# INCORPORATING UNCERTAINTY INTO DISPERSION CALCULATIONS

**Larry L. Gautney, Jr.**
Tennessee Valley Authority
Atmospheric Sciences Department

**Abstract**
Dispersion calculations are generally presented as a single value despite the recognition that for many situations a more appropriate presentation would be a range of values along with the probability of occurrence within the range. This paper describes a methodology that presents results in the form of probabilities by using frequency distributions rather than single values for performing calculations The software runs on a personal computer and is based on commonly used spreadsheets. The technique is demonstrated by estimating transport distances of particles. The results that incorporate uncertainty are compared to those obtained without this consideration.

## Purpose

Typically, dispersion estimates are based on the use of single values for each variable. Most variables, however, can take on any value within a range, which can often be represented by a frequency distribution. Although the need to account for the effect of this uncertainty on the final calculation is often mentioned, this has seldom been done because to do so has been an involved and time-consuming task.

The purpose of this paper is to describe and demonstrate a technique for incorporating uncertainty into calculations. Although the demonstrations are from atmospheric dispersion, the approach is applicable to any situation where there is a degree of uncertainty in the input that can be expressed in the form of a frequency distribution.

## Concept

Recently developed software makes the process of accounting for uncertainty a relatively easy process. This software is designed to allow the use of frequency distributions, rather that single values, in spreadsheets such as Excel and Lotus. The information defining the distribution is entered into cells on the spreadsheet in place of a single value, making it possible to easily modify existing spreadsheets.

The technique employed to account for the uncertainty of variables is to perform many iterations (typically about 1000), randomly drawing a value for each variable from its representative frequency distribution during each calculation. This technique, known as Monte Carlo simulation, has been used extensively for developing estimates of risk. The value assumed by each variable and the calculated result are used to compile information on frequency distributions and statistics. In addition, the software determines the sensitivity of the final calculation to changes of each of the variables.

Frequency distributions for the variables can be constructed from measurements, literature, experience, or simply a "best guess". Although measurements may be preferred they often do not exist. In this case, the literature may provide information on reasonable values, perhaps even frequency distributions. Finally, distributions can often be generated based on past experience; in some cases this may be the best source of information.

Fortunately, many of the most commonly used frequency distributions are incorporated into the software. The analyst provides only the information required to define the distribution for a situation. In addition, a custom distribution may be defined for cases that do not match a mathematical distribution.

## Application

Application of the technique will be demonstrated by calculating the distance particles are likely to travel before deposition. The use of a simple calculation facilitates a comparison of calculations with and without considering uncertainty in the input. Assuming relatively simple distributions for familiar parameters makes it possible to visualize the expected outcome and demonstrate that the results are reasonable.

## Settling velocity

The calculation of terminal settling velocity, $c_s$, of a particle falling through the atmosphere is described in many texts. The description below is from Friedlander[1].

$$c_s = \frac{\rho_p g d_p^2}{18\mu} C \left(1 - \frac{\rho}{\rho_p}\right)$$

where:

$c_s$ = the settling velocity (cm/s)

$\rho_p$ = the density of the particle (g/cm$^3$)

$g$ = the acceleration of gravity (980.6 cm/s$^2$)

$d_p$ = the particle diameter (cm)

$\mu$ = the viscosity of air ($1.818 \times 10^{-4}$ g/cm-s at 20° C)

$\rho$ = the density of air ($1.1884 \times 10^{-3}$ g/cm$^3$ at 20° C)

C, the slip correction factor (dimensionless), is given by:

$$C = 1 + \frac{2l}{d_p}\left(A_1 + A_2 \exp\left(\frac{-A_3 d_p}{l}\right)\right)$$

where $l$ is the mean free path between molecules (0.065 µm for normal air temperature and pressure). The constants $A_1$, $A_2$, and $A_3$ are:

$A_1$ = 1.257 (dimensionless)

$A_2$ = 0.400 (dimensionless)

$A_3$ = 0.550 (dimensionless)

Particles were assumed to be composed of cobalt (CO) with a density of 8.9 g/cm$^3$. Based on the above equations and assumptions the estimated settling velocities for CO particles with diameters of 1, 10 and 100 µm are 0.0310, 2.71, and 267.1 cm/s, respectively.

