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AN ANALYTICAL URBAN PUFF DISPERSION MODEL COMPARED WITH TRACER OBSERVATIONS IN JU2003

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Abstract: Puffs of SF_6 tracer gas were released near street level in a built-up urban center (Oklahoma City) during the Joint Urban 2003 (JU2003) field experiment. Nine real-time SF_6 samplers (with 0.5 s resolution) operated at downwind distances from about 100 to 1,100 m during about 30 puff releases over ten days. Here we address the maximum observed 0.5 s concentration, C, and the dosage for each sampler and puff time series. We also address the maximum concentration, C_{max}, over all samplers for each puff. The urban dispersion model is a simple analytical Gaussian puff formulation, with the dispersion parameter, σ, assumed equal for all three components. The formulation, $\sigma = \sigma_o + \sigma_{turb}$, is used. The turbulent dispersion component σ_{turb} in urban city centers is assumed to equal 0.17x, for all times of the day, where x is downwind distance along the puff centerline. σ_o represents the initial mixing in the first street canyon. Following earlier suggestions by McElroy and Pooler, σ_o is assumed to equal 30 m. The simple urban puff model is shown to be able to predict C and dosage with low mean bias but with a scatter of about a factor of two.

***Key words**: puff dispersion, urban dispersion, UDINEE, JU2003, urban puff tracer studies*

OBJECTIVES AND BACKGROUND

The authors are members of an international group of scientists who are evaluating urban puff dispersion models with the Joint Urban 2003 (JU2003) puff tracer observations. The project is named UDINEE (Urban Dispersion International Evaluation Exercise) and is described by Hernández-Ceballos et al. (2016). The European Commission's Joint Research Center (JRC) in Ispra, Italy, is coordinating the UDINEE project and producing statistical comparisons of the models' performance. With the support of the U.S. Defense Threat Reduction Agency (DTRA), the JRC could access the JU2003 database. The real-world scenario of concern to the European Commission is a release from an RDD (Radiological Dispersion Device) in a city. An RDD will be a puff release with significant heat from an explosion and significant amounts of aerosols. For obvious reasons, there are no research-grade field experiment data for an actual RDD release in a city. The JU2003 puff release trials are the closest field experiment to an actual RDD. SF_6 gas tracer was released (with no explosion or imbedded aerosols) by popping a 1 m diameter balloon at a height of about 1.5 m above street level in Oklahoma City, USA (Allwine and Flaherty 2006, Clawson et al. 2005, Zhou and Hanna 2007, Doran et al. 2007).

In addition to the JRC team, the UDINEE group consists of modelers from eight countries running nine different urban transport and dispersion models for the JU2003 puff scenarios. The models range in complexity from Lagrangian particle and puff models to CFD models. Initial comparisons of model results with the JU2003 puff data show significant scatter for all models and some cases of significant mean bias. The scatter was expected because the JU2003 puff observation analyses by Zhou and Hanna (2007) and Doran et al. (2007) showed significant scatter (with respect to empirical relationships) in their published plots. It has been pointed out that scatter is maximized for instantaneous puff releases because the data for a single puff is just one realization within an ensemble.

Having carried out several comparative model evaluation studies (e.g., Hanna and Chang, 2012), the authors recognize that, when there is significant scatter in the basic observations, it is difficult to show that one model's performance measures are significantly different than another model's. Consequently, we hypothesized that a simple analytical urban puff dispersion model would likely not perform significantly worse that the more advanced models. At the least, the simple urban model could provide baseline performance measures.

JU2003 PUFF TRACER DATA DESCRIPTION

The JU2003 continuous (i.e., 20 or 30 min duration) release data have become part of a standard urban field data archive used for evaluating urban transport and dispersion models (e.g., Hanna and Chang, 2012). Allwine and Flaherty (2006) provide a detailed summary of the entire JU2003 field experiment, and Clawson et al. (2005) describe the SF_6 puff releases and sampler technology. Characteristics of the JU2003 puff data are discussed by Zhou and

Hanna (2007) and Doran et al. (2007), who present their analysis of the data from the point of view of along-wind dispersion. There were many samplers and puffs where the puff "missed" the sampler, the observed concentrations were less than the instrument threshold, or there were unexplained large outliers. Zhou and Hanna (2007) suggest a set of 167 sampler/puff concentration time series for use in analysis, since they have significant concentrations with expected time series shapes. Doran et al. (2007) and Hernández-Ceballos et al. (2016) suggest slightly different sets, due to slight variations in criteria.

