Transport of Pollutants in the Atmosphere

The atmosphere is the environmental medium where we live and breath. Modeling of atmospheric pollution can be used to determine human exposure to existing pollution sources and to predict future exposures from industrial accidents. There are many sources of atmospheric pollution, including volcanoes, industrial smoke stacks, fugitive (or nonpoint) industrial emissions, gasoline stations, forest fires, industrial accidents, and automotive and railroad accidents. In Fate©, we will develop relatively simple models to predict the fate and transport of pollution released such sources.

First, we will compare other fate and transport models to the general atmospheric model. The aquatic models in Fate© were given only for one or two dimensions. Streams and lakes can be adequately modeled using one-dimensional models since most of the dispersion is in the longitudinal direction, while groundwater systems require at least two dimensions (x and y). Two dimensions are required in the latter system because the groundwater is not constrained by a river or lake bank, and dispersion can occur in all directions. Vertical dispersion, while important near a point pollution source, becomes less important when the groundwater system is bounded by confining layers above and below the aquifer of interest, which is why we used the simpler two-dimensional model in the instantaneous and pulse groundwater releases.

While the aquatic models may have seemed complicated, they are simpler than most atmospheric models. Because of wind currents and mixing, atmospheric models have to incorporate three dimensions, which automatically makes the governing equations more complex. As usual, we make many assumptions that make our model more manageable. For example, the models given in Fate® are not designed for gases that are more or less dense than the atmosphere, and therefore ignore buoyancy effects. The models distinguish between step and instantaneous sources, although actual atmospheric pollution episodes can lie between these two extremes. Unlike the aquatic models that allow first-order decay processes, our atmospheric models do not allow degradation of pollutants. This assumption is justified for models of a pollutant over relatively short distances (under10 000 meters or 7 miles) because most photochemical reactions (except for the production of smog) require the pollutant to be in the atmosphere over a much longer time frame (hours to days). The dominant force resulting in the reduction of the pollutant concentration is dispersion, which can rapidly dilute pollutant concentrations. However, understanding and accounting for dispersion can be very complicated. First, we will look at the movement of atmospheric gases over the Earth's surface.

A profile of the wind's velocity with increasing height has a steep increasing parabolic shape, with low velocity at the Earth's surface due to friction between the moving air and the ground. The surface wind velocity, is also subject to many complex variable, however. For example, the roughness of the Earth's surface can significantly impact the shape or steepness of the wind velocity-height profile. The wind velocity profile over an open grassland is illustrated in right-hand side of Figure 1, showing that wind speed rapidly approaches its maximum as height above the surface increases.

Compare this to an urban setting where tall buildings impede the path of the wind and slow its speed. This expands the velocity-height gradient well above the Earth's surface. The resulting lower wind velocity could decrease the turbulence and subsequent dispersion by slowing the wind velocity but may also result in stagnant pockets of the atmosphere that can contain clear or polluted air. Thus, the increase in the surface's roughness from the presence of building will greatly affect flow patterns and ground-level pollutant concentrations. Variables such as this demonstrate that, atmospheric processes are too complicated even for our most sophisticated models. In our brief introduction to we will simplify our model by assuming that an average wind speed can be used and, in general, we will not account for differences in surface roughness.