If the initial height, $z_i$, of the particle is known, the settling velocity can be used to estimate the time, t, required for the particle to fall to the ground, where $t = z_i/c_s$. Assuming the particle is transported downwind at a velocity equal to the average wind speed, U, the transport distance, x, is given by $x = Ut$, or $x = Uz_i/c_s$.

## Meteorological data

Wind speed from measurements at one of TVA's facilities is presented in table 1. The average of the upper and lower wind speeds defining seven wind speed categories from 0.6 to 24.4 mph was used to estimate the distance the particles would be transported before falling to the ground. The transport distance, in combination with the frequency of occurrence of the wind speed category, provides a measure of how far particles are likely to be transported.

## Example

The following example is presented in two parts. First, the estimates of transport distance based on the above information will be presented. This is followed by a presentation of estimates that directly incorporate the uncertainty in the wind speed and particle diameter.

### Without uncertainty

In addition to a summary of the meteorological data, table 1 presents estimated transport distances for three selected CO particle diameters. The results show that 100 μm particles are likely to be deposited within about 100 m of the vent, while the 10 μm particles can be expected to travel several thousand meters. The 1 μm particles have the potential to travel thousands of meters before settling to the ground.

The meteorological information implies there is about a 98 percent chance that particles 10 μm in diameter will be deposited within about 5432 m of the release point. For 100 μm particles this distance decreases to 54 m, illustrating that a factor of 10 increase in diameter results in a factor of 100 decrease in travel distance.

The results illustrate that the travel distance of particles depends on their initial height above ground, wind speed, particle diameter, and particle density. Particles with a diameter of about 10 μm and greater can be expected to be transported a few thousand meters or less before deposition. Smaller particles, however, may be transported much greater distances. This information, in combination with the wind speed frequency data, provides an estimate of how far particles of a particular size can be expected to be transported. For a mixture of particle sizes, however, the quantification of expected transport distance becomes more difficult because the effect of uncertainty in two parameters must be considered.

### With uncertainty

For comparison consider an evaluation which incorporates frequency distributions, rather than single values, for the particle diameter and the wind speed. The use of add-in software makes it possible to use frequency distributions in a spreadsheet cell in place of a single value. The specific software used was Excel 4.0 and Crystal Ball 3.0[2] running on a Macintosh. IBM-PC versions of the same software are available. (The PC version of Crystal Ball also works with Lotus.) In addition, other software products are available which perform the same function as Crystal Ball. This software allows a direct calculation of the expected distribution of travel distance which accounts for the uncertainty in both wind speed and particle diameter. In addition, the software provides statistical information on the results as well as a sensitivity analysis to identify the most critical parameters.

For this example the wind speed frequency is available from measurements and corresponds to that used above. Particle diameter measurements do not exist, but experience indicates that particle size distributions are often lognormal, so this form will be assumed. Specifically, the particle diameter was assumed to be lognormal with a mean diameter of 10 μm and a standard deviation of 3. The diameter and wind speed were assumed to be uncorrelated. (The software is capable of treating correlated distributions.) The distributions of wind speed and particle diameter as assumed and as used in the calculations are displayed in figure 1. A comparison confirms that the distributions used closely match those specified for each of the variables.

The frequency distribution based on estimated travel distance accounting for uncertainty in wind speed and particle diameter is presented in figure 2. Recalling that the distribution of particle diameter was assumed to be lognormal and observing that the wind speed distribution is also lognormal the distribution of distance traveled is as expected. One notable difference, however, is that the 98 percent level travel distance appears to be more than 5432 m. In fact, the 98 percent confidence level is estimated to be about 15,000 m., with 5,432 m corresponding to the 83.3 percent confidence level.

Figure 2, while helpful for investigating the effect of uncertainty in wind speed and particle diameter travel distance, represents only a small portion of the information available. For reference, a full report generated by the software is presented in the appendix. Following is a description of each page in the report.

Page 1 of the appendix presents information on the starting and ending time of the simulation and a trend chart. The trend chart is useful for investigation the cascading effect of uncertainty when forecasts depend on each other. A common example is the effect of uncertainty on successive estimates over time. The trend chart is meaningful only if forecasts depend on each other, therefore it is meaningless in the above example and is presented only to illustrate the capability of the software.

Page 2 contains the sensitivity chart, which provides information on how sensitive the forecast of travel distance is to assumptions about the wind speed and particle diameter. For the above example the estimated travel distance is strongly dependent on both parameters.

