J18.2 URBAN HPAC/SCIPUFF AND A SIMPLE URBAN DISPERSION MODEL COMPARED WITH THE MADISON SQUARE GARDEN 2005 TRACER OBSERVATIONS IN NEW YORK CITY

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ABSTRACT

The Hazard Prediction and Assessment Capability (HPAC) model system, which contains the SCIPUFF dispersion model, is widely used by the U.S. Department of Defense and other agencies. Version 5.0 SP1 (January 2008) of HPAC has been significantly updated to improve urban wind speed profile estimates and to add a model to calculate detailed flow and dispersion around individual buildings (MicroSwift/Spray, or MSS). Evaluations with urban tracer data sets are underway, and the most recent evaluations presented in this paper use data from the Madison Square Garden 2005 (MSG05) field experiment, which included detailed supporting meteorology and six different perfluorocarbon tracers (PFTs) released during four periods on two days in March, 2005. The MSG domain contains several very tall buildings with heights greater than 150 m, and is marked by deep street canyons. HPAC/SCIPUFF is run using three different urban dispersion module options (Urban Canopy (UC), Urban Dispersion Model (UDM), and MSS) and three different input meteorology options (observed average winds, basic default airport, and mesoscale meteorological model). For comparison purposes, a simple Gaussian-format urban dispersion model has also been run for the same MSG05 data base. The evaluations focus on hourly-averaged concentrations paired in space. It is shown that the urban HPAC/SCIPUFF options produce reasonable performance for samplers 200 to 400 m downwind of the source release area, although similar performance is also found for the simple urban dispersion model. The urban HPAC options tended to underpredict (by a factor of 10 to 100) the concentrations at the surface samplers close the source release area and the samplers on rooftops. The exception was that the MSS model sometimes could match these close-in and rooftop concentrations.

1. OBJECTIVES AND BACKGROUND

Meteorological and tracer data taken during a series of recent urban field experiments are being analyzed, in order to increase understanding of urban flow and dispersion in built-up downtown areas, to evaluate and perhaps modify dispersion models using the data, and to provide guidance for emergency response. The urban dispersion model comparisons discussed in this paper make use of the Madison Square Garden 2005 (MSG05) field experiment, which took place on 10 and 14 March 2005.

Besides the MSG05 field experiment described here, the Joint Urban 2003 (JU2003) field experiment (Allwine et al., 2004) has been used, and the Manhattan Midtown 2005 (MID05) field experiment (Allwine and Flaherty 2007) will be used to test the urban models discussed here

The current study focuses on a widely-used model system - the Hazard Prediction and Assessment Capability (HPAC) (DTRA, 2008), which includes the SCIPUFF atmospheric transport and dispersion (T&D) model (Sykes et al., 2007). The HPAC version 5.0 SP1 model, released in January 2008, was evaluated by Hanna et al. (2008) with the JU2003 SF_6 tracer data, yielding good performance, although there is an overprediction bias at night.

The current paper extends the urban HPAC 5.0 SP1 evaluations to the MSG05 data set. For comparisons, a simple urban dispersion model (described by Hanna and Baja, 2009) is included in the evaluations with the HPAC model.

2. HPAC URBAN OPTIONS TESTED

The components of HAPAC/SCIPUFF are described by Sykes et al. (2007). Several enhancements to the urban modules were included in HPAC in Version 5.0 SP1. For example, modifications were made to the SWIFT diagnostic meteorological model to remove errors in urban canopy winds in version 4.04. Also the MicroSwift-Spray (MSS) urban diagnostic wind and Lagrangian particle model are included in version 5.0 SP1. The current evaluations use the following HPAC/SCIPUFF urban options:

UC - Urban Canopy (a parameterization of the urban wind and turbulence profiles in SCIPUFF)

UDM - Urban Dispersion Model

MSS - MicroSWIFT/SPRAY (a new addition in version 5.0 SP1)

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The current runs use three alternate sets of meteorological data inputs:

Single (SNG) - Average wind speed and direction from all rooftop anemometers in urban area (Hanna et al., 2007). The wind speed is assumed to be 5.0 m/s at a height of 100 m on both days, and the wind direction is 285° on 10 March and 315° on 14 March.

Upwind (UPW) – National Weather Service (NWS) default (airport data). For MSG05 the Laguardia airport (LGA) wind data are used.

MEDOC – Mesoscale Meteorological Model – Version 5 (MM5) MEDOC outputs using special 4 km resolution runs by the National Center for Atmospheric Research (NCAR). MEDOC is a special format used just for inputs to HPAC.

Note that SWIFT (or MicroSWIFT for the case of MSS) is always triggered in HPAC for all meteorological input options except for MEDOC, where no additional diagnostic analysis of winds is performed.

The evaluations are carried out for predicted and observed 60-minute averaged C/Q paired in space (i.e., for each sampler and release trial). Note that both C_o and C_p had to exceed the Level of Quantification (LOQ)

3. SIMPLE URBAN DISPERSION MODEL

The simple urban dispersion model is thoroughly described by Hanna and Baja (2009), who present results of evaluations of the model with the JU2003 and MSG05 field data. The current paper uses these same MSG05 tracer concentration estimates as a basis for comparisons with the urban HPAC concentration estimates.

The model assumes that the crosswind plume concentration distribution has a Gaussian shape. It is based on earlier urban dispersion models suggested by Gifford and Hanna (1973) and Hanna et al. (1982), and uses so-called urban dispersion formulas suggested by Briggs (1973). Those formulas were partly based on the St. Louis field experiment (McElroy and Pooler, 1968), plus assumptions about enhancements of turbulence in urban areas.

It is assumed that the source is emitted near ground level. The Gaussian formula can be written:

$$C/Q = (1/(\pi u \sigma_y \sigma_z)) * \exp(-y^2/2\sigma_y^2)\exp(-z^2/2\sigma_z^2) \quad x > 0 \qquad (1)$$

where C/Q has units s/m^3, z is height of the receptor or sampler above ground level, and y is the lateral distance from the plume centerline. The plume centerline lines up with the average wind direction at the building tops (285 degrees on 10 March and 315 degrees on 14 March for MSG05). The wind speed, u, is the averaged vector wind speed for the plume as it is transported in the urban canopy. σ_y is the lateral cross-wind standard deviation of the concentration distribution and σ_z is the vertical cross-wind standard deviation of the concentration distribution.

The standard deviations are assumed to be made up of two parts, an initial σ_o due to the mixing in the street canyons at the source location, and a turbulent σ_t due to the usual ambient turbulence, which exists over all types of terrain. McElroy and Pooler (1968) suggest that the initial $\sigma_{yo} = \sigma_{zo} = 40$ m. We then have the following formulas:

$$\sigma_y = \sigma_{yo} + \sigma_{yt} = 40 \text{ m} + 0.25 x \qquad (2)$$

$$\sigma_z = \sigma_{zo} + \sigma_{zt} = 40 \text{ m} + 0.25 x \qquad (3)$$

The parameter (or "constant") 0.25 is in Briggs' (1973) urban sigma formulas for neutral conditions. The stability is assumed nearly neutral because of the daytime conditions in March and the moderate wind speeds. It is expected that, at night, the stabilities may be on the stable side of neutral, and the constant is reduced from 0.25 to 0.08 (this reduction was verified for the JU2003 nighttime runs (see Hanna and Baja, 2009).

