A PRELIMINARY INVESTIGATION OF MODEL EVALUATION DATA NEEDS

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INTRODUCTION

1.3. Dispersion models are used to assess the possible extent and severity of accidental and terrorist releases of toxic materials. Most of the current operational dispersion models provide only a characterization of what is observed on average (1st-moment) given the stated conditions. Knowledge of the variability in the possible outcomes about the 1st moment prediction can be important in hazard assessments. The variability can be characterized as coming from two primary sources, 1) wind field (trajectory) variability, and 2) unresolved (diffusion) variability not currently characterized by the model parameterizations. For this study an analytical scheme was developed to characterize more completely the variability in the dispersion. The algorithms were incorporated in a Lagrangian puff model, INPUFF (Petersen and Lavdas, 1986). The effects of variability in the dispersion were simulated using Monte-Carlo methods. The variability in the plume trajectory was investigated in a preliminary sense by tracking the divergence in trajectories from releases adjacent to the actual release location. This modified version of INPUFF provides a means for characterizing the distribution of possible outcomes as a consequence of natural variability in puff transport and diffusion.

1.4. Using this modeling system, we can investigate, in a controlled analytical environment, the problems associated with developing model evaluation procedures. For instance, since the "real-world" contains stochastic effects, how many realizations are needed in order to derive a reliable estimate of the average (1st-moment) surface-level concentrations as might be sampled during a tracer field experiment. Having a quantitative answer to this question is of some importance as ASTM D 6589 Statistical Evaluation of Atmospheric Dispersion Model Performance suggests analyzing tracer experiment results that have been grouped together for analysis.

DISCUSSION

Crosswind Concentration Profile Variations

INPUFF characterizes diffusion by assuming that the vertical and crosswind profiles of each puff has a Gaussian profile, until such time as the puff is well-mixed by convective mixing, at which time the vertical distribution of mass is assumed to be uniform. The widely-used Gaussian approximation for characterizing the crosswind distribution of mass of a dispersing plume as it is carried downwind provides a smoothed view of the individual realizations of what is really seen in the world.

Fig 1 illustrates the observed concentration, averaged over 10 minutes, seen by near-surface sampling along a 50 m arc downwind of a near-surface point-source release of sulfur-dioxide. For each 10 minute experiment or realization, the crosswind receptor positions, y, relative to the observed center of mass along the arc have been divided by σ_y, which is the second moment of the lateral concentration distribution along the arc, for that experiment, and the observed 10-minute concentration values have been divided by $C_{\max} = C^Y / (\sigma_y \sqrt{2\pi})$, where C^Y is the crosswind integrated concentration along the arc. Looking at the visual impression given by all the individual experiments plotted on the figure, the crosswind concentration profile is seen to have a Gaussian shape on average, but is not Gaussian in particular on any one experiment.

Previous investigations of the concentration fluctuations about the Gaussian profile have determined that they can be well characterized using a lognormal distribution (*Irwin and Lee,* 1996). To extend these results, an analysis was conducted of thirteen tracer dispersion experiments each of which had intensive near-ground level sampling along crosswind-arcs at various distances downwind of the release. A Gaussian fit (as described above) was

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computed for each release at each arc, and the Geometric standard deviation (GeoStd) was computed for all c/Cmax ratio values (where c is the observed concentration) for "centreline" receptors ($y < |0.67\sigma_y|$). Results were tabulated only for arcs having at least 50 ratio values for analysis. Fig 2 depicts the results obtained, where the results have been summarized into six groups. The Near-surface Simple group is Prairie Grass, Round Hill, Hanford-30, Green Glow I, and Hanford-67 and involves releases at or below 2 m in nearly flat terrain with steady-state meteorology. The Near-surface Complex group is Green Glow II, Ocean Breeze and Dry Gulch and involves releases at or below 2 m in complex non-steady meteorological conditions. The Elevated Simple group is Hanford-67 and Hanford-64 and involves elevated releases mostly at 26 m and 56 m with few at 111 m over nearly flat terrain. The last three groups (Kincaid, Lovett and Indianapolis) involved tracer injected into the exhaust gases of operating electric power generation plants. The stacks were 187 m, 145 m and 87 m in height for Kincaid, Lovett and Indianapolis, respectively. Kincaid is located in rural Illinois with relatively flat terrain. Lovett is located in complex terrain in rural New York. The Indianapolis release and initial sampling arcs were in the suburbs and the final sampling arcs were in city center.