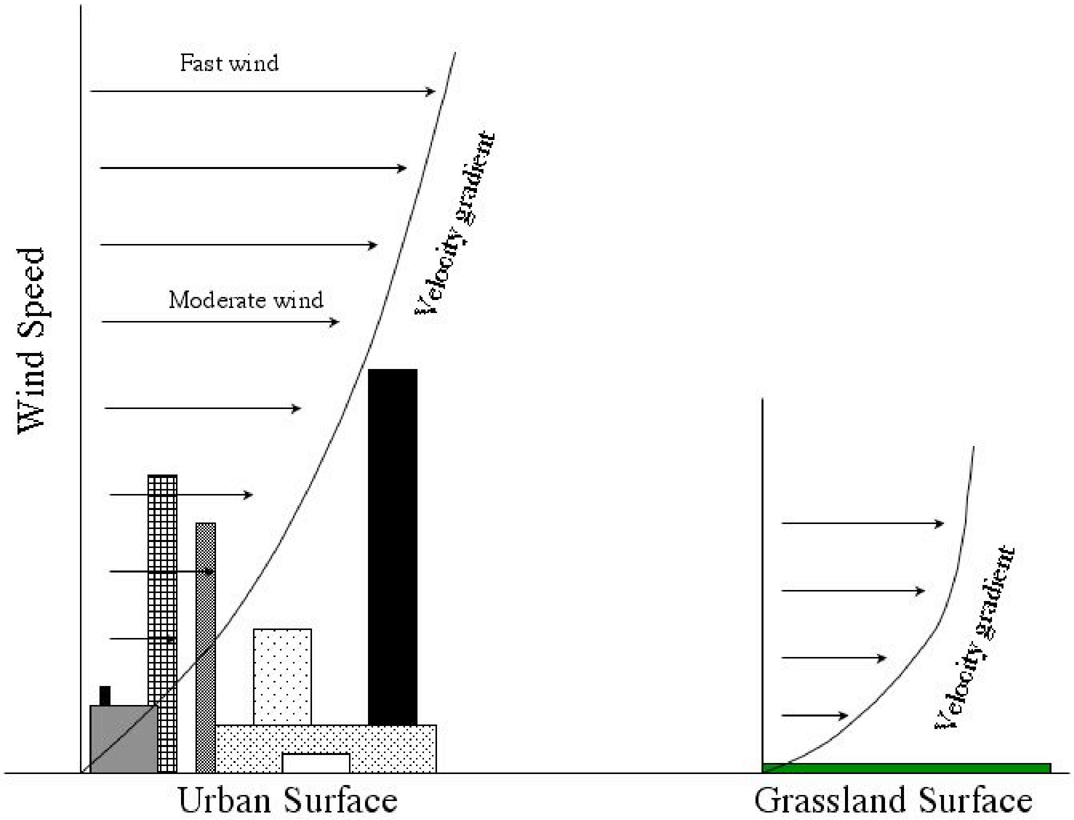


Figure 1. The effect of surface roughness on wind speed.

While surface roughness can greatly affect turbulence and mixing, the magnitude of wind speed can also increase mixing. We will refer to this mixing as dispersion, since the net result is a dilution of pollutant concentrations. If we combine the effects of wind velocity and the atmospheric temperature as a function of height above the surface, we obtain the three basic turbulence scenarios shown in Figure 2. We will start with an isolated pocket of atmosphere at nighttime temperatures (shown in Figure 2a). This type of condition occurs where a thick cloud layer prevents the Earth from radiating its heat to space as it cools during the night. Under theses conditions, an emission from an industrial stack will take the shape of the plume shown in Figure 2a. The released gases will rise or sink until their density (temperature) matches that of the surrounding (diluting) atmospheric gases. Then the plume will take the shape of a thin layer.