Because the cloud of material is assumed to spread out into a hemispherical shape around the source area (even in the upwind direction), the right-hand side of eq (1) is multiplied by $\exp(-x^2/2\sigma_{xo}^2)$ when $x < 0$. σ_{xo} is assumed to also equal 40 m.

For samplers at distances from the source less than about 100 m, and/or when the line-of-sight is unobstructed between the release point and the sampler, it is assumed that the plume remains in the initial street canyon or courtyard and travels more or less unimpeded without being extensively mixed laterally by the multiple large buildings. In this case, we assume that the initial lateral dispersion ($\sigma_{yo} = \sigma_{xo}$) is smaller. A value of 10 m is assumed. This condition applies to samplers 8, 10, and 15 (see Section 4 for a description of samplers setup), for which observed concentrations indicate that the plume sometimes traveled straight towards that receptor, even though it may be upwind or in a lateral direction from the source.

An estimate of the urban wind speed is needed. Hanna et al. (2007) show that the average magnitude of the street-level (z = 3 m) wind speed is about 2 m/s during MSG05. Because the tracer plume is being transported across the urban area at the vector-average wind speed, it is assumed that the vector average u equals 1.5 m/s for the MSG05 field experiment.

4. DESCRIPTION OF MADISON SQUARE GARDEN 2005 (MDG05) FIELD EXPERIMENT

The MSG05 field experiment (Allwine and Flaherty 2006, Watson et al. 2006, Hanna et al.,

2006) is part of a recent series of urban experiments in the U.S. (see Allwine, 2007). The Joint Urban 2003 (JU2003) experiment in Oklahoma City (Allwine et al., 2004, and Clawson et al., 2005) has been the most extensive of the series, with more tracer releases and more observing systems, and was also the subject of recent evaluations of the HPAC/SCIPUFF version 5.0 SP1 model (Hanna et al., 2008). The Manhattan Midtown 2005 (MID05) experiment followed the MSG05 experiment, with focus on the Midtown area, and took place on six days in August.

The science goals for MSG05 were to increase understanding of flow and dispersion in deep urban canyons and of rapid vertical transport and dispersion in recirculating eddies adjacent to very tall buildings in a large urban area. MSG05 took place on 10 and 14 March 2005, Allwine and Flaherty (2006) and Allwine (2007) describe the experiment in general and give some of the preliminary results. Watson et al. (2006) describe the tracer releases and sampling methodology. Hanna et al. (2006) present some comparisons of five different Computational Fluid Dynamics (CFD) model applied to MSG05, and Hanna et al. (2007) discuss the wind and turbulence observations. The average building heights are found to be about 60 m in the MSG area, and there are several buildings with heights above 150 or 200 m within a few blocks. For example, the One Penn Plaza (OPP) building just north of MSG has a height of 223 m.

The two Intensive Observation Period (IOP) days during MSG05 included several types of meteorological measurements. For example, there were seven sonic anemometers at street level and three sonic anemometers on building roofs, with two on very tall buildings (at z > 150 m). The flow patterns are complicated, but the effects of the building wakes and street canyons can generally be fairly well simulated by CFD models, as seen in the comparison of five CFD models for this domain reported by Hanna et al. (2006).

As in any complex site, the decisions during MSG05 concerning placement of meteorological instruments and PFT samplers represented a compromise among many considerations. For example, all street level anemometers and tracer samplers were obviously not far from buildings, street corners, and other complications. The general rule followed at street level was that the instrument should be as far away from the building wall and obstructions as possible, but should not be placed near enough to the street that it might be hit by vehicles. Consequently, most street level instruments were located on the street edge of the sidewalk.

Both MSG05 IOP days were marked by similar wind speeds (about 5 m s^{-1}) and directions (WNW to NNW) at rooftop. Temperatures were also similar, slightly below 0.0 C, during both IOPs. Both experiments took place during the daytime, between 7 am and 12:30 pm EST, with partly-cloudy skies.

The two days of wind observations from the tall buildings during MSG05 suggest that there is a range in wind speed of about a factor of two and in wind direction of about 40 to 60 degrees across the several rooftop sites on each IOP day. Since these two days were more or less optimum from the viewpoint of excellent weather and moderate persistent winds, these ranges in wind speed and direction can be expected to be less than those on most days.

The MSG05 field experiments included concurrent one-hour duration releases of six different perfluorocarbon tracer gases, from five point sources near street-level (at z = 1.5 m) on the sidewalk at the four corners of MSG, and just north of OPP (See Figure 1). Note that two PFTs were released from one location for quality control. Figure 2 shows the 20 street-level and seven rooftop PFT sampler locations. Table 1 gives the UTM coordinates and the latitude and longitude of each release location and sampler. The heights of the seven rooftop samplers are also given in Table 1.

Watson et al. (2006) describe the details of the PFT methods used for MSG05 and Allwine and Flaherty (2006) review the PFT part of the experiment in their comprehensive summary of MSG05. There are three major advantages of PFTs over other types of tracers – 1) the global backgrounds of most PFTs are very low, 2) the samplers can measure concentrations down to parts per quadrillion (i.e., 1 ppq = 10^{-15} parts per part volume), and 3) multiple PFTs can be released simultaneously and sampled and distinguished by the same sampler. Thus small amounts of PFT gas can be released and still be detected above the global background. And different PFTs can be released at the same time and their individual concentrations detected by the same sampler.

For MSG05, six PFTs were used, and their characteristics are given in Table 2. Even though they have high molecular weights, they act like neutral or passive gases once they are emitted to the atmosphere because their concentrations are so low. The release mechanism consisted of a small tank and tubing on a small tower on the sidewalk near the street. Each release was from a height of 1.5 m and was of duration 60 minutes. During each IOP day, there were two releases, starting at about 9 am and about 11:30 am. The exact timing and release mass are given in Table 3. Thus, even though there were only four release periods during the two days, there were 24 sets of tracer data. This is because there were six PFTs released during each period.

Each sampler collected the PFTs in 10 adsorption tubes during each day. The sampler pumps were adjusted so that each adsorption tube represented a 30-minute sample. Therefore the total duration of sampling on each day lasted from 9 am to 2 pm. The samples were analyzed in the laboratories at BNL and QA/QC procedures applied (see Watson et al., 2006). Table 4 gives the background concentrations and the derived uncertainty (expressed as a standard deviation, or Stdev) for each PFT. Also listed are the Level of Detection (LOD) and the Level of Quantification (LOQ), which are assumed to equal three and ten times the Stdev, respectively.

The final PFT data set that was entered in the data archive and distributed to researchers contained concentrations expressed as the original raw values minus the sum of the background and the Stdev. It is necessary to subtract the background concentration from observations to properly represent the tracer plume. Allwine and Flaherty (2006) chose to be conservative in estimating the background for removal by defining it as the measured background plus the Stdev rather than as just the measured background. After removing the background, the final step in determining "background-adjusted" values is to set all negative values to zero.

