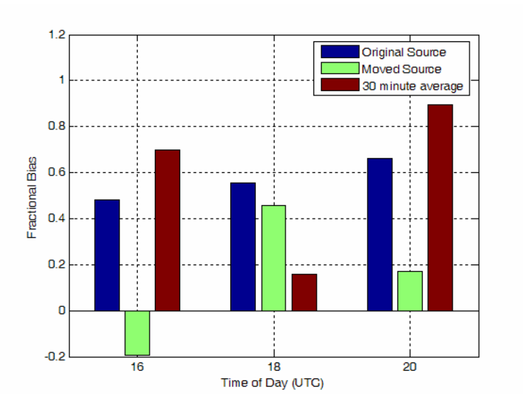

Figure 13: FB error for simulations

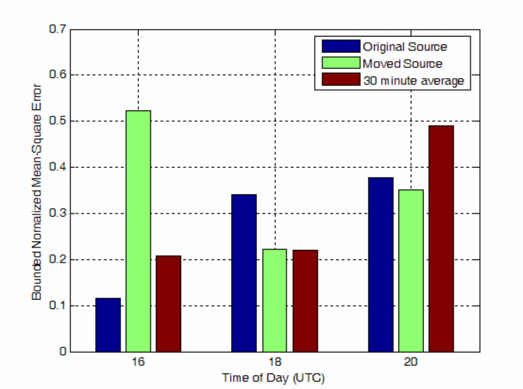

Figure 14: BNMSE for simulations

In all of the figures, the blue bar (left) indicates the original source location using 5-minute averages. The green bar (middle) shows a moved source using a 5-minute average and the red bar (right) shows the original source using a 30-minute average. In analyzing these figures, it is apparent that none of the cases minimize all of the error parameters. The 5-minute average with the original source location on average best minimizes the overall error.

The concentration plot for 1600-1630 UTC is shown in Fig 15. Fig 15 indicates that the simulation predicts the general pattern of the plume well, but underestimates its spread to the west.

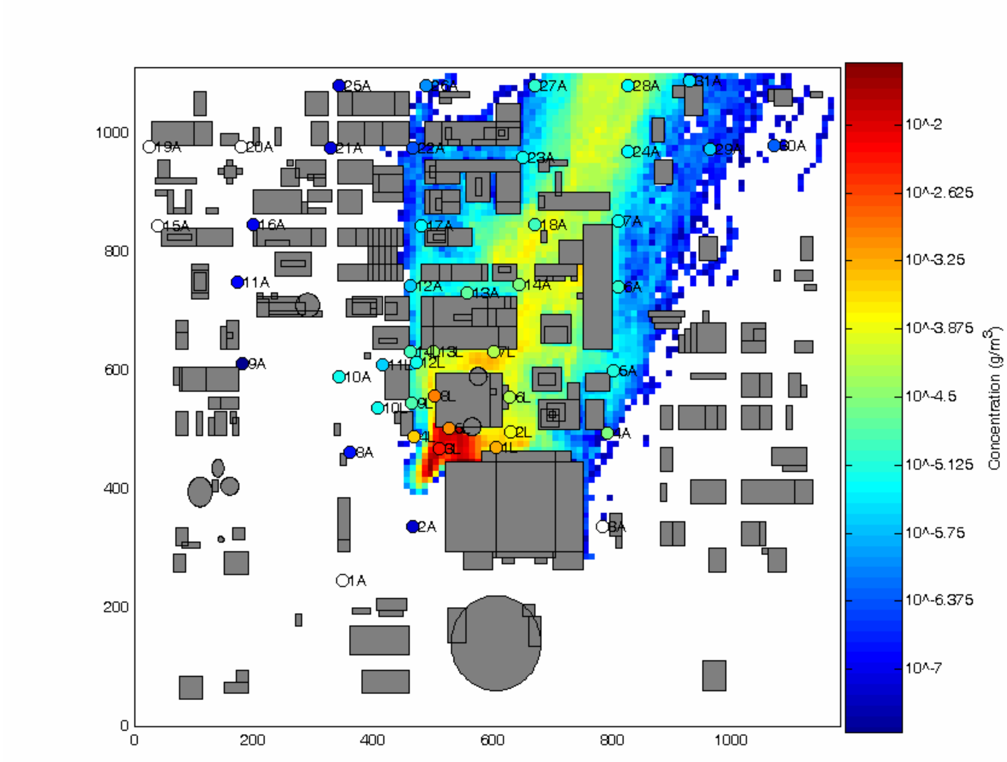

Figure 15: 30-minute averaged concentrations1600-1630 UTC

The point to point concentration comparison shown in Fig 16 shows that just over half of the points lie with a factor of 5. There is still a need to reduce the model error. In particular, almost half of the points that are observed to have a measured concentration are not simulated to have any concentration, indicating that the simulated plume is missing this region entirely.