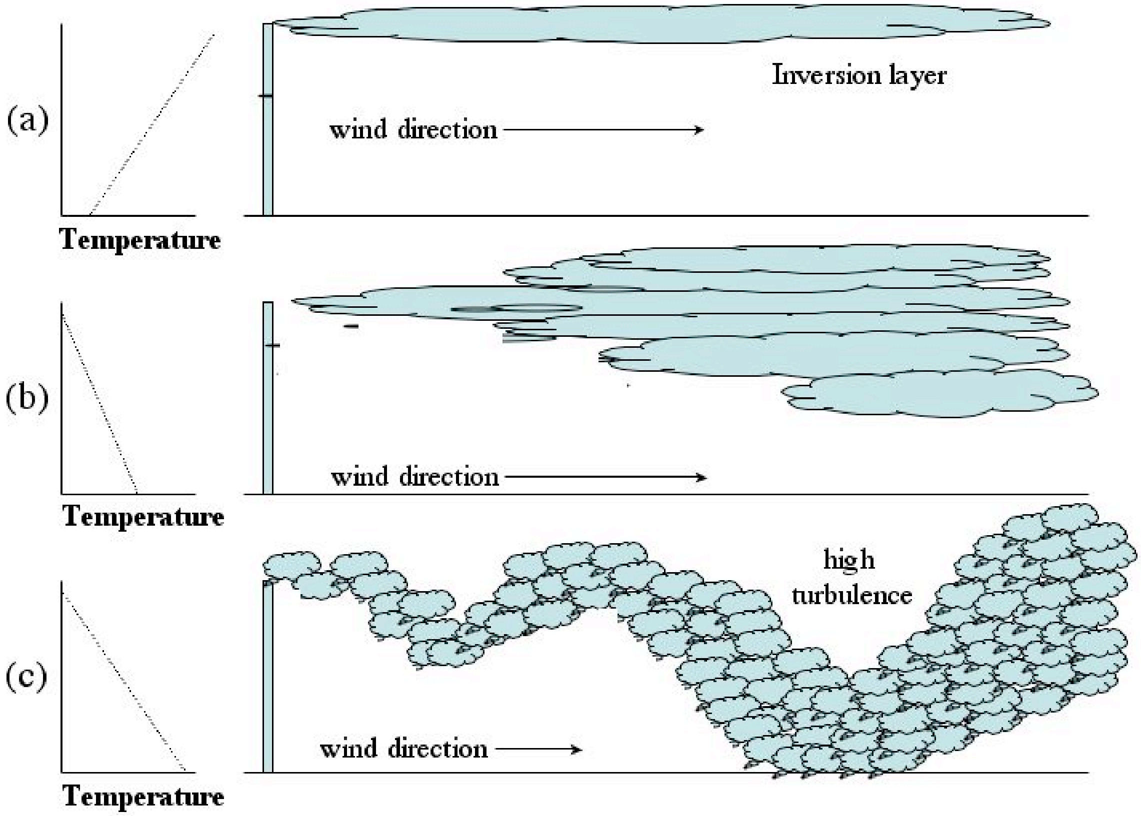


Figure 2. Three basic turbulence scenarios for plumes.

Under daytime heating conditions, the temperature-height profile will be similar to the one shown in Figure 2b. In a steady wind, the plume will spread in all directions, but mostly in the longitudinal direction. With a lower temperature-height gradient and a higher wind velocity, extreme turbulence will be observed (Figure 2c). In order to attempt the modeling of these conditions, we must greatly simplify the temperature and wind relationships.

We will start our simplification process by attempting to combine the effects of wind velocity, temperature-height profiles, and cloud cover into a set of atmospheric stability categories. As we do this, remember that our goal is to come up with a way to characterize dispersion (mixing) of the pollutant with the atmospheric gases. Table 1 shows a qualitative approach to the combined effects of wind speed and cloud cover collected for rural settings in England. Cloud cover is a good reflection of heat back to the Earth. The categories range from strongly unstable (category A reflected in Figure 2c) to very stable (category G) and distinguish between day and night conditions.

Table 1. Pasquill Stability Categories

Day, Degree of Cloud Insolation				Night	
Wind speed (at 10 m elevation m/s)	Strong	Moderate	Slight	Thinly overcast or greater than 50% low clouds	Less than 50% cloud cover
< 2	A	A-B	B	G	G
2 – 3	A-B	B	C	E	F
3 – 5	B	B-C	D	D	E
5 – 6	C	C-D	D	D	D
>6	C	D	D	D	D

Source: Turner (1994) and Pasquill (1961)

Turner (1994) adds the following notes on selecting the appropriate category:

1. Strong insolation corresponds to sunny midday in midsummer in England; slight isolation to similar conditions in midwinter.
2. Night refers to the period from 1 hour before sunset to 1 hour after sunrise.
3. The neutral category D should also be used, regardless of wind speed, for overcast conditions during day or night and for any sky condition during the hour preceding or following night as defined in note number 2.

Next, the somewhat qualitative categories in Table1 are used to mathematically predict values for horizontal dispersion coefficients (Table 2), which are estimates of mixing in the x and y directions. We do not have a way to accurately mathematically predict these values, and the data in Tables 1 and 2 are empirical (based on experimental observations). We usually assume that dispersion in the x and y directions is the same; thus Table 2 can be used to estimate $\square_x$ and $\square_y$ simultaneously. The equations given in Table 1 were used to draw the lines in Figure 3. Note that dispersion increases as you move away from the point source of pollution. This should be intuitive since mixing continues and the wind causes more mixing as you move away from the point source and the wind will also cause more mixing as you move away from the source. So, for every pollutant concentration you attempt to estimate, you must select a distance from the point source. The unfortunate result of this is that Fate© can only plot a slice of the concentration in the y and z planes. You will have to manually plot the concentration gradient in the x, or longitudinal, direction.