Of the six PFTs released, five gave "good" data. However, one of the PFTs, PECH, was determined to have too much uncertainty and was therefore not used in subsequent analyses. In addition, as recommended by Allwine and Flaherty (2006), our analysis used a conservative approach for determining background-adjusted values that are significantly different from zero. That is, only those observed final concentrations that exceeded the LOQ (10 Stdev) were used in our analysis.

5. METHODS

The predictions of the HPAC urban model options and the simple urban Gaussian model were compared with the PFT observations during MSG05. Tables were created containing predicted and observed concentrations for each sampler and each PFT release. Maximum 60-minute averaged concentrations were determined for each sampler and each release. Pairs of model predictions and observations were included in the comparison only if both the predicted and observed concentration exceeded the LOQ (i.e., 10 times the Stdev). Table 4 lists the LOQ for each PFT. This assumption resulted in over ½ of the street-level and aloft (V) samplers (e.g., numbers 5-7, 9, 11-14, 16-18, 20, V3 –V6, and V7) not being used in the comparisons at all. Numbers 9 and 20 collected no good data, and sampler V7 (at the top of the New Yorker Hotel) was later determined to have been inside the hotel. Only a few of the sampler locations (e.g., numbers 1, 2, 3, 4, 10, V1, and V2) had significant concentrations most of the time. Some of the samplers (numbers 8, 15, 19, and V6) were occasionally hit, for specific release locations.

The comparisons used scatter plots, as well as quantitative performance measures. The performance measures in the BOOT statistical model evaluation method (Chang and Hanna, 2004) were used. Assume that X = C/Q in the following definitions:

Fractional Mean Bias

$$FB = 2(\overline{X_o - X_p})/(\overline{X_o} + \overline{X_p}) \qquad (4)$$

Normalized Mean Square Error

$$NMSE = \overline{((X_o - X_p)^2)}/(\overline{X_o} * \overline{X_p}) \qquad (5)$$

Geometric Mean

$$MG = \exp((\overline{\ln X_o}) - (\overline{\ln X_p})) \qquad (6)$$

Geometric Variance

$$VG = \exp\overline{((\ln X_o - \ln X_p)^2)} \qquad (7)$$

Fraction of X_p within a factor of two of X_o (*FAC2*) (8)

In addition, the median, average, and maximum of X_o and X_p are determined and listed. Subscripts p and o refer to predicted and observed, and the overbar represents an average.

The simple urban model runs have been completed and the results evaluated by Hanna and Baja (2009). These results are presented in scatter plots and in tables of performance measures, where separate results are given for four groups: all samplers, surface samplers, aloft (building top) samplers, and surface samplers for the PFT release (PTCH) from the OPP site.

Because the HPAC urban model runs are still undergoing final review, only a few results are shown below. These include scatter plots for the average C/Q at each sampler for all PFTs for a given IOP and release time for the UC and the MSS urban model options. The UDM urban model option results are still under review.

6. RESULTS

As mentioned in the previous two paragraphs, the simple urban model runs for MSG05 were completed, reviewed, and are being published by Hanna and Baja (2009). Consequently, comprehensive evaluation results are available and are summarized below in Section 6.1. However, the urban HPAC computer runs are still under review for some options, such as the UDM option, and comprehensive evaluation results are not yet available. Consequently, in Section 6.2 we present only a few scatter plots, for the UC and MSS urban options, and have not completed the tables of performance measures. We do discuss some specific quantitative conclusions for specific samplers and some general conclusions below.

6.1 Results for Simple Urban Model

Scatter plots of X_o versus X_p for the simple urban model are given in Figures 3, 4 and 5 for all samplers, for only the surface samplers, and for only the aloft samplers, respectively. If there were perfect agreement, all points would be oriented on a straight line at a 45 degree slope on the figures. But since perfect models never happen in the atmospheric sciences, we look to see if the agreement is "within the range" of other air quality models. Generally an air quality model for this type of application is said to be acceptable if its mean bias is less than a factor of two, and its scatter is less than a factor of two or three most of the time (Chang and Hanna, 2004). It is also desirable that the model be able to match the observed maximum concentration within about a factor of two.

Figure 3 is the scatter plot for all sampler data. It shows the middle of the cloud of points roughly falling along the 45 degree line, but with many points in the upper left of the diagram indicating an overprediction for several of the low observed concentrations. Figure 4 contains data only for the surface samplers, showing that most of the area of points with overpredictions have been eliminated.

Figure 5, for the aloft (building-top) samplers, shows the simple urban model overpredictions occurring at low observed concentrations. The model predicts C/Q of 255 at Sampler V1 and 142 at Sampler V2 for the PFT released at location B, on the NE corner of MSG for all four releases, because a constant vector average wind of 1.5 m/s was assumed. These match fairly closely the maximum observed C/Qs of 205 and 140 at those locations, which was the intent of the model development. But there are some release trials when observed C/Q was less at those locations.

Table 5 contains the quantitative performance measures for the simple urban model data in Figures 3, 4, and 5, as well as for two other subsets of the data – the surface data for the release near OPP, and the surface data from the close-in samplers (8, 10, and 15). It is seen that, for all data and for the surface data, the max C_p/Q is about one-half of the max C_o/Q. However, for the aloft data, the max C_p/Q is about 25 % larger than the max C_o/Q.

For the average or the median C/Q, at the surface, the predicted values are within 15 % of the observed values. FAC2 is 0.45 for all surface data.. Thus almost ½ of the predictions are within a factor of two of the observations.

The scatter plots and quantitative performance measures for the simple urban model are within the ranges for "good" model performance listed by Chang and Hanna (2004) for other model evaluation exercises.

6.2 Results for HPAC Urban Options

The HPAC results are shown in scatter plots in Figures 6 and 7, and in Table 6.

Figure 6 contains scatter plots for the UC HPAC urban model option. The three plots on the left are for all PFT releases and the three plots on the right are for only the four MSG releases (i.e., not the PTCH release on the north side of One Penn Plaza). The top, middle, and bottom rows of plots are for the SNG, UPW, and MEDOC meteorological input options, respectively. The points represent averaged C/Q over the four or five PFT releases at that day and release period. Note that IOP1 is 10 March and IOP02 is 14 March 2005. There were two release periods (R1 and R2) on each day. Different symbols are used in the plots for the four different tracer release periods. It is seen that there is much scatter, although there are a few points near the dark line that indicates perfect agreement. Most of the points indicating good agreement are from samplers 1 through 4, which are at 200 to 400 m downwind, roughly along the line of the rooftop wind direction. The top two rows also indicate that the six highest observed C/Q values are underpredicted by a factor of 100 or more. These points are all from sampler 10, which is close the MSG on the NE side; or from samplers V1 or V2, which are at a height of 48 m on setback roofs on the One Penn Plaza building, just north of MSG. The predicted plume is obviously missing those samplers most of the time.

The bottom row of Figure 6 is for the MEDOC meteorological option as used in the UC model. These scatter plots initially look better than those in the top two rows, but the reason is that the high observed C/Q values from samplers 10, V1, and V2 are not on the plots, because of extremely low predicted values. Recall that a pair of observed and predicted C/Q values for a certain PFT are retained for the evaluations only if both exceed the LOQ (minimum accepted concentration).