Pages 3 and 4 present a statistical and graphical summary of the particle settling velocity. Similar information can be generated for any intermediate calculation.

Pages 5 and 6 present a statistical and graphical summary of the estimated travel distance. As an illustration of one of the presentation options available, the graph of distance traveled is presented as a frequency distribution rather than the reverse cumulative distribution in figure 2. In addition, note that this page provides the previously mentioned 83.3 percent confidence level travel distance of 5,432 m.

Finally, page 7 presents a summary of the assumptions used in the calculations.

## Summary

The technique presented above describes a method for accounting for uncertainty when performing calculations. Although the example is simple enough to allow visualization of the outcome prior to running the model, this is not the case for more complex situations. Complex situations, however, are precisely those where quantifying the implications of uncertainty is most important. A sensitivity analysis, for example, can identify the parameters where a refinement is most likely to have a significant effect on the final outcome of calculations. By taking the process a step further and associating a cost to the refinement of each parameter the likely cost and potential benefit of different resource allocation options can be compared.

For example, much work is currently under way to satisfy the permitting requirements of Title V of the clean air act. These requirements call for permit applicants to provide estimates of pollutants not previously reported and/or emissions from sources that were not previously covered under air permits. While it is important that a realistic estimate of emissions of a pollutant be provided on the permit application, but at the same time the applicant knows that the emission rate varies due to fuel quality, operating conditions, temperature or some other influence. Incorporating this uncertainty into estimates of emissions can provide information on the probability that future emissions testing will find the source exceeding the permit limit and possibly being out of compliance.

## References

1. Friedlander, S. K.,"Smoke, Dust, and Haze", John Wiley & Sons, Inc., 1977.
2. "Crystal Ball 3.0 User Manual", Decisioneering Inc., 1993.

Table 1. Travel distances for cobalt particles with diameters of 1, 10 and 100 μm and frequency of occurrence of measured wind speed.

| Wind speed | | Freq. | Cum. freq. | Distance traveled (m) before deposition for particle diameter of: | | |
|---|---|---|---|---|---|---|
| (mph) | (m/s) | (%) | (%) | 1 μm | 10 μm | 100 μm |
| 1.00 | 0.45 | 6.04 | 6.04 | 47542 | 544 | 6 |
| 2.45 | 1.10 | 36.24 | 42.28 | 115113 | 1318 | 13 |
| 4.45 | 1.99 | 26.65 | 68.93 | 209083 | 2393 | 24 |
| 6.45 | 2.88 | 15.58 | 84.51 | 303052 | 3469 | 35 |
| 9.95 | 4.45 | 13.76 | 98.27 | 467499 | 5352 | 54 |
| 15.45 | 6.91 | 1.21 | 99.48 | 725916 | 8310 | 84 |
| 21.45 | 9.59 | 0.07 | 99.55 | 1007825 | 11537 | 117 |

• Release height was assumed to be 32.61 m.

Figure 1. Frequency distribution of wind speed and particle diameter as assumed and as used to perform calculations.