Table 2. Pasquill-Gifford Horizontal Dispersion Parameters (Turner, 1994)

$$\square_y = 1000 * \tan(T)/2.15$$

where x is the downwind distance (in km) from the point source and T is one-half Pasquill's □ in degrees. T, as a function of x, is determined by each stability category from Table1.

Stability	Equation for T
A	T = 24.167 – 2.5334 ln(x)

B	T = 18.333 – 1.8096 ln(x)
C	T = 12.5 – 1.0857 ln(x)
D	T = 8.333 – 0.7238 ln(x)
E	T = 6.25 – 0.5429 ln(x)
F	T = 4.167 – 0.3619 ln(x)

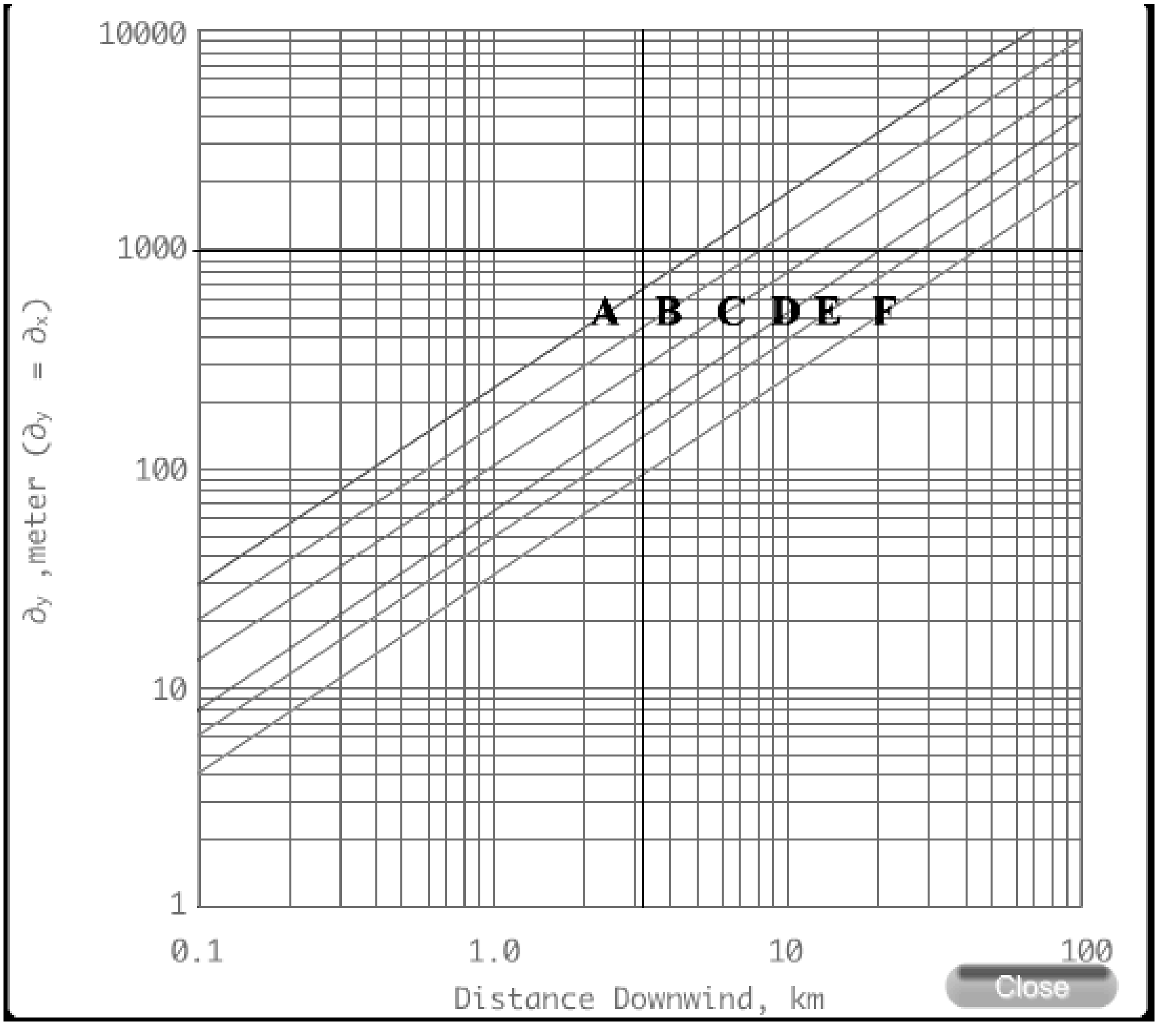


Figure 3. Pasquill-Gifford Horizontal Dispersion Parameters (Turner (1970) and Pasquill (1961))

Dispersion in the vertical (z) direction is somewhat more complicated to predict and again is based on experimental observations. We can estimate the vertical dispersion coefficient, σ_z, by using the same atmospheric stability categories from Table 1 but with a more precise treatment of the wind speed. The equation governing the estimate of vertical dispersion is

$$\sigma_z = a\,x^b,$$

where x is the distance in km

a and b are fitting parameters obtained from Table 3.

A plot of the dependence of vertical dispersion coefficients on distance from the point source is shown in Figure 4. We have been describing dispersion, but what exactly is it? As we have noted, dispersion is a function of the distance from the point source. Dispersion is a mathematical description of mixing between the pollutant plume and the natural atmospheric gases. The values you read from the graph or calculate using the equations are given in meters or kilometers. Thus, the values given represent the width of the pollutant plume at the specified distance from the point source and thus reflect the amount of atmosphere the pollution has mixed with.