Figure 7 is the same as Figure 6 except Figure 7 is for the MSS HPAC urban option. Note that MSS is able to account for recirculating vortices in street canyons and behind buildings. The MSS performance is similar to the UC performance with the exception that MSS is able to better account for the high concentrations at samplers V1 and V2, at a height of 48 m on the OPP building. However, MSS performance for sampler 10 is only slightly better than that of UC.

Scatter plots for the UDM HPAC urban option are still undergoing quality checks and are not ready for inclusion here.

Table 6 presents quantitative comparisons between observed and predicted C/Q for some of the key samplers whose points are plotted in Figures 6 and 7. We have not yet calculated the set of performance measures (e.g., FB and NMSE) shown in Table 5 (for the simple urban model), because we are waiting for the final UDM runs to be completed. When two samplers are indicated, the maximum from the two has been entered in the table.

Samplers “1 or 4” represent the two downwind samplers along the rooftop wind direction at the approximate 200 m distance (see Figure 2). Samplers “2 or 3” represent the 400 distance along the rooftop wind direction. Sampler 10 often records high concentrations and is to the northeast of MSG, close to some of the source release locations. Samplers (V1 or V2) also record high concentrations and are on the 48 m level of the One Penn Plaza building, close to some of the source release locations.

To aid understanding of Table 6, the predicted C/Q values are shaded green if they are within a factor of two of the observation, and are shaded yellow if they are within a factor of five. If the predicted C/Q value has no color, it has a greater than factor of five difference with the observed C/Q. Note that nearly all (46 of 48) predicted C/Q values are green or yellow for samplers 1 or 4 and 2 or 3, in the first eight rows of the table. 21 of the 48 are yellow, indicating agreement within a factor of two. Thus the urban model options are performing fairly well for those samplers, with no obvious “better” or “worse” urban model option or meteorological input option.

As the scatter plots suggest, the model options usually underpredict C/Q at sampler 10 by a large amount. The exception is for release 2 on 10 March, when the observed C/Q was less (by a factor of 5 to 7) than for the other three releases, and the model options predict slightly higher C/Q than for the other three releases.

The samplers V1 and V2 at a height of 48 m on the OPP building record large observed concentrations. The UC urban options predict several orders of magnitude too low C/Q values for most combinations. The MSS urban option is able to do much better than the UC option with these samplers, probably due to MSS’s capability to account for recirculating vortices around MSG, OPP, and the Two Penn Plaza buildings.

There is not much obvious difference in performance between the three meteorological input options (SNG, UPW, and MEDOC) for any of the urban models.

The performance of the UC and MSS urban options is "not too bad" (often within a factor of two) for downwind samplers 1, 2, 3, and 4, which are 200 to 400 m from the source. However, the model options usually predict more of a drop-off in C/Q from 200 m to 400 m than is observed. Thus the model bias changes with distance.

No model option simulates the C/Q observed at 24 to 50 μs/m^3 at sampler 8 during IOP01 with the NW MSG release location. That sampler (see Figure 2) is a half a block to the north. The windward vortices near MSG and OPP plus street canyon channeling were likely causing that hit. The same type of "miss" by HPAC happens for sampler 15 where C/Q is observed at 13 to 18 μs/m^3 for the SW release during IOP02. Sampler 15 is a half a block to the south. A similar type of miss happens at sampler V6, which hangs over the roof of the Post Office building, at a height of only 20 or 30 m, just west of the SW release in IOP02. It observes 40 to 100 μs/m^3 for the SW MSG release in IOP02. This is obviously due to a street canyon vortex.

No model option simulates anything other than 0.0 concentrations at samplers 3 and 4 at the top of the One Penn Plaza building (about 229 m). However, the observed C/Q averaged 1 to 3 μs/m^3. This is about 1 to 3 % of the C/Q at street-level next to OPP and about 10 to 30 % of the C/Q at street level at distances of 200 to 400 m.

Because it can account for vortices near buildings, MSS does better than the other model options at some of the samplers off the centerline suggested by the direction of the rooftop wind. For example, MSS can simulate the upwind (towards the NW) plume motion for the NE MSG release with large impact on sampler 10 (which is located to the NW of the release point). This flow to the NW was found by the sonic anemometers and is simulated by the CFD models (see the Hanna et al. (2006) article with the five CFD model results). It is caused by a straightforward windward vortex on Two Penn Plaza. MSS is the only model to simulate (within a factor of two) significant C/Q at the aloft samplers V1 and V2 on the setback roof of OPP at a height of about 48 m. Observed C/Q there was almost as high as at street level. The other urban models predicted nearly zero there.

MSS continues its tendency (found for JU2003 by Hanna et al., 2008) to have a few very large overpredictions (such as a 200 μs/m^3 value at samplers 3 and 4 (distance of 200 m) for the release north of OPP).

The MSG05 field experiment may not be a good test of MM5/MEDOC because the wind flows were straightforward due to strong synoptic WNW flow (post cold front) on both IOP days. The situation should be different when the MID05 comparisons are carried out in the future, since there were lighter winds and more of a challenge.

7. LIMITATIONS

With 20 surface samplers and 7 samplers aloft, and six different PFT releases during four release periods, there could have been as many as 27 x 6 x 4 = 648 good data pairs (i.e., with both observed and predicted concentrations above the sampler threshold). The final count of good data pairs was only 80, due to some samplers data being missing, one PFT (PECH) not being used, and many observed concentrations below the sampler threshold. This is enough data to arrive at useful conclusions for MSG05, but it is expected that many more good data will be available from MID05, which involved more IOP days, more samplers, and more tracer gas released.

The MSG05 field experiment was of course site specific, as any urban experiment would be. This is another reason to look forward to analyzing the MID05 data, which were taken a few blocks from MSG05. However, because both MSG05 and MID05 took place during the day, there is still a need to test the models at night.

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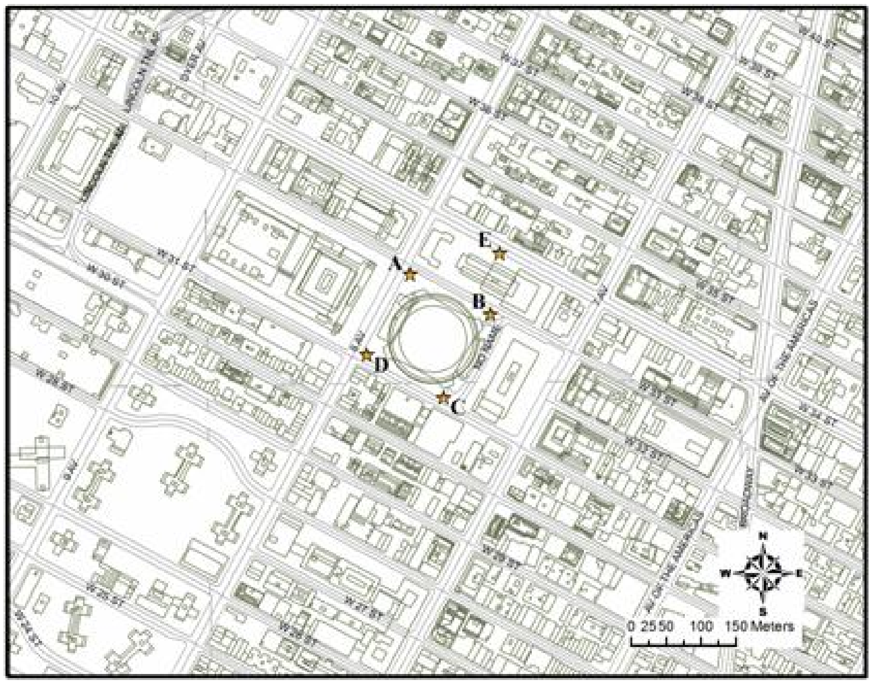

Figure 1. The five tracer release locations during MSG05 (from Allwine et al., 2006). Table 1 lists the precise locations in UTM and lat-long. Figure from Allwine and Flaherty (2006).

