THE GAUSSIAN ATMOSPHERIC TRANSPORT MODEL AND ITS SENSITIVITY TO THE JOINT FREQUENCY DISTRIBUTION AND PARAMETRIC VARIABILITY

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ABSTRACT

Reconstructed meteorological data are often used in some form of long-term wind trajectory models for estimating the historical impacts of atmospheric emissions. Meteorological data for the straight-line Gaussian plume model are put into a joint frequency distribution (JFD), a three-dimensional array describing atmospheric wind direction, speed, and stability. Methods using the Gaussian model and JFD inputs provide reasonable estimates of downwind concentration and have been shown to be accurate to within a factor of four. We have used multiple JFDs and probabilistic techniques to assess the Gaussian plume model and determine concentration-estimate uncertainty and model sensitivity. We examine the straight-line Gaussian model while calculating both sector-averaged and annual-averaged relative concentrations at various downwind distances. The sector-average concentration model was found to be most sensitive to wind speed, followed by horizontal dispersion (σ_Z), the importance of which increases as stability increases. The Gaussian model is not sensitive to stack height uncertainty. Precision of the frequency data appears to be most important to meteorological inputs when calculations are made for near-field receptors, increasing as stack height increases.

INTRODUCTION

Estimates of the historical impacts of radiological emissions, e.g.., dose reconstruction, are usually determined after a substantial effort to reconstruct meteorological data for the period of interest. These data are then used in some form of long-term wind trajectory model, most commonly a Gaussian plume formulation. Meteorological data for the straight-line Gaussian plume model is generally packaged into a "joint frequency distribution", or a three-dimensional array of probabilities of winds blowing in a given direction, within a given wind-speed range, and under the influence of a given atmospheric stability. The joint frequency distribution (JFD) is then used to model downwind atmospheric concentrations as the basis for the majority of the dose reconstruction activities. Additionally, the Gaussian model, in conjuction with historical JFD inputs, is sometimes used to estimate hypothetical impacts under various release scenarios.

The JFD is typically obtained by compiling a large number of hourly-averaged meteorological observations over a long period, on the order of years. The NRC, in Regulatory Guide 1.109 (1977), recommends using JFDs that have been compiled over a five-year period. Presumably, a large JFD database results in a more representative set of data for simple atmospheric modeling; however, these larger datasets may tend to mask site specificity, resulting in a less meaningful assessment. Methods using the Gaussian model and JFD inputs provide reasonable estimates of downwind concentration and have been shown to be accurate to within factors of two to four when compared to measured concentration data (Miller and Hively 1987).

Uncertainty assessment techniques may utilize Monte Carlo methods to vary the JFD while calculating downwind atmospheric concentrations. Studies of this type may use five-year joint frequency distributions and apply random uncertainties to the values of windspeed, stability, and direction in order to estimate the uncertainties related to simulating historical conditions. This, however, does not appear to be an appropriate method for uncertainty estimates of air concentrations for historical analysis. Individual cells within the array of frequencies describing windspeed, stability, and direction may not vary by the same degree and may have complex correlations, therefore, random selection is inappropriate. The uncertainty lies in the fact that a meteorological dataset from one time period or location is being used to estimate concentrations in another time period or location. These uncertainties are best determined by examining the sensitivity of the Gaussian model to different data sets, whole data sets not variations in individual data. We, therefore, have used multiple JFDs as input to the Gaussian plume model to determine uncertainty, rather than a Monte Carlo error propagation method. This technique provides insight as to the sensitivity of the straight-line plume model to variation in its inputs under actual meteorological conditions, and thus may strengthen our confidence in concentration estimates of historical releases.

In this work, we have attempted to answer two questions regarding uncertainties in the Gaussian model: (1) how important are the concentration parameters, and (2) how important is the precision of the joint frequency data? These questions are answered by examining the straight-line Gaussian model while calculating both sector-averaged and annual-averaged relative concentrations at various downwind distances. Sector-averaged concentrations are made site-specific only by the use of specific windspeed averages, release heights, and downwind elevation data. In addition to these parameters, the annual-averaged concentrations are site-specific when meteorological frequency data are used that describe the probability of the winds blowing in a given direction, with atmospheric characteristics described by particular stability and windspeed categories.

METHOD

We have determined the sensitivity of the Gaussian plume model to its various inputs by examining it in two parts. First, the sensitivity of the model to parametric variability was determined by calculating sector-averaged concentrations using Monte Carlo techniques, independent of a specific JFD. Second, to estimate model sensitivity to the joint frequency distribution, we calculated annual-averaged relative concentrations for each of sixteen sectors using twenty-four different JFDs from a variety of locations.