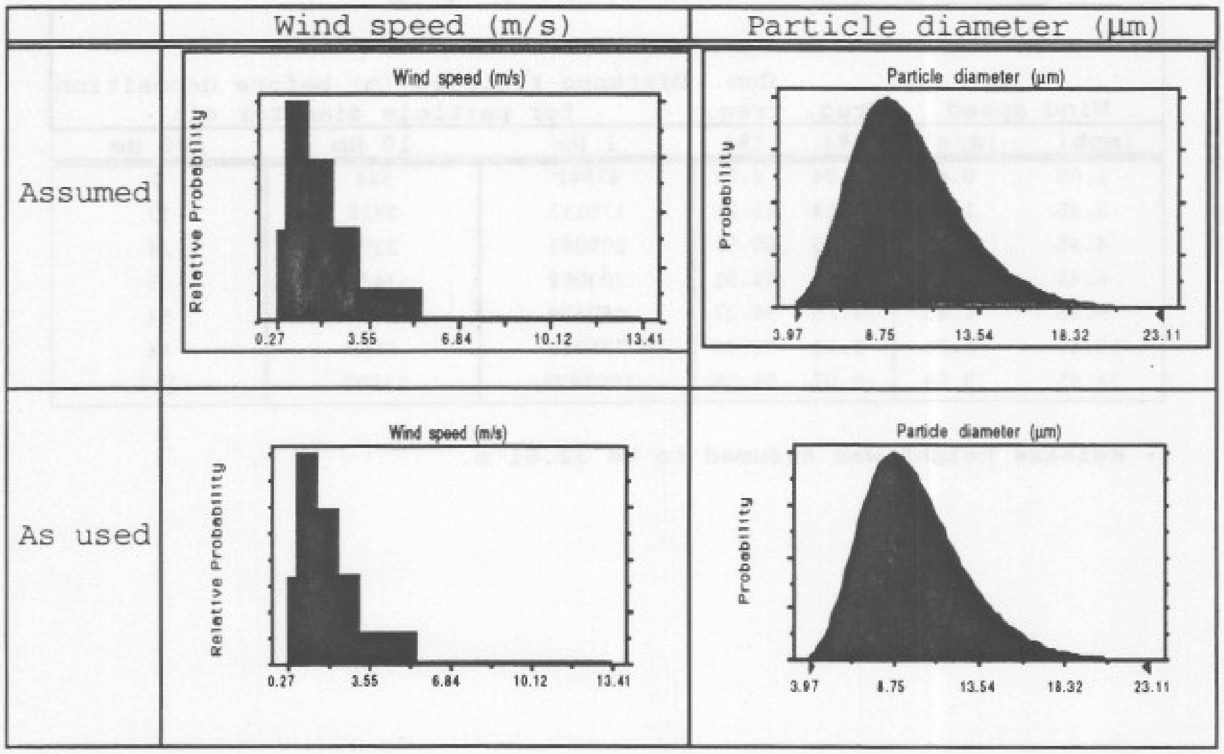
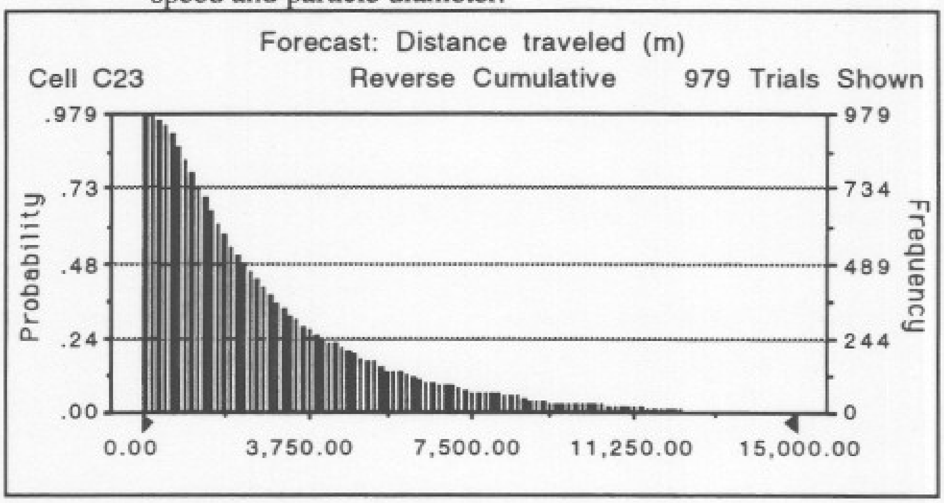
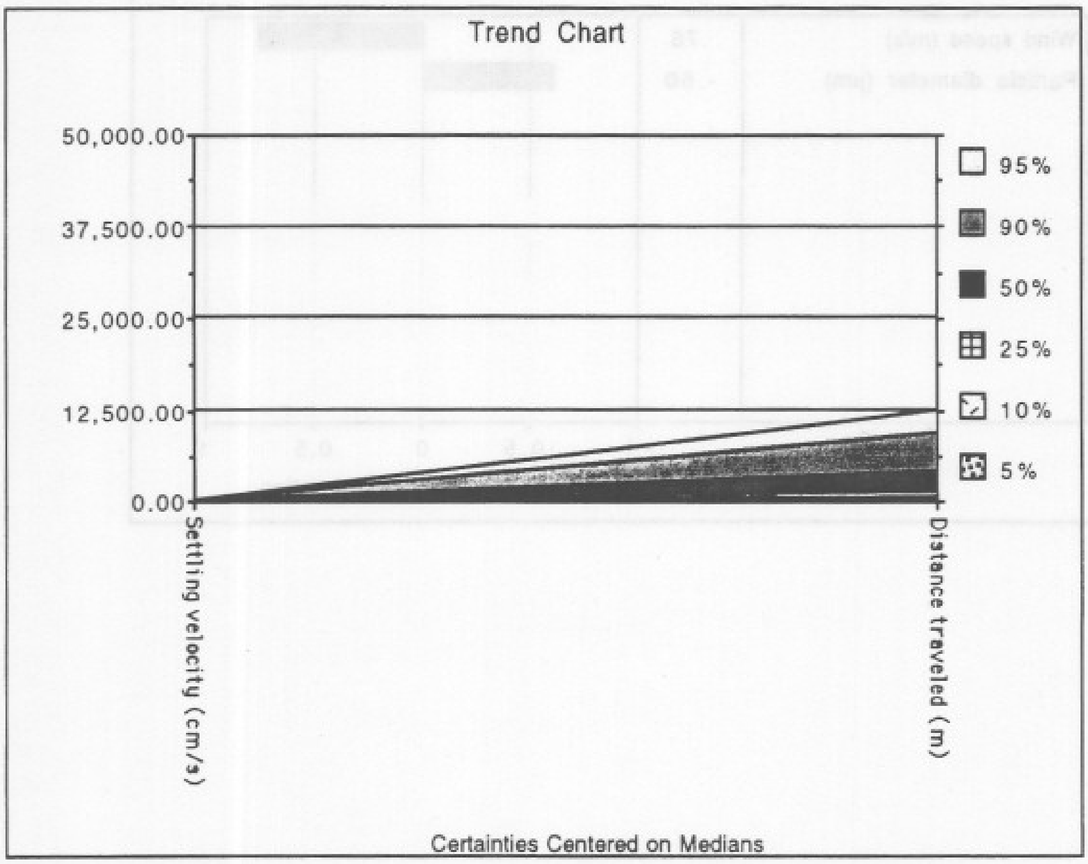