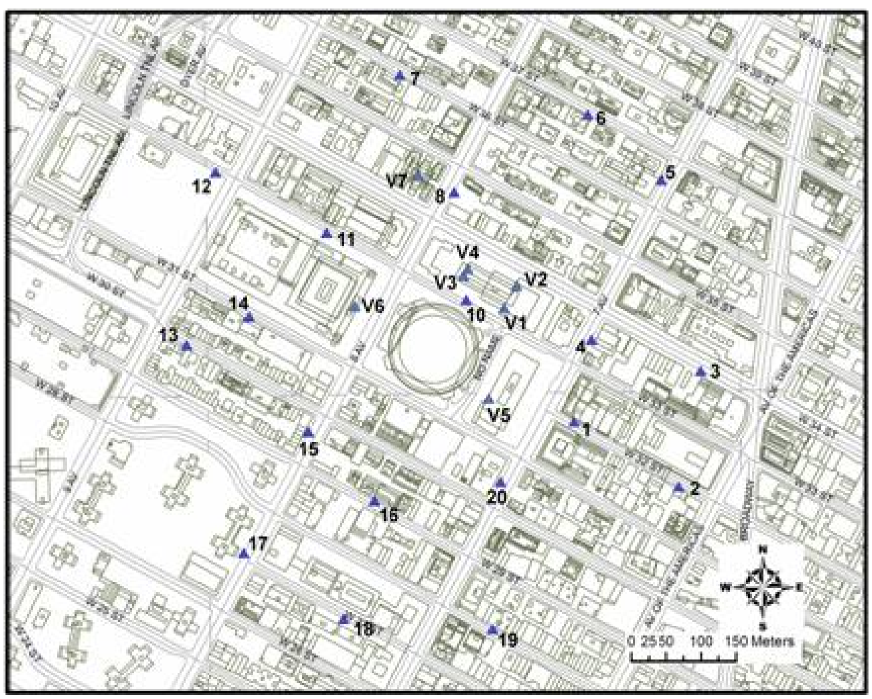

Figure 2. The PFT sampler locations during MSG05. Samplers with labels beginning with V are located above street level on buildings. Table 1 lists the precise locations in UTM and lat-long. Figure from Allwine and Flaherty (2006).

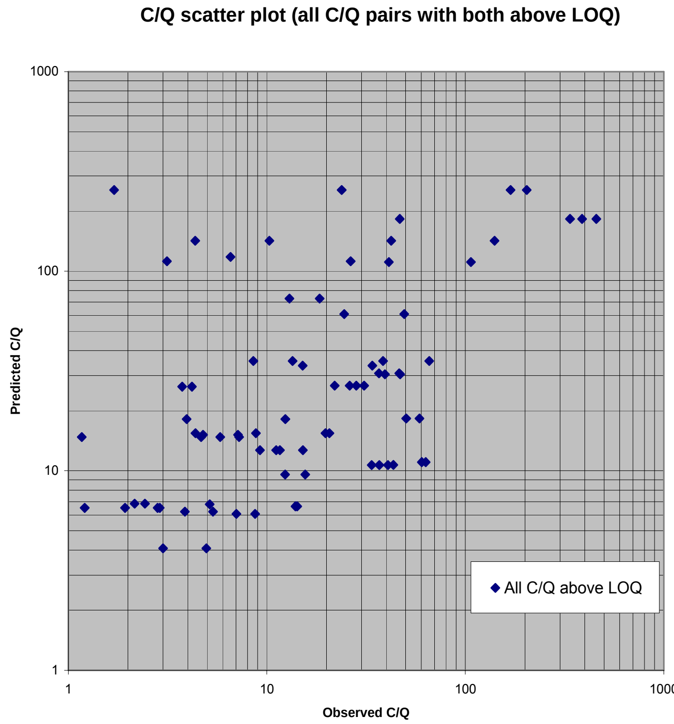

Figure 3. Simple urban dispersion model scatter plot of all data (N = 80) with both observed and predicted C above the LOQ. Units of C/Q are s/m^3 times 10^6.

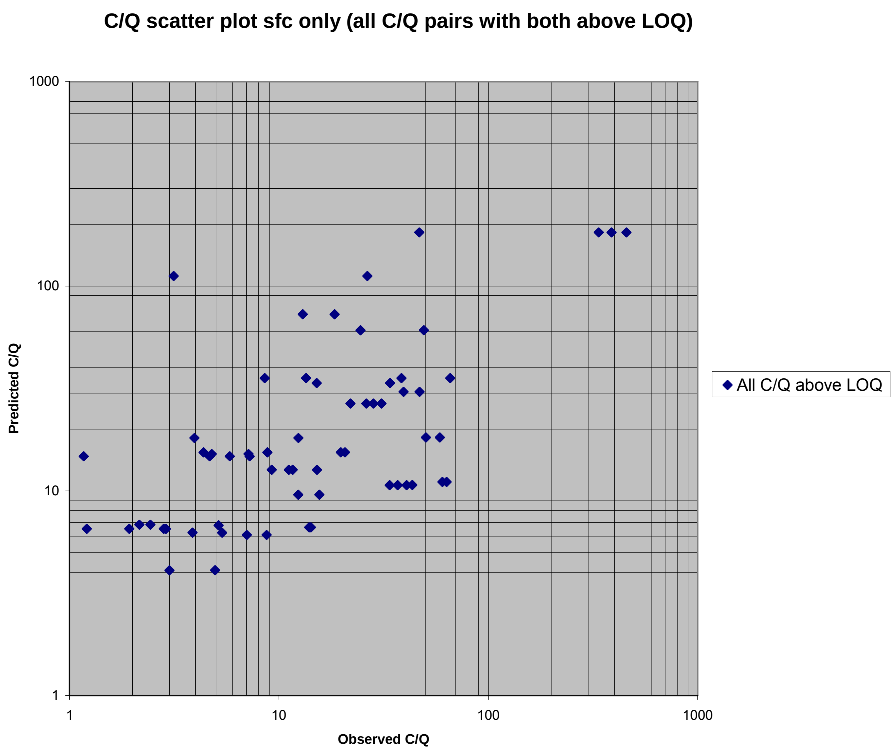

Figure 4. Simple urban dispersion model scatter plot of all surface data (N = 65) with both observed and predicted C above the LOQ. Units of C/Q are s/m^3 times 10^6.