In both instances, vertical dispersion factors (σ_Z) for stability categories A through F were calculated using a power function algorithm to describe the familiar Pasquill-Gifford curves (Pillinger and Huang 1986). Three parameters for each of two regions of the P/G curves are used in the equation,

$$\sigma_Z = Ax^B + C, \tag{1}$$

to estimate values of σ_Z. Values of the coefficients, dependent on downwind distance, x, are provided in Table 1. Dispersion factors for stability category G are calculated using the relationship,

$$\sigma_Z(G) = \exp[2 \cdot \log(\sigma_Z(F)) - \log(\sigma_Z(E))]. \tag{2}$$

Parameter sensitivity. In order to determine the sensitivity of the Gaussian model to each of its input parameters, independent of the JFD, we have examined the sector-averaged relative concentration, $\left[\frac{\mathrm{X}_k}{Q}\right]_S$, for each of the 16 cardinal wind directions (k) using,

$$\left[\frac{\mathrm{X}_k}{Q}\right]_S = \frac{6.385}{\sigma_Z \pi x \bar{u}_k} \exp\left[\frac{-h^2}{2\sigma_Z^2}\right], \tag{3}$$

where σ_z is the vertical dispersion coefficient for downwind distance x, $\bar{u}_k$ is the average windspeed in sector k, and h is the physical stack height. Parameters in Eq. (3) were allowed to vary as follows: the vertical dispersion coefficient was assumed to be lognormally distributed with a geometric standard deviation determined as a function of downwind distance (Table 2); windspeed was varied by stability class; and physical height was assumed to vary about it's stated value by ±3% as a triangular distribution.

The uncertainty of the vertical dispersion coefficient, σ_Z, was varied with downwind distance and stability class in a manner consistent with the fundamental form of the Pasquill-Gifford functions (Turner 1967). Distributions describing σ_Z for all downwind distances and stability classes were assumed to be lognormally distributed with geometric standard deviations (GSD) determined as follows (Fig. 1). First, midpoint values between the individual Pasquill-Gifford curves were determined by logarithmic interpolation as a function of downwind distance.

Estimates of uncertainty were then taken as the average of the upper and lower ratios of the midpoint values to the mean dispersion coefficients as calculated with Eqn. (1) at a given downwind distance. These ratios were assumed to contain 95% of the estimates of dispersion coefficient, i.e., two geometric standard deviations. The GSD was then calculated using,

$$GSD = \exp\left[\frac{\ln(R)}{1.96}\right], \tag{4}$$

where R is the average ratio of midpoint values to the mean.

This method of determining the uncertainty of the vertical dispersion coefficient suggests that uncertainty increases with downwind distance and decreases as the atmosphere becomes more stable. The numerical data indicate that the GSDs of the vertical dispersion factors range from 1.07 to 1.77 for distances ranging from 0.1 to 50 km downwind (Table 2).

At times, atmospheric conditions and downwind distances dictate that the value of σ_Z be constrained to the average height of the inversion layer. During these conditions, primarily in unstable air and at large receptor distances, we have assumed that no uncertainty exists in the estimate of σ_Z because it is a defined and fixed value. Uncertainty in this case is related to the height of the inversion layer. We have assumed, therefore, that uncertainty in the mean inversion height is described by a normal distribution with a mean of 1000 meters and a standard deviation of 5%.

Windspeed distributions were derived from meteorological data collected at each of eight onsite towers at the Savannah River Site. Frequency-weighted average windspeeds were calculated and plotted (Fig. 2) against joint frequency data over all eight tower locations. These plots, therefore, represent the input distributions for windspeed as a function of atmospheric stability. Windspeed values within categories were given equal weight during parameter-value sampling.

Parameter values for multiple calculations of sector-averaged relative concentration (X/Q) were assigned using a Latin hypercube sampling (LHS) routine. The method considers the range of each parameter to be composed of a given number of non-overlapping intervals of equal probability. For a given parameter, values are selected at random from each interval based on the probability density function in the interval. The Latin hypercube approach is a constrained random sampling technique that results in added precision over conventional random sampling methods (e.g., simple random sampling) since the entire range of the distribution is sampled in a more systematic manner. Thus, fewer iterations are needed in order to provide adequate statistical input for the probabilistic dose estimate.

One thousand X/Q estimates were calculated using the Gaussian model and the parameter assignments described above. The Latin hypercube routine selected 10 parameter values from each of 100 intervals within each parameter distribution. The Latin hypercube method provided frequency distributions of X/Q with mean standard errors of less than 0.01%. Statistics of the probability distributions obtained by this method were not improved significantly by increasing the number of trials above 1,000.

Model Sensitivity and the JFD. One of the most critical inputs to the Gaussian plume model for calculating annual average air concentrations is the joint frequency distribution of meteorological data. Questions often arise as to the regularity with which these data should be gathered, the proximity of the release point to the meteorological tower, and the appropriateness of using simplified default values, e.g., D stability and an average site windspeed. The importance of these questions will come to light when examining the sensitivity of the Gaussian model to the JFD inputs.