For those near-surface releases in nearly flat terrain with steady-sate meteorology the GeoStd is about 1.5 for all downwind distances. The GeoStd for the other groups is about 2.0. The average GeoStd for all the results depicted is 1.8 with a standard deviation of 0.62. A GeoStd equal to 1.8 means that 95% of the centreline c/C_{MAX} ratio values are within about a factor of 3 of C_{MAX}.

Dispersion Parameter Variability

INPUFF has several options for characterizing the growth of the vertical and lateral dimensions of each puff, and we selected to use the Pasquill-Gifford dispersion parameters. The vertical and lateral Pasquill-Gifford dispersion parameters are a set of seven curves that describe the growth puffs as a function of downwind distance, with separate curves for each stability category (A through F, where A is very unstable, F is very stable, and there are separate curves for neutral-day and neutral-night). A limitation in the current version of INPUFF is that the stability category is assumed to be the same over the entire domain of the model simulation.

Irwin (1984) calculated the bias in the dispersion parameter (σ_y and σ_z) estimates, and observed that the bias varied from one site to the next, and also calculated the random errors about the systematic bias at each site. To further explore these uncertainties, an analysis was conducted of the tracer field experiments from 26 different sites listed and discussed in *Irwin* (1983). For each experiment we: 1) computed the average and geometric mean of ratio P/O, where P is the predicted and O is the observed growth rate of the dispersion, and 2) computed the standard deviation and geometric standard deviation of P/O ratio values. We limited the analysis to transport distances of less than 5 km. For the current analysis, Model 3 as described in *Irwin* (1983) was used for the predictions. Table 1 summarizes the results obtained from the analysis described. A log-normal distribution was seen to be a reasonable characterization for all of the random error distributions, even though a normal distribution is seen to be indicated at nine experiment sites (see notations in Table 1). We looked to see if the variability in the growth rates had a distance dependence or release height dependence but such was not seen.

If we assume that the random biases and random errors come from independent log-normal distributions, we can model the variability in the growth rates of the dispersion parameters as

$\Delta\sigma_{y,z} = b_{y,z} r_{y,z} \Delta\sigma^{o}_{y,z}$, where the subscripts y and z respectively refer to the lateral and vertical dispersion, b and r are random bias and error factors, $\Delta\sigma^{o}_{y,z}$ is the model's estimate of the increase in the dispersion parameter, and $\Delta\sigma_{y,z}$ is the simulated increase including the effects of variability. We can use the Table 1 results to characterize the distributions of b and r. We can characterize the 26 biases as a log-normal distribution with a GeoSD of 1.48 (e.g., $b_{y,z}$), and we can characterize the 26 GeoSD values by their average, 2.02 (e.g., $r_{y,z}$,). Note, a log-normal distribution with a GeoSD of 1.5 means 90 % of the values are within a factor of 2.

When we simulated the variability in the growth rate of the dispersion coupled with the variability in the lateral profile for non-Gaussian effects, it was seen that variability in the growth rates affected centreline concentration values in the near-field when the puffs are small and the growth rates are at a maximum (see Fig. 3). Once puffs attain some size, the centreline fluctuations are primarily due to the fluctuations imposed on the lateral concentration profile.