Table 3. Pasquill-Gifford Vertical Dispersion Parameter

Vertical Dispersion Parameter: $\sigma_z = a\,x^b$, where x is in km				
Stability	Distance (km)	a	b	σ_z at upper boundary
A	> 3.11			5000
	0.5 – 3.11	453.85	2.1166	
	0.4 – 0.5	346.75	1.7283	104.7
	0.3 – 0.4	258.89	1.4094	71.2
	0.25 – 0.3	217.41	1.2644	47.4
	0.2 - 0.25	179.52	1.1262	37.7
	0.15 – 0.2	170.22	1.0932	29.3
	0.1 – 0.15	158.08	1.0542	21.4
	< 0.1	122.8	0.9447	14.0
B	> 0.35			5000
	0.4 - 35	109.30	1.0971	
	0.2 – 0.4	98.483	0.9833	40.0
	> 0.2	90.673	0.93198	20.2
C	all values of x		61.141	0.91465
D	> 30.	44.053	0.51179	
	10. – 30.	36.650	0.56589	251.2
	3 – 10.	33.504	0.60486	134.9
	1 - 3	32.093	0.64403	65.1
	0.3 - 1	32.093	0.81066	32.1
	< 0.3	34.459	0.86974	12.1
E	> 40.	47.618	0.29592	
	20. – 40.	35.420	0.37615	141.9
	10. – 20.	26.970	0.46713	109.3
	4 – 10.	24.703	0.50527	79.1

	2 - 4	22.534	0.57154	49.8
	1 - 2	21.628	0.63077	33.5
	0.3 - 1	21.628	0.75660	21.6
	0.1 – 0.3	23.331	0.81956	8.7
	< 0.1	24.260	0.83660	3.5
F	> 60	34.219	0.21716	
	30. – 60.	27.074	0.27436	83.3
	15 – 30.	22.651	0.32681	68.8
	7 - 15	17.836	0.4150	54.9
	3 - 7	16.187	0.4649	40.0
	2 - 3	14.823	0.54503	27.0
	1 - 2	13.953	0.63227	21.6
	0.7 - 1	13.953	0.68465	14.0
	0.2 – 0.7	14.457	0.78407	10.9
	< 0.2	15.209	0.81558	4.1

Source: Turner (1970) and Pasquill (1961)