Our original database of JFD files[*] consisted of a set of 476 JFDs originating from National Weather Service data recorded at airports across the United States. That set was narrowed to 269 useable datasets based on the following criteria: (1) the file is in its original form; (2) it contains 5 consecutive years of data; and, (3) the data were collected within the general time period from 1950 to 1965. Dose reconstruction projects for the Department of Energy are focused on the early years of nuclear-weapons production, and since these are the databases that are being reconstructed, it is important to use data for this analysis that were obtained with similar instrumentation. Confining our data to these years also better ensures that it was obtained in similar fashion at all airports.

Of the useable datasets, twenty-four were chosen for use in the analysis. These datasets were purposefully selected to cover areas all over the United States, locations that incorporate various geographical and topographical features (Table 3). The final datasets included twenty-

[*] STAR datafiles obtained from Mr. Barry Parks, U.S. Department of Energy, Germantown, MD.

three states, sites in the coastal plains, on large islands, in deserts, mountains, plateaus, plains, and rolling hills. Five of the files were from southern states, four from the southeast, three from the northeast, three from the mid-west, four from the northwest, four from the west, and one from the Hawaiian Islands. By choosing such diverse locations, estimates of model sensitivity are maximized.

Once the datasets were selected, an electronic spreadsheet was developed to calculate relative concentration (X/Q) as a function of distance for all stability classes, wind-speed categories, and wind directions using each of the twenty-four JFDs. Values of sector-averaged X/Q were calculated as in Eqn. (3) and values of annual-averaged relative concentrations were determined using,

$$\left[\frac{\mathrm{X}_k}{Q}\right]_A = \sum_{ij}\left[\frac{\mathrm{X}_k}{Q}\right]_S \cdot \left[f_{ij}\right]_k, \qquad (5)$$

where f_{ij} represents the JFD array and is the frequency of winds blowing in a given wind-speed category (i) and in a given stability class (j). As in Eqn. (3), k represents compass direction from the release point to the receptor.

All input parameters, except frequency values associated with the JFD, were held constant and mean values were used for each wind-speed category so as to isolate the joint-frequency inputs in determining model sensitivity. Dispersion coefficients were calculated as above and the average inversion height was assumed to be 1000 meters, thus constraining σ_Z to this maximum value.

RESULTS AND DISCUSSION

Parameter sensitivity. Parameter sensitivity was determined by Monte Carlo techniques and multiple iterations of the sector-average Gaussian model. Probabilistic output distributions of relative concentration averaged over the width of a compass sector at a given downwind distance were generated using Eqn. (3) and by varying wind-speed, physical stack height, and the vertical dispersion coefficient. All output distributions were lognormally distributed. Median and range values were recorded for each of 70 output distributions, i.e., an array of seven stability classes by ten downwind distances from 0.1 to 50 km. The measure of relative range was calculated as the difference of output distribution values at the 97.5^{th} percentile and the 2.5^{th} percentile value, divided by the median. Model sensitivity was determined by calculating the contribution-to-variance in the output from each parameter as a function of downwind distance, stability class, and stack height.

Plots of mean downwind relative concentration versus distance and stability class (**Fig. 3**) are characteristic and indicate a loss of dependency on stability inputs beyond a distance of about 5 km. These data also suggest that the model is increasingly more sensitive at closer distances as the atmosphere becomes less stable.

Figure 4 shows that for unstable atmospheres (classes A and B) variations in the relative range of output distributions are minimal with all downwind distances, but generally as the air becomes more stable, the output ranges increase significantly at distances less than about 5 km. Beyond that point, output distribution ranges indicate less uncertainty in modeled concentrations.

The investigation of parameter sensitivity focuses on three variables: physical stack height, wind-speed, and the vertical dispersion coefficient. Sensitivity plots as a function of stability class and downwind distance are presented in Fig. 5 for three stack heights. The data indicate a number of interesting and complicated patterns of model sensitivity to the variables in the sector-average calculation.

Sensitivity of the Gaussian model to it's three primary inputs is quite difficult to assess. Model sensitivity shifts back and forth between wind speed and σ_Z depending on stack height, downwind distance, and atmospheric stability. Generally, the data of Fig. 5 indicate that the Gaussian model is more sensitive to wind speed than the vertical dispersion coefficient and that the stack height has little significance in overall sensitivity, with only slight importance in the near-field during stable conditions. However, if stack height increases, the model becomes more sensitive to the vertical dispersion parameter, σ_Z, and consequently, less sensitive to wind speed. Additionally, for those situations where the Gaussian plume may or may not reach the ground (i.e., tall stack, near-field receptor, stable air), the importance of σ_Z is very high while wind speed is of little significance.