The nine TGA fast-response SF_6 samplers were located at distances ranging from about 100 m to about 1,100 m from the source release location. Three alternate puff release locations were used, and the sampler locations could be moved from one IOP day to another (i.e., the experiment director wanted to be sure the puff "hit" the sampler network). The TGA SF_6 samplers' data are reported with a resolution of 0.5 s. Most of the observed concentration time series have similar shapes, characterized by a rapid rise to a concentration peak which persists for 1 or 2 minutes. There is a slower downtrend (as much as 5 to 10 min) as the puff departs. Spikes and dips of short duration are seen in all time series.

Clawson et al. (2005) explain that the minimum or threshold TGA concentration varied with sampler and IOP, but was typically a few hundred ppt. They also point out that the samplers were occasionally saturated (i.e., concentrations exceeded the maximum limit). This saturation value varies with sampler and IOP but averages about 23,000 ppt.

SIMPLE ANALYTICAL URBAN GAUSSIAN PUFF DISPERSION MODEL

The first author has been developing and testing simple urban dispersion models for over 45 years (e.g., see the review by Hanna 2014). In the 1970s, the models were for continuous area sources in urban metropolitan regions. With the rise in threat of terrorist releases of toxic chemicals in city centers in the late 1990s and early 2000s, several research programs (including JU2003) were initiated where urban tracer experiments were conducted and where new or revised urban transport and dispersion models were developed and evaluated. Hanna and Baja (2009) present the results of testing of a simple urban Gaussian continuous plume model using the JU2003 and the Madison Square Garden 2005 tracer data for continuous releases.

Our simple analytical urban Gaussian puff dispersion model assumes a Gaussian shape with equal dispersion coefficients in all directions (i.e., $\sigma_x = \sigma_y = \sigma_z = \sigma$):

$$C/Q = [1/(2^{1/2}\pi^{3/2}\sigma^3)]\exp(-y^2/2\sigma^2) \quad (1)$$

where, in this paper, C is the <u>maximum</u> 0.5 s concentration at each sampler for each puff, y is cross-wind distance from the puff center, and Q is mass released. It is also assumed that the puff release height and the sampler height are at z = 0, and equation (1) includes reflection at the ground. At all sampler locations, σ is large enough that the C solution, for the assumed release and sampler heights of z = 0, is not significantly different from the solution using the actual heights.

Note that equation (1) does not explicitly include wind speed, u. The wind direction, however, is used to determine the cross-wind location of the puff center with respect to each sampler location, allowing "y" to be calculated in equation (1). For simplicity, the assumed wind speed and direction are assumed to be constant over a given IOP, using the "All-Anemometer" wind averages listed by Hanna and Baja (2009).

Several recent urban boundary layer studies (e.g., Hanna et al., 2011) suggest that stabilities are always nearly-neutral in city centers (due to the anthropogenic heat inputs and the large amount of mechanical turbulence around buildings). We therefore assume that σ has no day-night variation in the city center. The assumed urban σ formula in our simple model is based on the Zhou and Hanna (2007) and Doran et al. (2007) analyses of the JU2003 puff data, considering the general suggestions by Hanna and Franzese (2000) for similarity formulas for along-wind dispersion of puffs. A simple linear formula is used, and includes an assumption of a significant initial σ_o = 30 m:

$$\sigma = \sigma_o + \sigma_{turb} = 30\text{ m} + 0.17x \quad (2)$$

The 0.17x term represents turbulent dispersion, σ_{turb}. It is assumed to have a linear dependence on downwind distance, x, in the city center distance ranges. The initial σ_o is explained by McElroy and Pooler (1968) as being due to mixing in the street canyon where the source is located. It is well known that there are strong eddies of scales proportional to the street width and the nearby building dimensions in street canyons. McElroy and Pooler suggest σ_o = 30 or 40 m based on their analysis of observations in St. Louis. Initial σ_o values in the same "ball-park" are seen in the plots of observed and modeled continuous plume concentration distributions for Midtown Manhattan 2005 (MID05) in Flaherty et al. (2007).

Since σ is a function of x in our model, a puff will have the same shape (distribution) at a given x, regardless of the wind speed. However, when dosage D (time integrated concentration) is calculated, it will be larger at smaller wind speeds since the puff will take longer to pass over the sampler. We carried out sensitivity studies using formulas suggested by Zhou and Hanna (2007) for σ as a function of travel time, t, but the performance measures were not much different than those reported here for σ as a function of x.