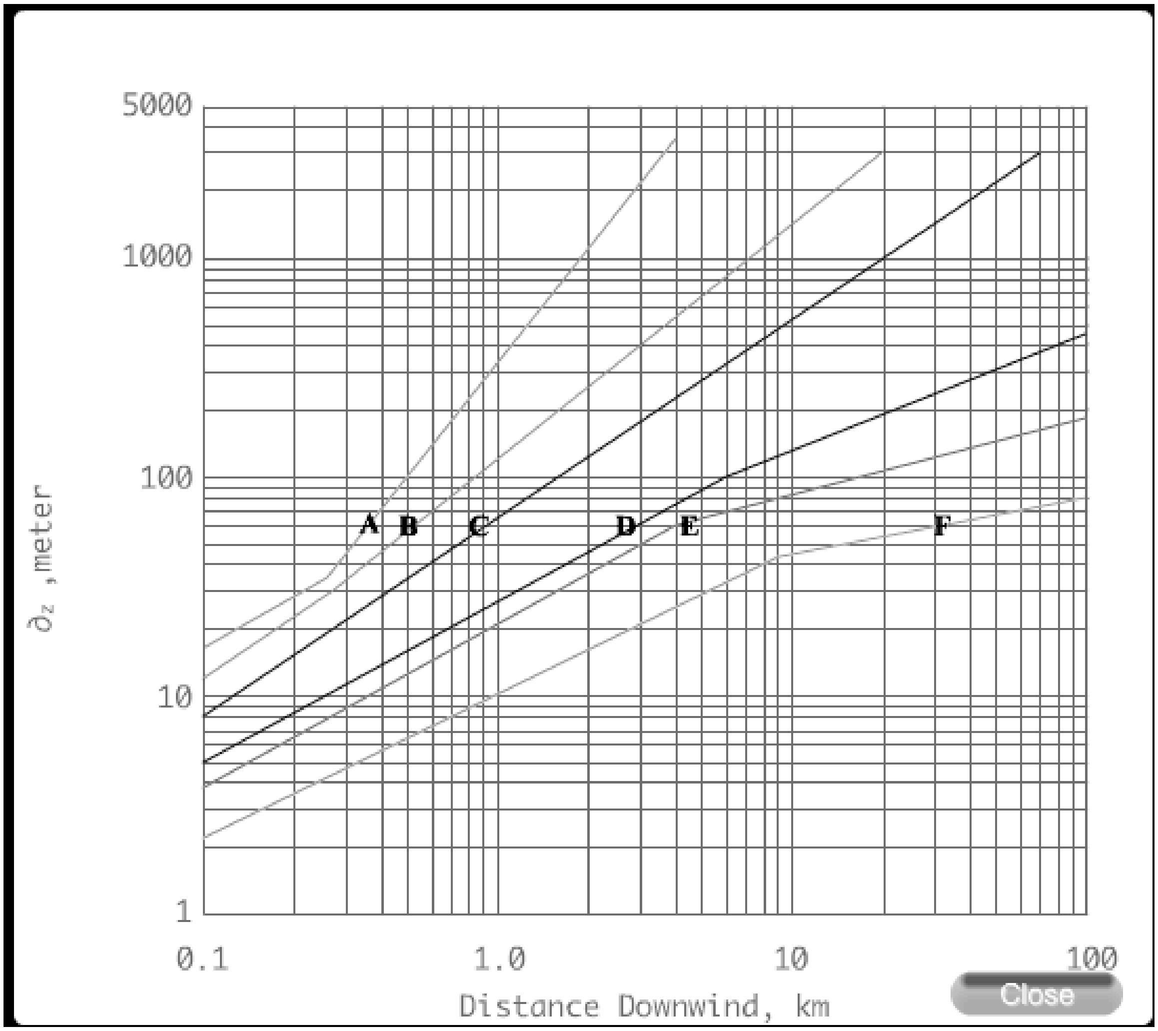


Figure 4. Pasquill-Gifford Vertical Dispersion Parameters (Turner, 1970)

Step Input (Plume Model) of Pollutant

Using the many assumptions stated earlier and the estimated horizontal and vertical dispersion coefficients, the plume model (Equation 1) can be derived, using differential equation techniques to estimate the pollutant concentration at any point (x, y, and z) downwind from the continuous source. This is referred to as the plume model.