The various plots in Fig. 5 show a general hyperbolic shape to the sensitivity of the vertical dispersion coefficient. Discontinuities in this shape are an artifact of constraining σ_Z; when the value of σ_Z is limited to the mean inversion height, essentially all model sensitivity is shifted to the wind-speed parameter. The value of σ_Z is constrained at distances ≥ 2 km in A stability, ≥ 10 km in B stability, and ≥ 30 km in C stability.

The data generally suggest that σ_Z has more importance in the near-field, even more so in stable conditions, and as receptor distance increases importance shifts to wind speed. This shift is seen to occur closer to the release location for shorter stack heights. Conversely, for a given stack height, the importance of σ_Z is highest in near-field stable conditions and in far-field unstable conditions. In a neutral atmosphere, the importance of wind speed peaks at a given downwind receptor distance that increases with stack height. And, in unstable air, the overall importance of σ_Z increases with stack height, such that σ_Z takes on extreme importance in very unstable air in the near-field.

Many more conclusions can be drawn by close examination of Fig. 5, but their utility would be limited to the conditions specific to a given release scenario. Thus, the general conclusions are more useful in assessing the sensitivity of the Gaussian model to its few input parameters.

Sensitivity to the JFD. Annual-average, relative air concentrations at ground-level were calculated for each of sixteen directions using twenty-four JFD input datasets with mean windspeeds in each windspeed/stability category. Mean values of these 384 relative concentration estimates, when plotted as a function of downwind distance and release height, exhibit characteristics expected of the straight-line Gaussian model (Fig. 6). Sensitivity of the annual-average model to the JFD was determined by examining two measures of the variability exhibited by the 384 output values. The significance of the joint frequency data as input to the Gaussian model is measured by how much variability exists in estimates of relative concentration using a variety of meteorological databases. The range and a coefficient of variation provide indicators of the amount of variability propagated through the model as a result of JFD inputs. The first measure provides an indication of how the range of estimates changes for various conditions, and the second measure shows variability about the mean of the concentration distributions. The range is calculated as the ratio of the maximum and minimum values while variability is quantified as the standard deviation divided by the mean of all output values.

Plots of both measures have similar shapes and trends, however, the coefficient of variation (Fig. 7) is the better measure of JFD importance because it is more sensitive to changes in physical stack height and downwind distance. For ground-level releases, the model produces very stable results over all distances. As the stack height increases to 10 meters, variability decreases indicating that the model is less sensitivity to the meteorological data and that the JFD has minimal importance. When the physical stack height increases above 10 meters, an increase of variability at distances closer than about 2 km results, hence putting more importance on the JFD. By contrast, beyond 2 km our sensitivity measures show that the variability in multiple calculations of X/Q is relatively small and that the joint frequency data has less importance in the far-field.

CONCLUSIONS

In an analysis of parameter sensitivity in the straight-line Gaussian dispersion model, it was found that the sector-average concentration model is most sensitive to wind speed, with that sensitivity generally decreasing as the receptor moves farther downwind. The Gaussian model appears to be more sensitive to variability in the horizontal dispersion parameter (σ_Z) in the near-field. This is evidenced by a convergence of relative concentration estimates and distribution range as a function of stability class (Figs. 3 and 4). This convergence implies that regardless of σ_Z input, concentration estimates and their uncertainty are quite similar with receptors in excess of about 5 km downwind. The data of Fig. 5 also indicate that the importance of σ_Z increases as stability increases. The model is not sensitive to physical stack height, primarily because of the lack of uncertainty in that parameter. With advancements in global positioning technology, terrain elevations can be determined with great precision relative to the other parameters of the Gaussian model.

Based on changes to probabilistic estimates of concentration (Fig. 7), the annual average model would seem to be most sensitive to frequency inputs of wind speed, direction, and stability when calculations are made for near-field receptors. With ground- or low-level atmospheric releases, the variability in concentration estimates is minimal and somewhat constant for all downwind receptor distances within the limits of the Gaussian model. That variability, however, increases dramatically in the near-field as stack height increases, but shows very little change beyond about 2 km.

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FIGURE CAPTIONS

Fig. 1 Pasquill-Gifford curves of horizontal dispersion coefficients and demonstration of the estimate of parameter uncertainty (Turner 1967).

Fig. 2 Wind speed probability as a function of stability category.

Fig. 3 Downwind sector-averaged relative concentration (sec/m^3) as a function of stability class.

Fig. 4 Distribution relative range as a function of stability class. Relative range is calculated as the difference between the output values at the 2.5th and 97.5th percentile divided by the median.

Fig. 5 Results of the sensitivity analysis for sector-averaged concentration estimates. Histograms of parameter sensitivity for stack height, wind speed, and horizontal dispersion are given as a function of stability class and downwind distance for release heights of (a) 10 m, (b) 30 m, and (c) 62 m.