The fundamental averaging time in our analysis is the resolution of the samplers (0.5 s) and our assumed σ formula is for that averaging time. For larger averaging times (say 10 s or 20 s), σ would be slightly larger (a rough rule of thumb is that σ is proportional to averaging time raised to the 0.2 power).

COMPARISONS OF MODEL PREDICTIONS WITH OBSERVATIONS

The simple urban Gaussian puff model described above was used to predict maximum short term (0.5 s) concentrations for each puff and each sampler. The reported mass release, Q, and average wind speed and direction were used as inputs. The UDINEE model comparison project in which our small study is imbedded is evaluating a much larger set of model outputs, including, for example, 3-D grids with time dependent solutions (Hernandez-Ceballos et al. 2016). Here we focus on three major types of model outputs:

i) For each puff and sampler: Maximum C(0.5 s); units ppt
ii) For each puff: C_{max}(0.5 s) over all samplers operating for that puff
iii) For each puff and sampler: Dosage D = integral of C over t; units ppt-s

Observations from the TGA samplers are available for each of these model outputs. Scatterplots of predicted versus observed values are used to allow quick "eyeball" assessment of the model performance. Figure 1 contains the scatterplot for maximum C(0.5 s) for each puff and sampler. Note that the blue points for daytime trials and the black points for nighttime trials approximately overlap each other and there is no obvious mean difference. Visual inspection also suggests that, although there is minimal mean bias, there is little correlation between observed and predicted C's, since the points have what is referred to as a "shotgun blast" pattern.

In our initial comparisons, we used all the puffs and samplers that had significant observed concentrations. However, we found that nearly all of the observed maximum C(0.5 s) values exceeded about 400 ppt, while there were about 10 % of the predicted maximum C that were much less than 400 ppt. To even up the comparisons (i.e., compare oranges with oranges), we restricted our scatterplots (such as Figure 1) and calculations of model performance measures only to puffs and samplers where <u>both</u> observed and predicted maximum C(0.5 s) > 400 ppt. Figure 1 shows that, as stated earlier. the observed C has a saturation-caused "cap" at about 23,000 ppt, and about 12 of the observed points are seen to be at that limit. However, we retain those points in the figure and in the subsequent quantitative analysis because they are very important from a health effects perspective

For the points in Figure 1, 39 % are within the ±FAC2 (factor of two) lines, satisfying Hanna and Chang's (2012) acceptance criterion of FAC2 > 0.30 for urban dispersion models. We also calculated the fractional mean bias FB to be -0.40 and the normalized mean square error (NMSE) to be 1.69, which satisfy the acceptance criteria that the magnitude of FB < 0.67 and the value of NMSE < 6. However, Figure 1 also shows that about 7 % of the predicted points indicate an "error" of more than an order of magnitude.