$$C(x,y,z) = \frac{Q_m}{2\pi\sigma_y\sigma_z u}\left[\exp\left(-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right)\right]\left[\exp\left(-\frac{1}{2}\left(\frac{z - H_r}{\sigma_z}\right)^2\right) + \exp\left(-\frac{1}{2}\left(\frac{z + H_r}{\sigma_z}\right)^2\right)\right] \qquad \text{Eqn 1}$$

where $C(x,y,z)$ is the concentration of pollutant in the plume as a function of x, y, and z (mass/length^3),

x, y, and z are distances from the source (length) (see Figures 3 and 4),

Q_m is the pollutant source (mass/time)

$\sigma_x = \sigma_y$ is the horizontal dispersion coefficient (length),

σ_z is the vertical dispersion coefficient (length),

u is the wind velocity (length/time), and

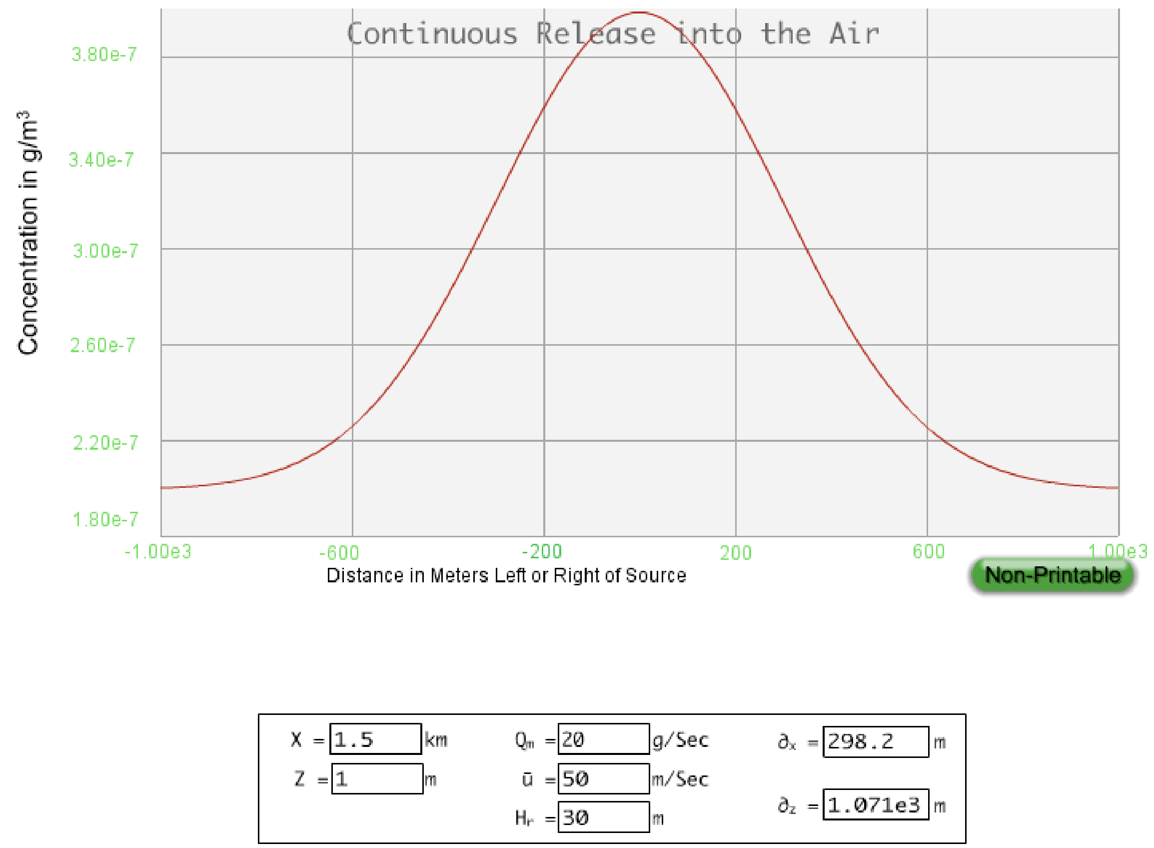
H_r is the height of the release (length).