Fig. 6 Mean downwind ground-level annual-averaged relative concentration (sec/m^3) as a function of stack height.

Fig. 7 Coefficient of variation (COV) of the annual-averaged relative concentration distributions as a function of stack height. The COV is calculated as the standard deviation divided by the mean.

Table 1. Values of the coefficients in Eqn (1) for determining vertical dispersion coefficients as a function of downwind distance.

Downwind Distance	Stability Category	A	B	C
100 - 1000 meters	A	0.00066	1.941	9.27
	B	0.0382	1.149	3.3
	C	0.113	0.911	0
	D	0.222	0.725	-1.7
	E	0.211	0.678	-1.3
	F	0.086	0.74	-0.35
> 1000 meters	A	0.00024	2.094	-9.6
	B	0.055	1.098	2
	C	0.113	0.911	0
	D	1.26	0.516	-13
	E	6.73	0.305	-34
	F	18.05	0.18	-48.6

Table 2. Geometric standard deviation of vertical dispersion coefficient uncertainty estimates (lognormal distributions).

Downwind	Stability Class						
Distance	A	B	C	D	E	F	G
100	1.07	1.09	1.12	1.10	1.09	1.12	1.12
200	1.09	1.09	1.11	1.11	1.10	1.13	1.13
500	1.25	1.19	1.14	1.13	1.11	1.12	1.12
1000	1.43	1.30	1.17	1.14	1.11	1.12	1.12
2000	-	1.48	1.22	1.17	1.11	1.12	1.12
3000	-	1.60	1.24	1.19	1.12	1.12	1.12
5000	-	1.77	1.29	1.23	1.13	1.13	1.13
10000	-	-	1.35	1.28	1.14	1.14	1.14
30000	-	-	-	1.38	1.18	1.17	1.17
50000	-	-	-	1.44	1.20	1.18	1.18

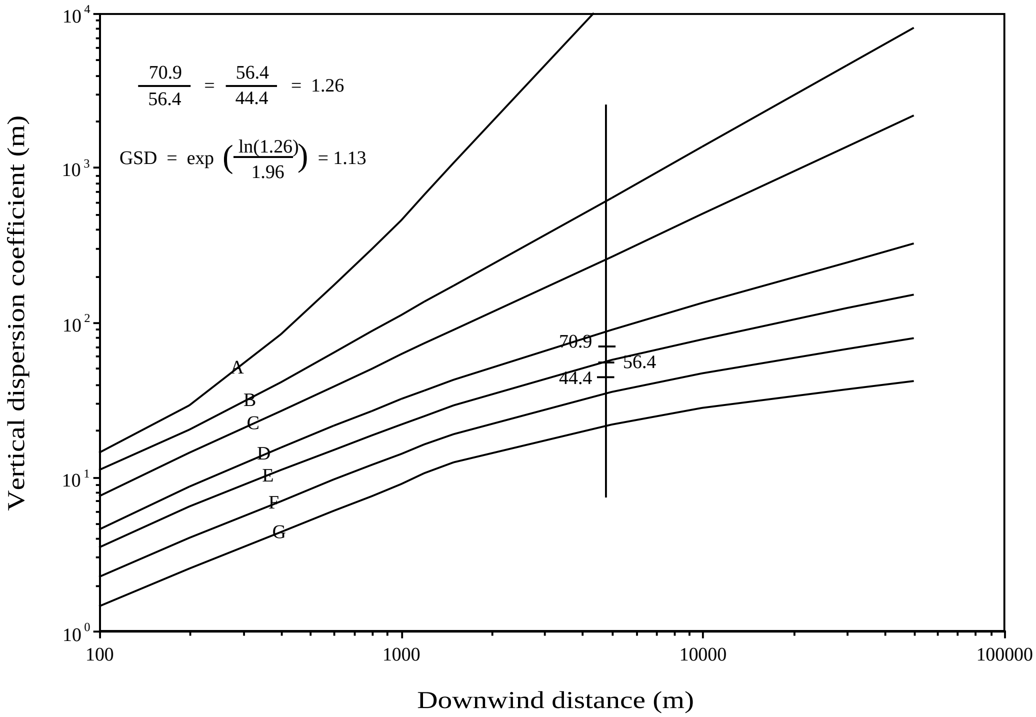
Note: For example, the calculated dispersion coefficient for a distance of 5000 meters in E stability is 56.4 meters. The assumed values of σ_z at 5000 meters and during E stability conditions, therefore, would be lognormally distributed with a geometric mean of 56.4 and a geometric standard deviation of 1.13.

The dashes (-) represent conditions in which the value of σ_z is constrained to 1000 m, the mean inversion height, with its uncertainty represented by a normal distribution and a standard deviation of ± 5%.