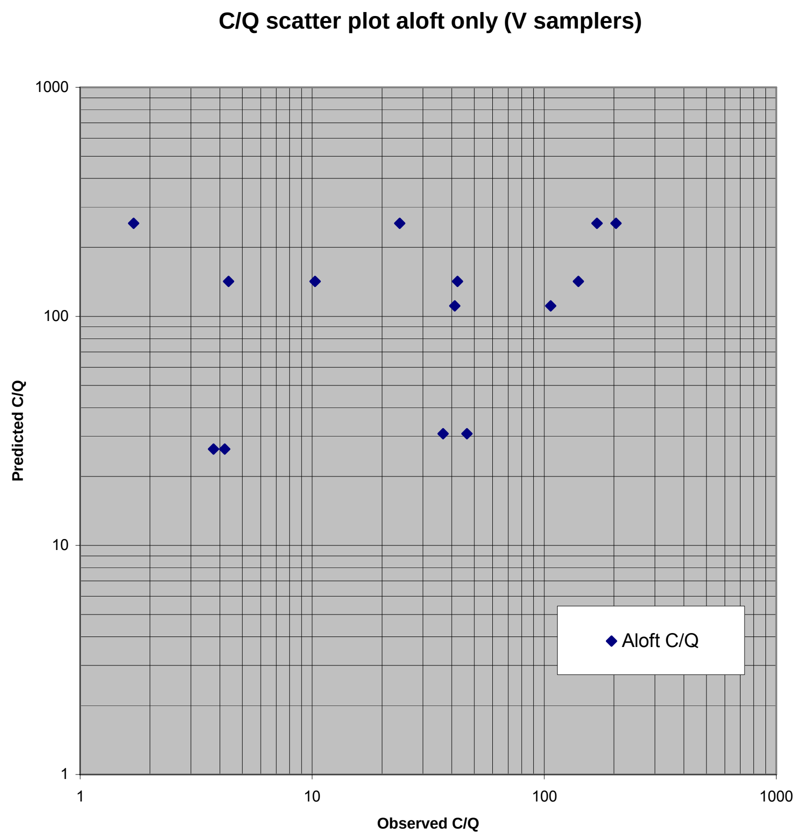

Figure 5. Simple urban dispersion model scatter plot of all aloft data (not at the surface) (N = 15) with both observed and predicted C above the LOQ. Units of C/Q are s/m^3 times 10^6.

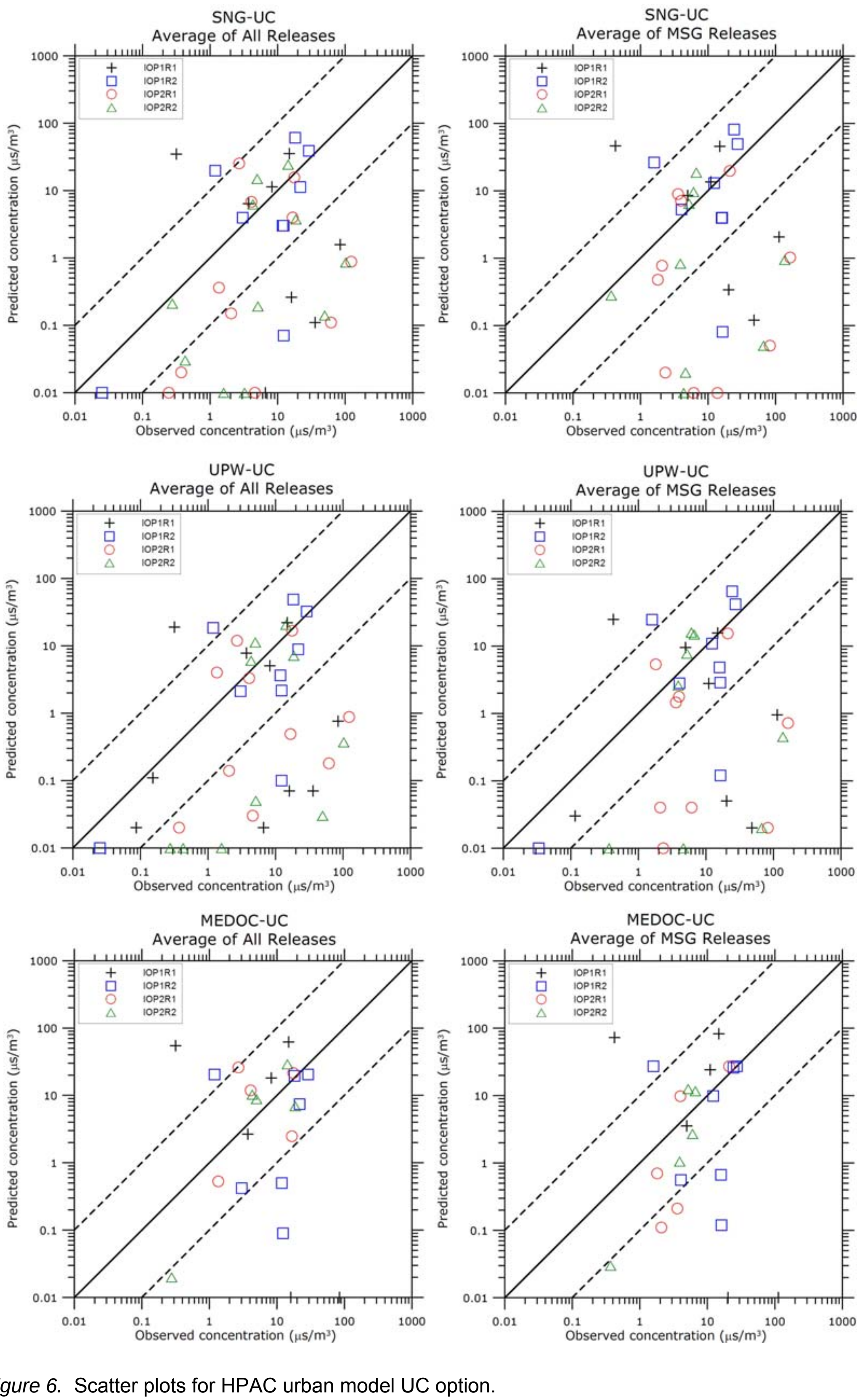

Figure 6. Scatter plots for HPAC urban model UC option.