Puff Trajectory Variability

As a preliminary investigation, we used approximately 30 24-hour ETA forecasts which are publicly available and have a horizontal grid size of 12-km. A limitation in the current INPUFF is that variations in the winds as a function of height are not treated, only variations in the horizontal. We selected four locations along the Eastern US (New York, Washington, Atlanta, and Miami) anticipating progressively more zonal (east-west) winds for the more southern locations. A puff was released at the start of the 0000Z forecast from each of the eight cells surrounding each central location plus one from the central location, and tracked for the 24 hours of the forecast. At the end of each hour, the median separation of the puffs from the central puff was determined as well as the central puff's σ_y. Analyses were conducted using the 10-m winds and the winds for the first layer (mid-level of which was 75 m) at each location. At all four locations, the separation of the puff trajectories for both sets of winds was greater than the puff's lateral dimensions at least out to 100 km.

CONCLUDING REMARKS

The preliminary results from our analyses suggest the following. The variability not described by the average Gaussian crosswind profile is substantial. Fig. 4 compares the uncertainty in determining the centreline average maximum, Cmax, as a function of the number of receptors distributed along an arc and the number of experiments grouped together for analysis. Fig 4's results can be approximated as $Std(C\max)/C\max = \sqrt{e^{\ln^2 GeoStd} - 1}/\sqrt{NS}$, where NS = NG*(NR/5), NG is the number of arcs grouped for analysis, and NR is the number of nonzero observed concentration values seen along the arc. The variability induced by growth rate variations does not appear to affect centreline concentrations except for locations very near the release. The variability in the transport is likely larger than the entire plume or puff width, which will preclude pairing in time and space of model and observation results for statistical evaluation of model performance.

Disclaimer

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Table 1. Summary of comparison of Model 3 of Irwin (1983) predictions of the growth rate of vertical and lateral dispersion with field data from 26 sites. GeoSD is the geometric standard deviation.

Elevated Lateral Dispersion Sites

Experiment Site	Number	Bias	GeoSD
Hanford(64)-56m	11	1.29	3.05*
Hanford(67)-56m	46	0.99	2.66*
Hanford(67)-26m	158	1.22	2.13
NRTS	80	1.10	1.22
Karlsruhe	26	2.44	2.55
Hanford	48	1.07	1.82*
Suffield	80	1.07	1.63

Elevated Vertical Dispersion Sites

Experiment Site	Number	Bias	GeoSD
Agesta	21	0.82	1.66*
Karlsruhe	58	1.12	2.24
Hanford	13	0.40	2.01*
NRTS	80	0.62	1.36*

Near-Surface Lateral Dispersion Sites

Experiment Site	Number	Bias	GeoSD
Mt. Iron	49	1.29	2.02
NRTS-B	31	0.98	2.24*
NRTS-A	66	0.71	1.67*
Hanford 30	83	1.19	1.75
Green Glow	44	1.30	1.67
Prairie Grass	251	0.81	2.02
Dry Gulch	98	0.62	2.03
Ocean Breeze	101	0.59	1.69
Round Hill II	47	0.75	1.62
Round Hill I	20	0.54	1.63*
Hanford(67)-2m	64	1.00	2.30

Near-Surface Vertical Dispersion Sites

Experiment Sites	Number	Bias	GeoSD
NRTS-B	74	1.69	3.03
NRTS-A	25	1.70	2.79*
Prairie Grass	154	0.92	1.92
Round Hill I	32	1.16	1.77

Values with * denote cases where a Normal distribution best characterizes the random errors, but for which, we also found a log-normal distribution fits nearly as well.

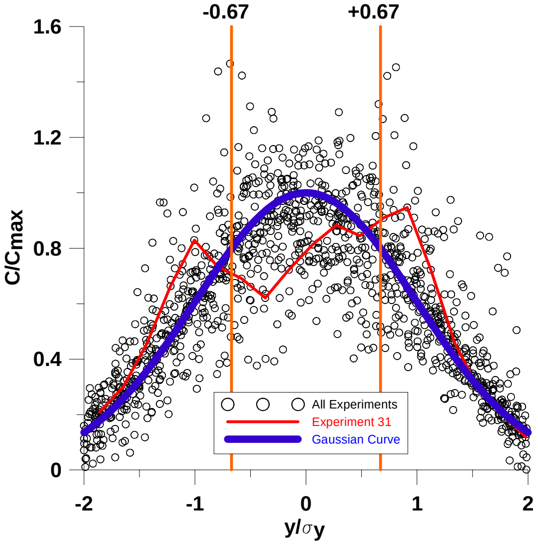

Fig. 1: Illustration of the natural variability that is not characterized in the crosswind of a dispersing puff or plume by a Gaussian puff or plume model, American Society for Testing and Materials(2000). Results depicted are for the 50 m downwind arc of the Project Prairie Grass experiment.