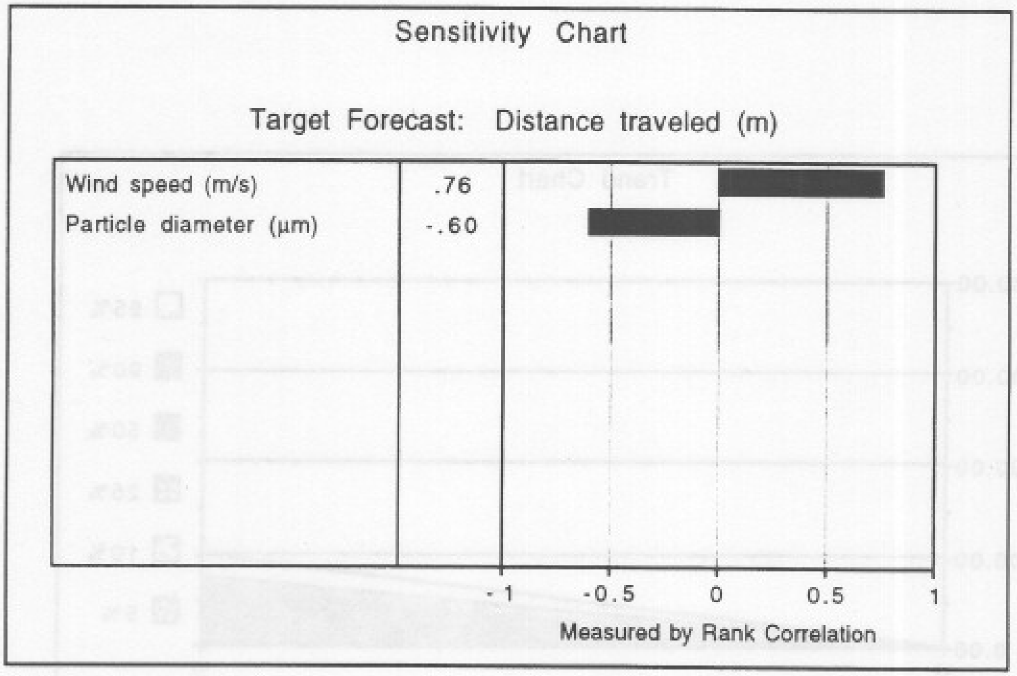

Figure 2 Estimated travel distance considering the uncertainty in wind speed and particle diameter.