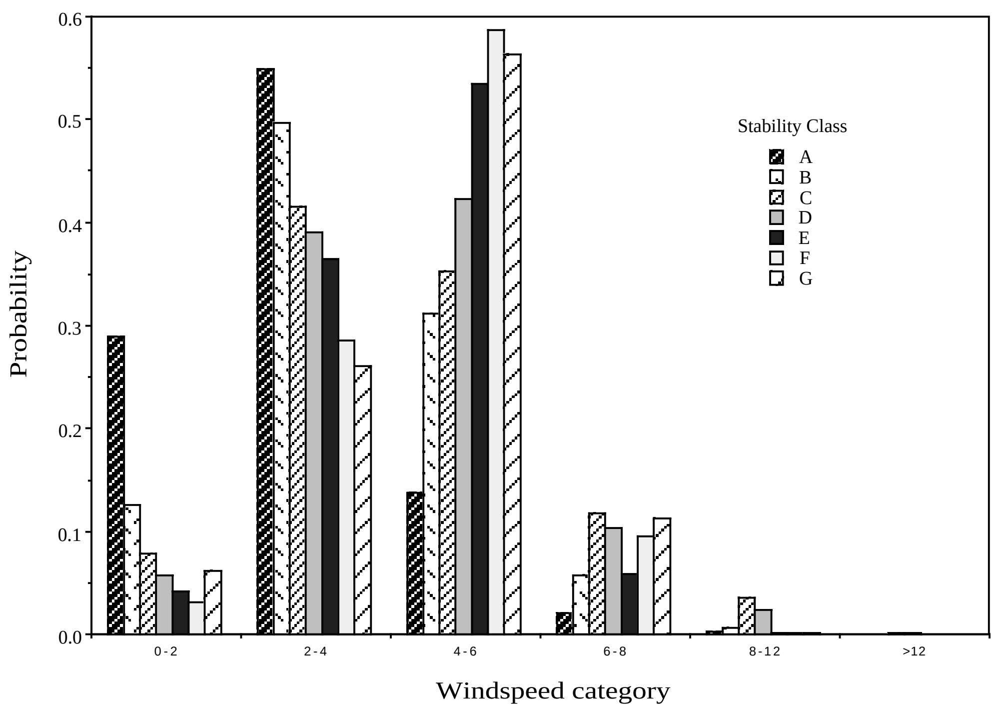
Table 3. Airport locations and 5-yr time period of the 24 STAR datasets used for the sensitivity analysis.

El Dorado, AR	01/50 - 12/54
Tucson, AZ	01/59 - 12/63
Oakland, CA	01/60 - 12/64
Denver, CO	01/60 - 12/64
Tampa, FL	01/60 - 12/64
Hilo, HI	08/62 - 07/67
Pocatello, ID	01/58 - 12/62
Glenview, IL	01/60 - 12/64
Paducah, KY	01/60 - 12/64
Augusta, ME	01/50 - 12/54
Kirksville, MO	01/50 - 12/54
Biloxi, MS	01/60 - 12/64
Winston Salem, NC	01/60 - 12/64
Dickinson, ND	01/60 - 12/64
Lincoln, NE	01/59 - 12/63
Teterboro, NJ	01/52 - 12/56
Albuquerque, NM	01/60 - 12/64
Santa Fe, NM	01/50 - 12/54
Astoria, OR	01/60 - 12/64
Philipsburg, PA	01/50 - 12/54
Anderson, SC	01/54 - 12/58
Galveston, TX	01/58 - 12/62
Walla Walla, WA	01/50 - 12/54
Morgantown, WV	01/50 - 12/54