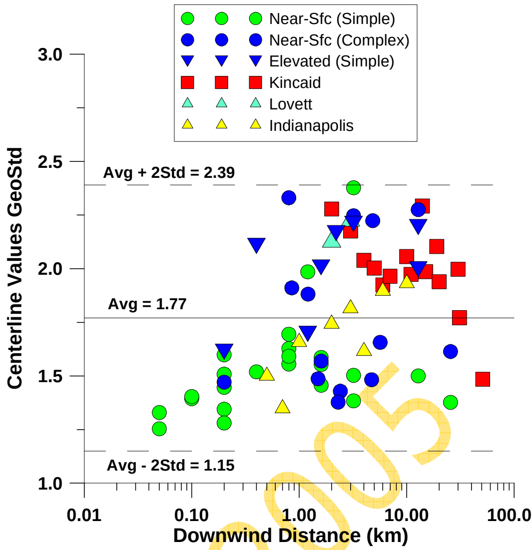

Fig. 2: Summary of GeoStd values determined for centreline concentration fluctuations.

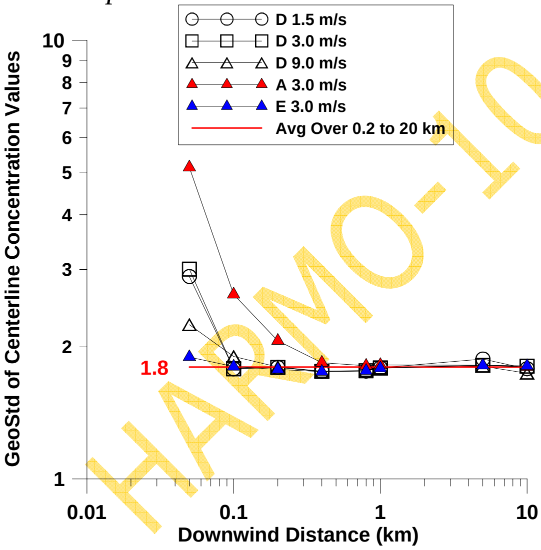

Fig. 3: GeoStd determined for the centreline concentration values for several idealized situations having steady-state conditions for 200 hours. In these simulations variability was simulated in the lateral concentration profile and in the growth rates of the dispersion.

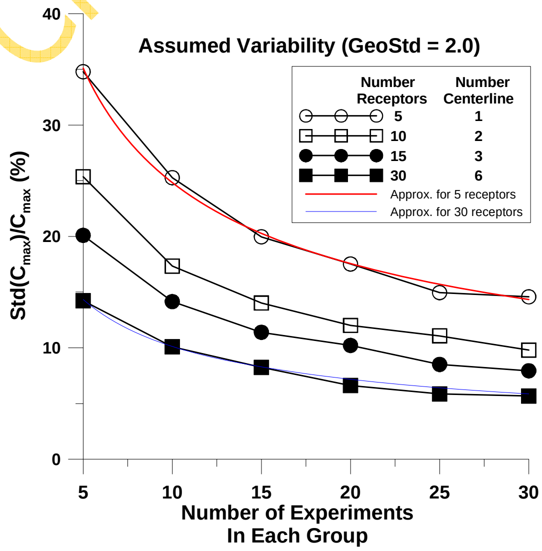

Fig. 4: Summary of uncertainty in the determination of Cmax, in terms of σy(Cmax)/Cmax, as a function of number of receptors along an arc and the number of experiments grouped together for analysis.