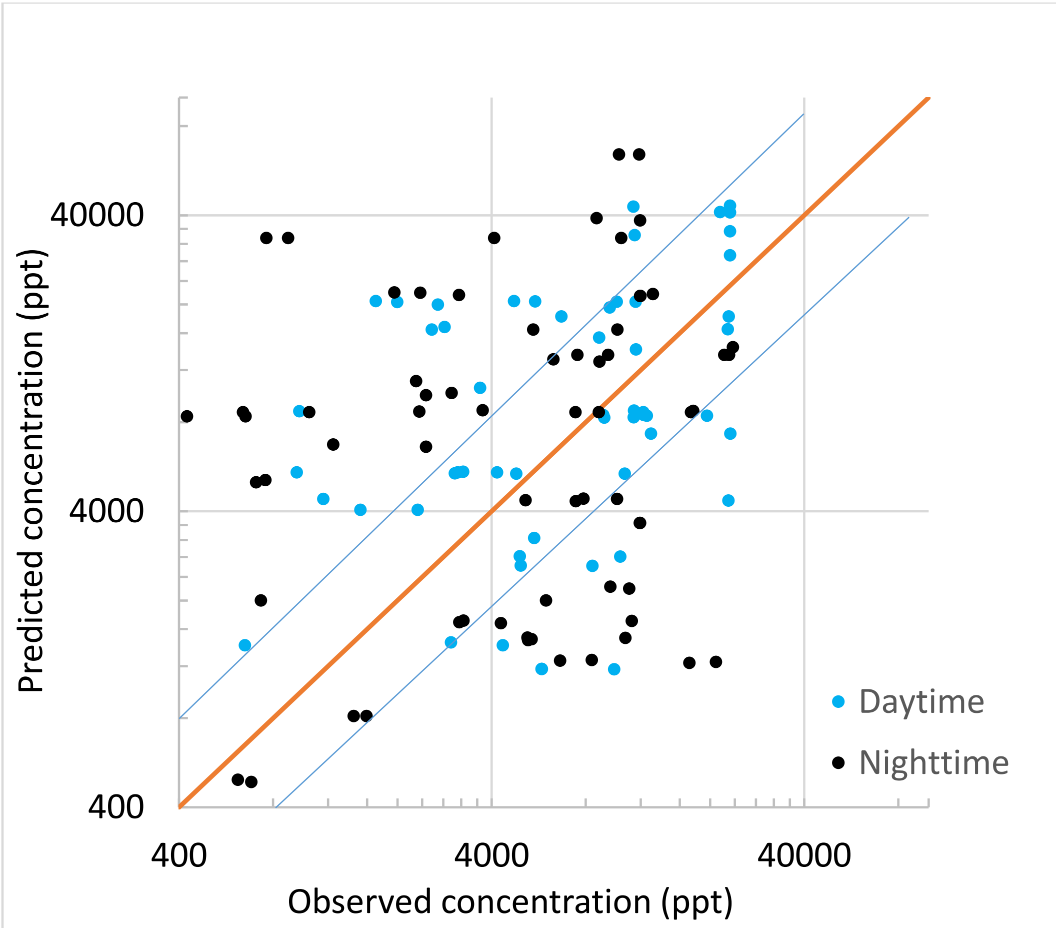

Figure 1. Predicted and observed maximum C(0.5 s) for each puff and sampler. The perfect agreement line is red and the ± FAC2 lines are blue. Day and night IOPs are distinguished.

A scatter plot was also produced for the maximum (C_{max}) for each puff over all samplers. A puff was included only if there were significant observed concentrations (C > 400 ppt) from at least one of the operating TGA samplers, and if predicted concentrations > 400 ppt at that sampler (see paragraph above). Here the saturation C of about 23,000 ppt is found to apply to about half of the 25 puffs. FAC2 = 0.39, which satisfies the acceptance criterion of FAC2 > 0.30. FB = -0.81, which barely does not satisfy the magnitude of FB < 0.67 criterion. NMSE = 1.65, which does satisfy the NMSE < 6 criterion. Although 80 % of the points are overpredictions, this would be lessened if some of the observed concentrations at the saturation value of 23,000 ppt were increased by a factor of two or three or more. The maximum predicted concentration is about 100,000 ppt while the maximum observed concentration is 23,000 ppt (the saturation value).

The scatter plot for dosage D is expected to be less sensitive to the saturation issue mentioned above, since the saturation (high concentration) usually occurs only for a small fraction of the total time period. The performance measures (FAC2 = 34%, FB = 0.13, and NMSE = 1.36) satisfy Hanna and Chang's (2012) urban dispersion model acceptance criteria (FAC2 > 30 %, magnitude of FB <0.67, and NMSE < 6), despite the fact that there is little evidence of correlation (i.e., another "shotgun blast").

CAVEATS

Most of the time, the predictions of the simple urban Gaussian puff model for the JU2003 puffs are seen to produce performance measures (FAC2, FB, and NMSE) that satisfy the model acceptance criteria proposed by Hanna and Chang (2012). There is much scatter, however, and there is minimal correlation between predicted and observed concentrations. These performance measures can be greatly dependent on the assumed minimum (now 400 ppt) and maximum (saturated) concentrations (now about 23,000 ppt).

As pointed out earlier, we have been involved in analyzing the JU2003 puff data for 13 or 14 years. Thus our model evaluations are not using "independent" field data. However, since there are no other high quality urban puff data, it is necessary to use JU2003.

We assumed that the wind direction was given by the "All-Anemometer" average over an IOP. With different wind directions, the C predictions and the performance measures would change. Also, our formula for σ is a function of x. However, Zhou and Hanna (2007) also suggest a best fit formula for σ as a function of time, t, after release. We included this $\sigma(t)$ formula in a sensitivity study with the above data, and found no difference in performance, so did not include those results in this brief paper.

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