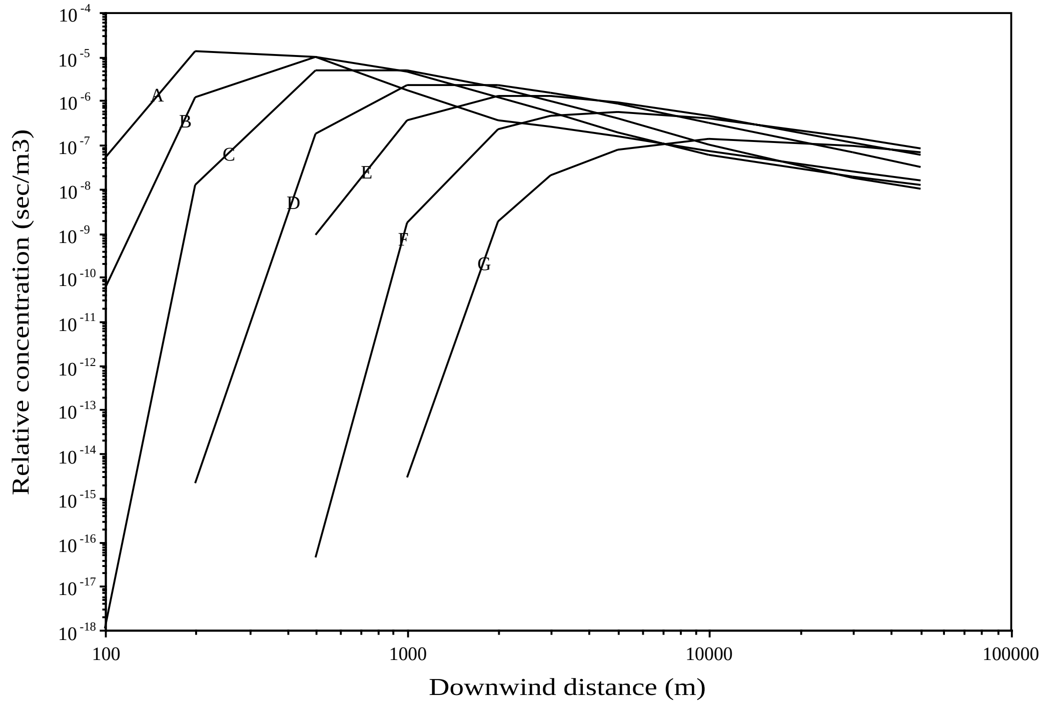
Pasquill-Gifford curves from Eqn. X



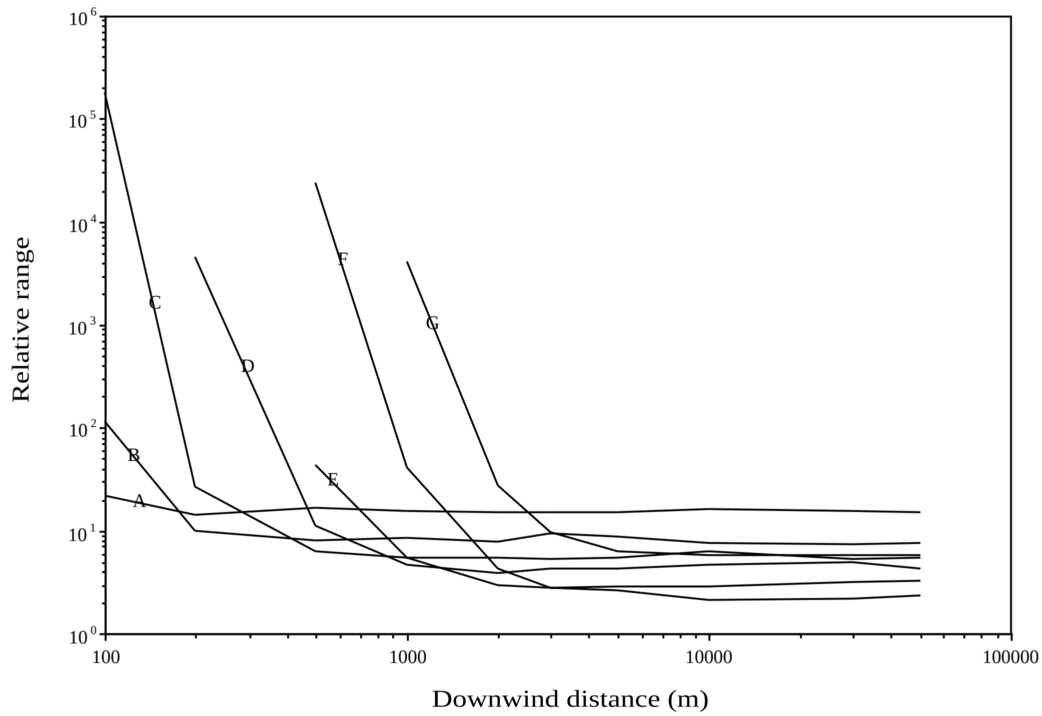
Windspeed Probability as a Function of Stability Category