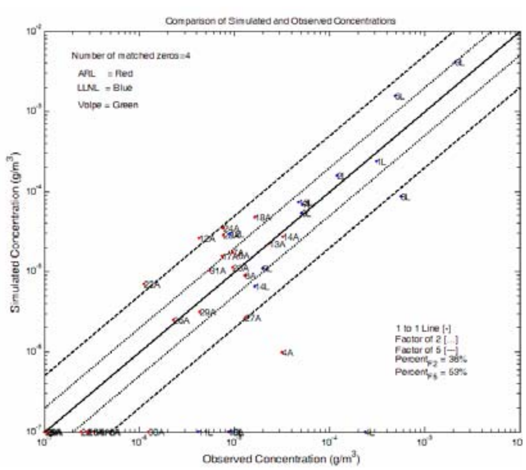

Figure 16: 5-minute average point to point concentration comparisons1600-1630 UTC

One of the sources of error discussed above is the accuracy of the GPS to define the true location of the individual sensors; to investigate this issues, an analysis was conducted to determine if moving sensor locations significantly decreased error. ARL sensors were located throughout the Oklahoma City domain and are used as an example here. Figure 16 shows a comparison of the measured and simulated concentration values as well as a comparison of the adjacent grid cell values. Figure 17 indicates that there are large numbers of sensors that are highly sensitive to location. By moving a specific sensor 1 grid cell away, the model error can be substantially reduced. The values shown below are only from the ARL sensors. An example of the significance of this analysis can be seen by looking at sensors number 22. The center of the grid does not even lie within a factor of 5 but an adjacent cell is approximately within a factor of 2 to the measured value. Note that the symbols shown in Figure 17 are described in Figure 6.

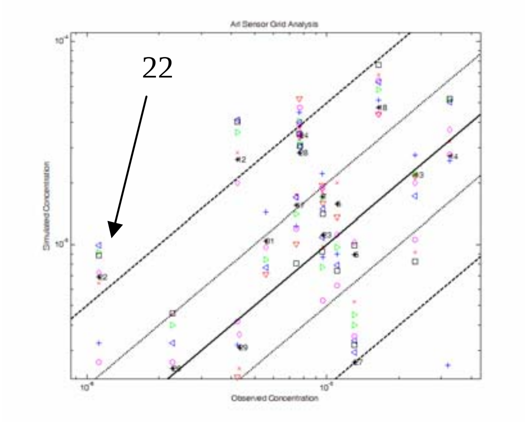

Figure 17: Adjacent grid cell analysis using 5-minute averages:1600-1630 UTC

4. SUMMARY

The comparison of the simulated and measured results shows the sensitivity of the QUIC to changes in inflow parameters as well as sensor placement and source placement. The comparison of the winds shows that over half of the wind speeds are being under predicted. The QUIC simulations show that the winds are predominately southerly while the measurements indicate that there is a wider range of wind directions. QUIC-URBs algorithm for channeling and recirculation may need to be investigated further. It was shown that shorter time averages of wind speed and direction (5 minutes) resulted in enhanced lateral dispersion of the plume. Even though the plume showed more lateral dispersion with a shorter averaging period, the model still under predicted the dispersion to the west. The plume width was also affected by the placement of the source, but the single modified source location tested did not improve the overall results. Concentration comparisons showed that many simulation points correlate well with the experimental data, but there are a number points near the edges of the plume and near buildings with poor correlations. The sensitivity of the sensor locations may have a lot do with this and should be analyzed further.

Future work will consist of quantifying the wind sensors error using a methodology similar to the one adopted here for the concentration sensors, including performing a grid analysis. This could help understand more about the errors associated with the comparison plots. Also, investigating winds at multiple heights and vertical dispersion of the plume may provide insight into error associated with the various QUIC algorithms as well as sensor location sensitivity.

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6. APPENDIX

Table 1: QUIC-URB Parameters

	1600-1630 UTC	1800-1830 UTC	2000-2030 UTC
Rooftop Recirculation	ON	ON	ON
Street Canyon Algorithm	ON	ON	ON
Upwind Cavity Algorithm	ON	ON	ON
Interstection Algorithm	ON	ON	ON

Table 2: QUIC-Plume Parameters

	1600-1630 UTC	1800-1830 UTC	2000-2030 UTC
Gas Type	Ideal Gas	Ideal Gas	Ideal Gas
Total Mass Released	8.89 kg	5.44 kg	5.44 kg
Release Type	Continuous	Continuous	Continuous
Particles Released	201,600	201,600	201,600
Conc. Averaging Time	1800 sec	1800 sec	1800 sec

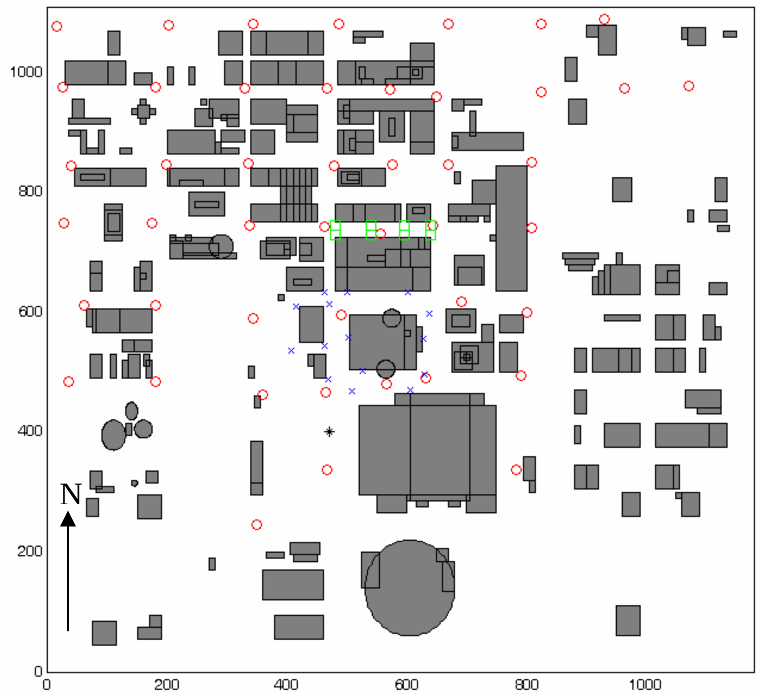

Figure 18: Source location (black star); ARL (red circle), LLNL (blue x) and Volpe (green square) sensor locations