**Crystal Ball Report**

Simulation started on Sat, Oct 1, 1994 at 11:39:49 AM
Simulation stopped on Sat, Oct 1, 1994 at 11:42:09 AM




Sensitivity Chart
Target Forecast: Distance traveled (m)
Wind speed (m/s)
.76
Particle diameter (µm)
-.60
-1
-0.5
0
0.5
1
Measured by Rank Correlation

**Forecast: Settling velocity (cm/s)** **Cell: C18**

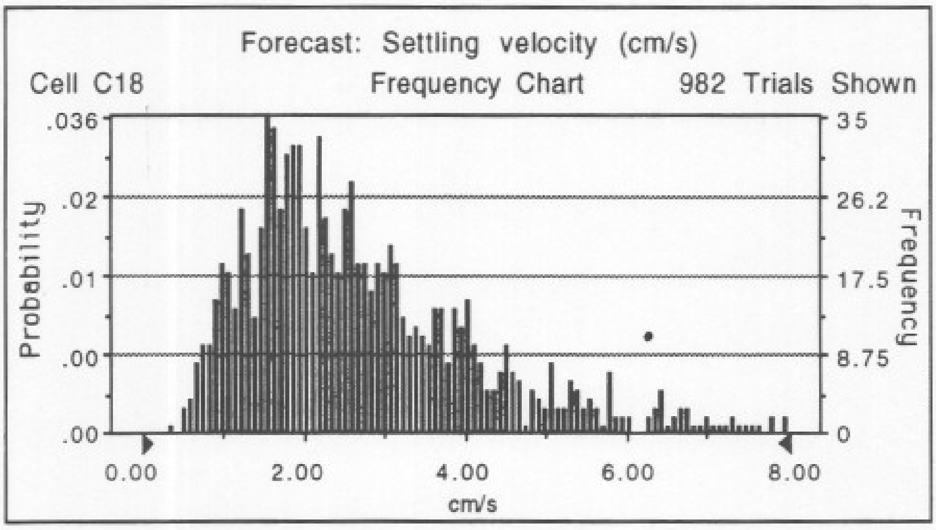
Summary:

Display Range is from 0.00 to 8.00 cm/s

Entire Range is from 0.33 to 15.93 cm/s

After 1,000 Trials, the Std. Error of the Mean is 0.06

| Statistics: | Value |
|---|---|
| Trials | 1000 |
| Mean | 2.86 |
| Median (approx.) | 2.44 |
| Mode (approx.) | 1.81 |
| Standard Deviation | 1.77 |
| Variance | 3.13 |
| Skewness | 2.07 |
| Kurtosis | 10.42 |
| Coeff. of Variability | 0.62 |
| Range Minimum | 0.33 |
| Range Maximum | 15.93 |
| Range Width | 15.60 |
| Mean Std. Error | 0.06 |



**Forecast: Settling velocity (cm/s) (cont'd)** **Cell: C18**

Percentiles:

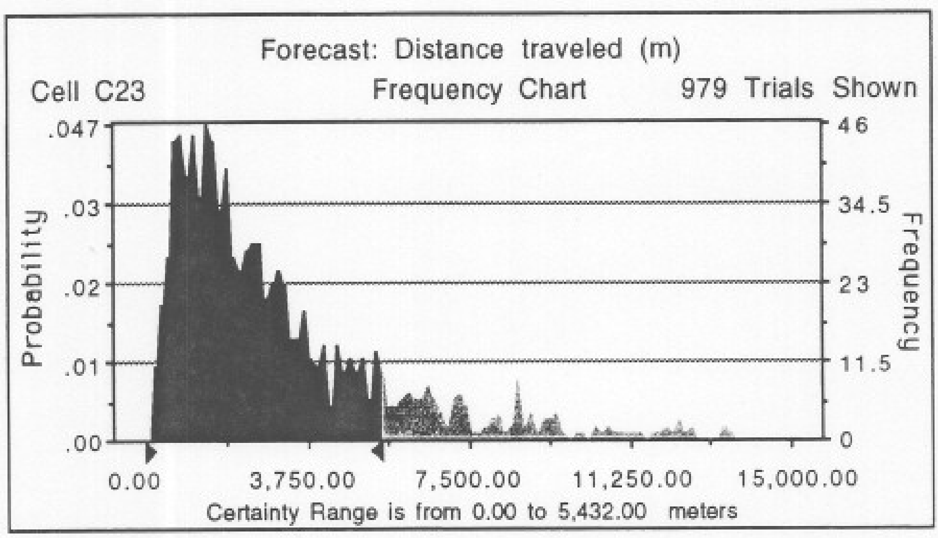
| Percentile | cm/s (approx.) |
|---|---|
| 0% | 0.33 |
| 10% | 1.18 |
| 20% | 1.55 |
| 30% | 1.82 |
| 40% | 2.10 |
| 50% | 2.44 |
| 60% | 2.81 |
| 70% | 3.26 |
| 80% | 3.93 |
| 90% | 5.09 |
| 100% | 15.93 |