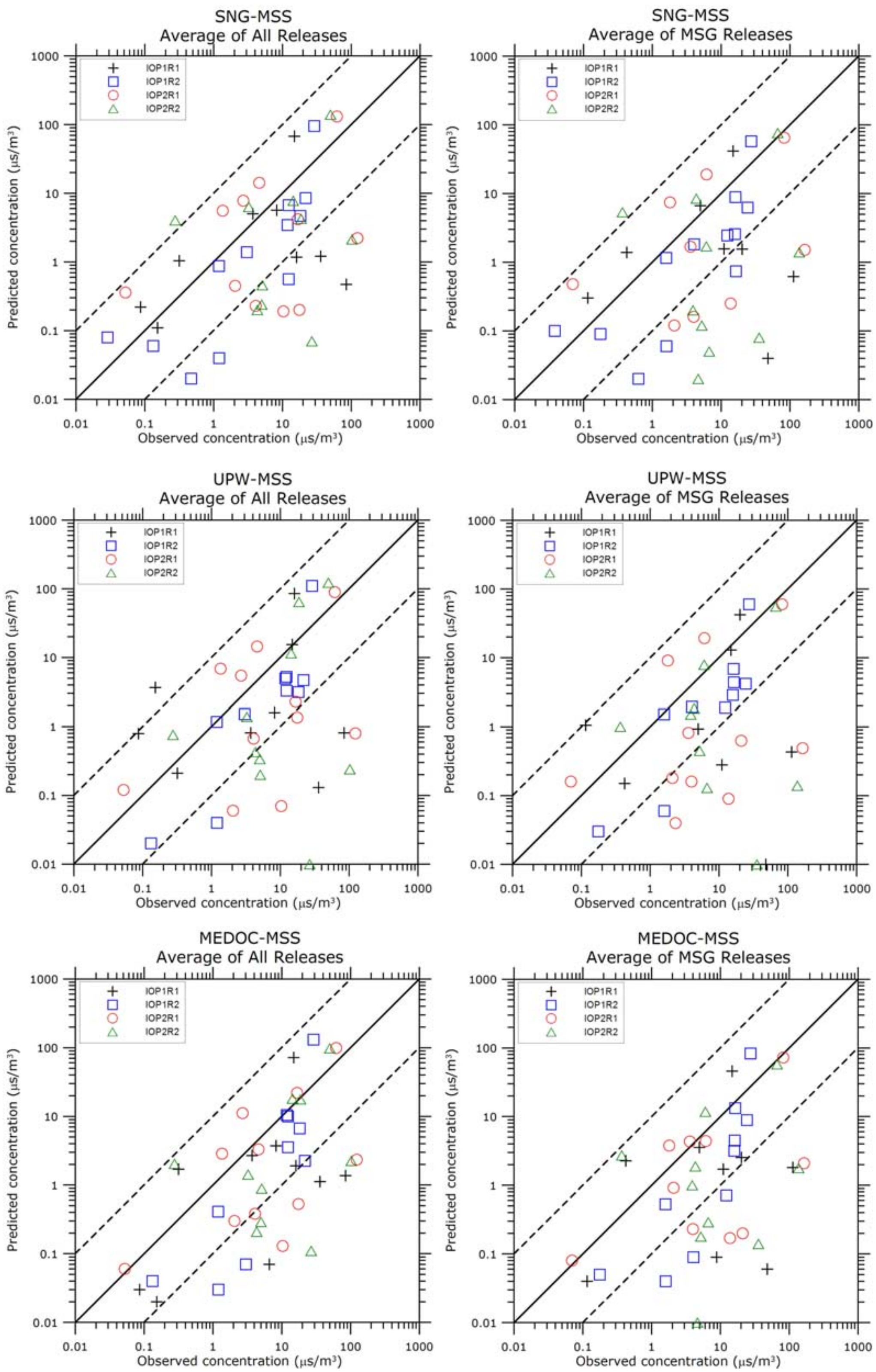

Figure 7. Scatter plots for HPAC urban model MSS option

Table 1. PFT Instrument/Sampler and Release Locations. Figures 1 and 2 Showed These on a Map of MSG05. Samplers 1 through 20 were at Heights of 3 m. Samplers V1 – V7 were at Elevations of 48 m, 48 m, 227 m, 227 m, 133 m, 42 m, and 117 m, Respectively. From Watson et al. (2006) and Allwine and Flaherty (2006).

Instrument	Location Description	Easting	Northing	Latitude	Longitude
1	7th & 32nd In front of the Hotel Pennsylvania - North side of street	585172	4511447	40.74957	-73.99109
2	west of 6th & 32nd In front of the Blarney Stone Bar - South side	585322	4511354	40.74872	-73.98932
3	34th & Broadway South side - In front of Footlocker	585353	4511518	40.75019	-73.98894
4	Midway between 34th & 33rd East side of 7th - In front of McDonald's	585197	4511563	40.75061	-73.99078
5	Between 36th & 37th In front of Bates Worldwide - West side of 7th	585297	4511789	40.75264	-73.98956
6	232 W. 37th south side In front of West Tandori Club - Midway 7th & 8th	585192	4511882	40.75349	-73.99079
7	Midway 8th & 9th on 36th In front of 320 Goldie Restaurant - S side	584923	4511938	40.75402	-73.99397
8	In front of McDonald's Midway 34th & 35th - East side of 8th	585000	4511772	40.75251	-73.99308
10	One Penn Plaza - Middle of building North side of 33rd	585017	4511619	40.75113	-73.99290
11	In front of the Post Office South side of 33rd - Between 8th & 9th	584818	4511714	40.75201	-73.99525
12	Across from St. Michael's Church South side of 33rd - Between 9th & 10th	584659	4511800	40.75280	-73.99712
13	9th and 30th 370 W. 30th - South side of 30th close to 9th	584617	4511555	40.75060	-73.99765
14	South side of 31st midway 8th & 9th - Across from bay 16 of the Post Office	584707	4511595	40.75095	-73.99658
15	West side of 8th #393 Midway btn 30th & 29th - In front of 8th Ave Garden	584792	4511432	40.74947	-73.99559
16	In front of 29th St Marketplace North side of 29th - Between 7th & 8th	584886	4511334	40.74858	-73.99449
17	8th & 27th Middle of T-bone intersection - West side 8th	584699	4511260	40.74793	-73.99672
18	In front of Nagler Hall on the S side of 27th	584842	4511167	40.74708	-73.99504
19	North side of 28th In front of Center Floral Design - Between 6th & 7th	585056	4511152	40.74692	-73.99250
20	In front of Seven Penn Plaza Between 30th & 31st - West side of 7th	585067	4511361	40.74881	-73.99234
V1	12th story Penn One 33rd St side	585072	4511607	40.75102	-73.99225
V2	12th story Penn One 34th St side	585090	4511639	40.75131	-73.99203
V3	Top of Penn One 33rd St side	585013	4511653	40.75144	-73.99294
V4	Top of Penn One 34th St side	585019	4511663	40.75153	-73.99287
V5	Top of Penn Two	585050	4511479	40.74987	-73.99253
V6	Top of Post office 8th and 33rd	584858	4511610	40.75107	-73.99479
V7	Top of New Yorker Hotel	584949	4511796	40.75274	-73.99368
Release A	8th and 33rd – North corner of MSG	584937	4511643	40.75136	73.99385
Release B	33rd midway between 7th & 8th – East corner MSG	585052	4511585	40.75083	73.99249
Release C	31st midway between 7th & 8th – South corner MSG	584985	4511465	40.74975	73.99330
Release D	8th and 31st – West corner MSG	584875	4511527	40.75032	73.99460
Release E	34th between 7th & 8th – middle of Penn One	585065	4511673	40.75162	73.99233

Table 2. Perfluorocarbon Tracer Characteristics and Conversions. From Watson et al. (2006) and Allwine and Flaherty (2006).