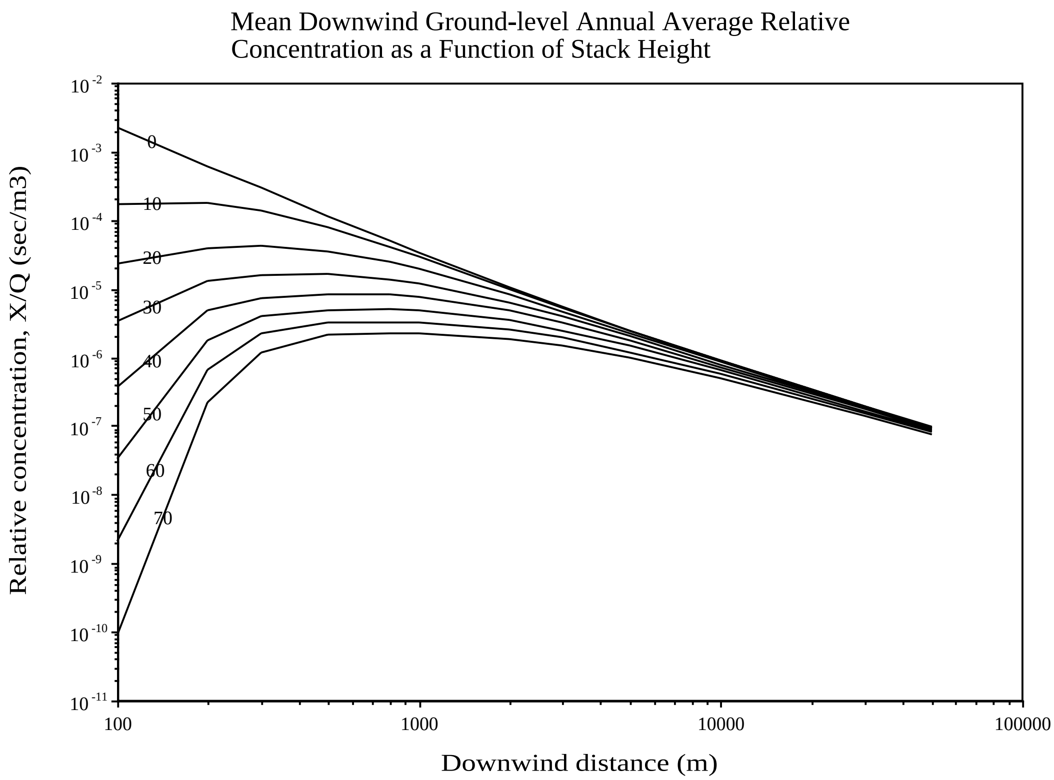


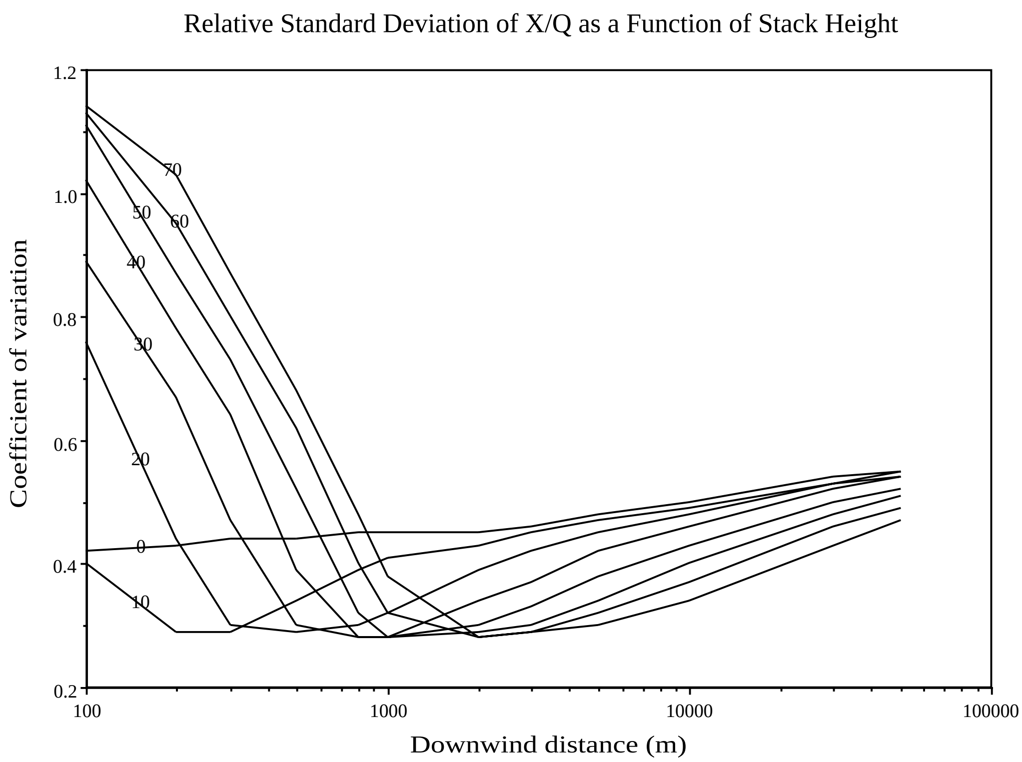
Downwind Sector-Averaged Relative Concentration as a Function of Stability Class



Distribution Relative Range (95%) as a Function of Stability Class




Mean Downwind Ground-level Annual Average Relative
Concentration as a Function of Stack Height
Relative concentration, X/Q (sec/m3)
Downwind distance (m)
0
10
20
30
40
50
60
70
100
1000
10000
100000


Relative Standard Deviation of X/Q as a Function of Stack Height
Coefficient of variation
1.2
1.0
0.8
0.6
0.4
0.2
100
1000
10000
100000
Downwind distance (m)
70
50
60
40
30
20
0
10