End of Forecast

**Forecast: Distance traveled (m)** **Cell: C23**

Summary:
- Certainty Level is 83.30%
- Certainty Range is from 0.00 to 5,432.00 meters
- Display Range is from 0.00 to 15,000.00 meters
- Entire Range is from 176.34 to 49,844.00 meters
- After 1,000 Trials, the Std. Error of the Mean is 123.29

| Statistics: | Value |
|---|---|
| Trials | 1000 |
| Mean | 3,471.27 |
| Median (approx.) | 2,340.02 |
| Mode (approx.) | 1,418.03 |
| Standard Deviation | 3,898.71 |
| Variance | 15,199,974.14 |
| Skewness | 4.18 |
| Kurtosis | 32.63 |
| Coeff. of Variability | 1.12 |
| Range Minimum | 176.34 |
| Range Maximum | 49,844.00 |
| Range Width | 49,667.66 |
| Mean Std. Error | 123.29 |



**Forecast: Distance traveled (m) (cont'd)** **Cell: C23**

Percentiles:

| Percentile | meters (approx.) |
|---|---|
| 0% | 176.34 |
| 10% | 745.45 |
| 20% | 1,094.80 |
| 30% | 1,459.42 |
| 40% | 1,827.57 |
| 50% | 2,340.02 |
| 60% | 2,919.89 |
| 70% | 3,663.42 |
| 80% | 4,977.55 |
| 90% | 7,129.81 |
| 100% | 49,844.00 |

End of Forecast

## Assumptions

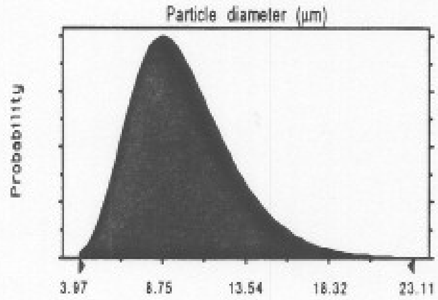
**Assumption: Particle diameter (μm)** **Cell: C11**

Lognormal distribution with parameters:

| | |
|---|---|
| Mean | 10.00 |
| Standard Dev. | 3.00 |

Selected range is from 1.00 to 100.00

Mean value in simulation was 9.87

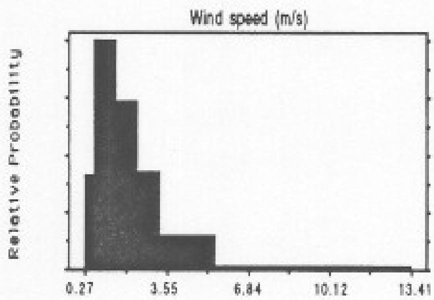



**Assumption: Wind speed (m/s)** **Cell: C21**

Custom distribution with parameters:

| | | | | Relative Prob. |
|---|---|---|---|---|
| Continuous range | 0.27 | to | 0.63 | 0.060400 |
| Continuous range | 0.63 | to | 1.52 | 0.362400 |
| Continuous range | 1.52 | to | 2.41 | 0.266500 |
| Continuous range | 2.41 | to | 3.31 | 0.155800 |
| Continuous range | 3.31 | to | 5.54 | 0.137600 |
| Continuous range | 5.54 | to | 8.22 | 0.012100 |
| Continuous range | 8.22 | to | 10.91 | 0.000700 |
| Continuous range | 10.91 | to | 13.41 | 0.004500 |
| Total Relative Probability | | | | 1.000000 |

Mean value in simulation was 2.20




End of Assumptions