Acronym	**Chemical Name**	**Formula**	**Mol. Wt. (g/mol^{-1})**	**Conversion from ppqv to µg/m^3**
PMCP	Perfluoromethyl-cyclopentane	C_6F_{12}	300	1.34E-5*
PMCH	Perfluoromethyl-cyclohexane	C_7F_{14}	350	1.56E-5
oc-PDCH	Perfluoro-1,2-dimethyl-cyclohexane	C_8F_{16}	400	1.78E-5
PECH	Perfluoroethyl-cyclohexane	C_8F_{16}	400	1.78E-5
i-PPCH	Perfluoro-isopropyl-cyclohexane	C_9F_{18}	450	2.0E-5
1PTCH	Perfluoro-trimethyl-cyclohexane	C_9F_{18}	450	2.0E-5

***Thus 1 ppqv = 1.34E-5 µg/m^3**

Table 3. PFT Release Locations, Start Times, Release Durations, and Release Masses during MSG05. From Watson et al. (2006) and Allwine and Flaherty (2006).

Modified form of Table 3 of the BNL Tracer Report
Tracer Release Data for March 10, 2005
Release duration was nominally 1hr. Tracer releases were terminated at 10:00 and 12:30.
Release mass was computed using 1 atm and 0 degC, which was similar to ambient conditions.
Tracer mass has an error of +/- 3%

3/10/2005 9:00 EST	Tracer Release Location	Start Time	Release Duration (min)	Release Mass (g)
oc-PDCH	A	9:00	60	0.316
PMCP	B	9:05	55	4.624
PMCH	C1	9:00	60	1.739
i-PPCH	C2	9:00	60	0.082
PECH	D	9:02	58	0.592
1PTCH	E	9:16	44	0.090

3/10/2005 11:30 EST	Tracer Release Location	Start Time	Release Duration (min)	Release Mass (g)
oc-PDCH	A	11:30	60	0.320
PMCP	B	11:30	60	5.261
PMCH	C1	11:30	60	1.777
i-PPCH	C2	11:30	60	0.084
PECH	D	11:30	60	0.641
1PTCH	E	11:30	60	0.123

Modified form of Table 4 of the BNL Tracer Report
Tracer Release Data for March 14, 2005
Release duration was nominally 1hr. Tracer releases were terminated at 10:00 and 12:30.
Release mass was computed using 1 atm and 0 degC, which was similar to ambient conditions.
Tracer mass has an error of +/- 3%

3/14/2005 9:00 EST	Tracer Release Location	Start Time	Release Duration (min)	Release Mass (g)
PECH	A	9:06	54	0.570
PMCP	B	9:07	53	4.408
PMCH	C1	9:00	60	1.477
i-PPCH	C2	9:00	60	0.068
oc-PDCH	D	9:06	54	0.269
1PTCH	E	9:00	60	0.116

3/14/2005 11:30 EST	Tracer Release Location	Start Time	Release Duration (min)	Release Mass (g)
PECH	A	11:30	60	0.669
PMCP	B	11:30	60	5.044
PMCH	C1	11:30	60	1.889
i-PPCH	C2	11:30	60	0.089
oc-PDCH	D	11:30	60	0.320
1PTCH	E	11:30	60	0.121

Table 4. Estimates of PFT Backgrounds and Uncertainties, Based on Number of Data Points Indicated. Uncertainties are Expressed as a Standard Deviation (Stdev), Level of Detection (LOD = 3 times Stdev), and Level of Quantification (LOQ = 10 times Stdev). From Watson et al. (2006) and Allwine and Flaherty (2006).

PFT	Number of Data Points Used to Determine Background	Background C in ppqv	Stdev in ppqv	LOD in ppqv	LOQ in ppqv
PMCP	239	19	2.2	6.6	22
PMCH	342	17	2.1	6.3	21
ocPDCH	347	3	0.7	2.1	7
iPPCH	401	6	1	3	10
1PTCH	302	3	1.2	3.6	12
PECH	93	1	3	9	30

Table 5. Statistical Performance Measures for Simple Urban Model. Note that C/Q has units of s/m^3 times 10^6. Equations (4) through (8) Define the Performance Measures. N is the Number of Samplers with Pairs of Observed and Predicted C/Q Exceeding the LOQ.

Performance Measure	All Data Simple Model	All Sfc Data Simple Model	All Sfc Data for OPP Release Simple Model	All Near-Field (8, 10, 15) Sfc Data Simple Model	Aloft Data (Not at Sfc) Simple Model
N	80	65	10	10	15
Max Co/Q	457	457	63	457	204
Max Cp/Q	256	183	34	183	256
Average Co/Q	40.7	37.1	38.0	136.3	56.1
Average Cp/Q	51.9	32.1	21.7	122.4	136.2
Median Co/Q	14.2	13.7	43.1	36.6	36.7
Median Cp/Q	18.1	15.0	18.3	112	142
FB	-0.24	0.14	0.55	0.11	-0.83
NMSE	2.36	2.64	1.04	1.12	1.68
MG	0.61	0.76	1.44	0.43	0.22
VG	6.00	3.15	3.03	11.29	93.9
FAC2	.43	.45	.30	.20	.33

Table 6. Comparison of Observed and Predicted C/Q at Specific Samplers for HPAC Urban Model Options UC and MSS. Note that C/Q has units of s/m^3 times 10^6. A Given C/Q is the Average Over the Five PFTs for a Certain Date and Release. Green Indicates Predicted C/Q that are within a Factor of Two of the Observations. Yellow Indicates Accuracy within a Factor of Five. No Color Indicates a Difference in C/Q of Greater than a Factor of Five.

Release Number and (Sampler Number)	Obs C/Q	Pred UC SNG	Pred UC UPW	Pred UC MEDOC	Pred MSS SNG	Pred MSS UPW	Pred MSS MEDOC
1 on Mar 10 (1 or 4)	**14.9**	62.4	22.0	62.4	67.5	15.4	71.7
2 on Mar 10 (1 or 4)	**29.0**	20.5	32.4	20.5	95.1	111	131.3
1 on Mar 14 (1 or 4)	**17.6**	25.3	16.9	26.1	7.8	5.45	11.1
2 on Mar 14 (1 or 4)	**14.4**	24.3	20.5	29.2	7.8	11.5	18.2
1 on Mar 10 (2 or 3)	**8.26**	18.2	7.79	18.2	5.66	1.59	3.74
2 on Mar 10 (2 or 3)	**21.8**	7.4	8.85	7.42	8.5	4.68	2.25
1 on Mar 14 (2 or 3)	**16.6**	6.8	3.32	11.8	4.2	2.27	21.9
2 on Mar 14 (2 or 3)	**18.7**	6.3	7.14	8.84	4.2	64.5	17.8
1 on March 10 (10)	**85.0**	0.01	0.76	0.01	0.47	0.81	1.37
2 on March 10 (10)	**18.3**	19.5	48.8	19.5	4.68	3.14	6.69
1 on March 14 (10)	**123.4**	0.88	0.88	0	2.23	0.8	2.35
2 on March 14 (10)	**103.0**	0.66	0.37	0	2.13	0.24	2.25
1 on Mar 10 (V1 or V2)	**36.1**	0.10	0.07	0.01	1.21	85.3	1.91
2 on Mar 10 (V1 or V2)	**12.3**	0.50	3.65	0.50	6.69	5.24	10.5
1 on Mar 14 (V1 or V2)	**62.1**	0.15	0.18	0.53	132	89.5	98.9
2 on Mar 14 (V1 or V2)	**50.1**	0.21	0.05	0.02	140	123	98.5