Notice the terms we need to use this mode: the mass of pollutant released, the wind speed, the x, y, and z coordinates that yield estimates of dispersion (mixing), and the height of the release above the Earth's surface. All of these are relatively simple to estimate using the techniques described earlier.

For the concentration along the centerline of the plume ($z = 0$, and $H_r = 0$), we can use a simplification of Equation 1:

$$C(x,y,0) = \frac{Q_m}{\pi\sigma_y\sigma_z u}\left[\exp\left(-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right)\right] \qquad \text{Eqn 2}$$

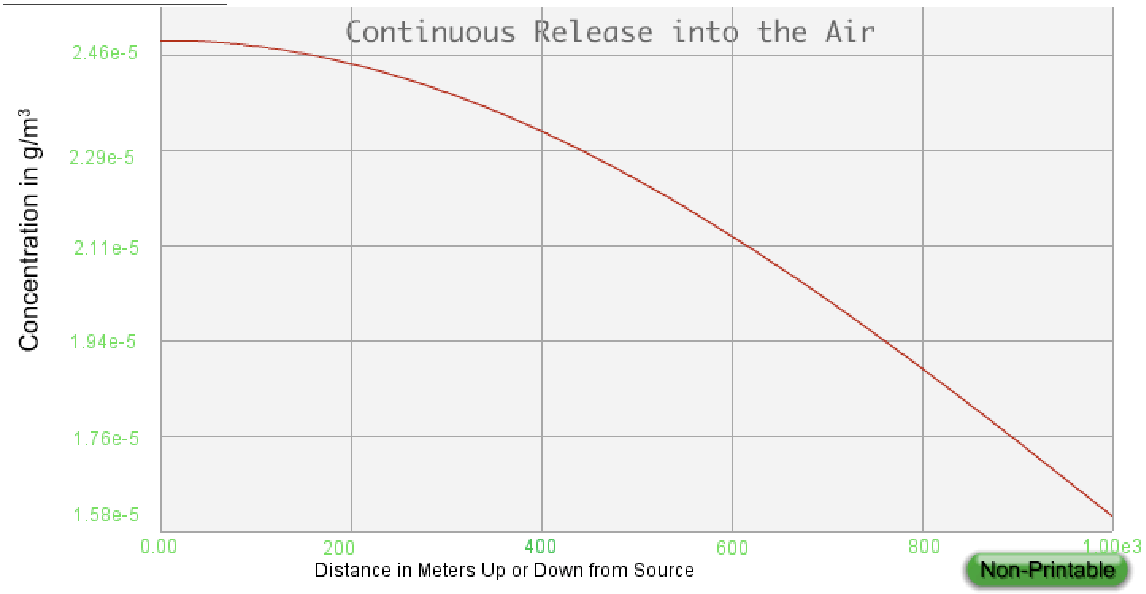
A typical simulation of downwind pollutant concentration is shown in Figure 5 for a 1.0 meter z value (height above ground level), a y distance of 0.0 km (along the x-z axis), and an x value (distance downwind) of 1.5 km. In Figure 5, the height of the Gaussian-shaped plot is along the center x axis (a y value of zero), and 1 meter above ground or about nose level for a tall human. The pollutant concentration declines as you go to the left or right of the centerline (an increase or decrease of y values). Note that the width of the main plume concentration covers a range of approximately 1200 meters (from –600m to the left to +600m to the right).

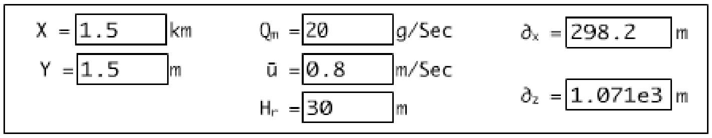


X = 1.5 km
Z = 1 m
Q_m = 20 g/Sec
$\bar{u}$ = 50 m/Sec
H_r = 30 m
∂_x = 298.2 m
∂_z = 1.071e3 m

Figure 5. Output from Fate© for a continuous release (plume) of pollutant into the atmosphere as you look along the x-axis.

A similar output would be obtained by plotting a y value of 0.0 (along the center line), an x distance of 1.5km, and calculating the pollutant concentration as you move up in the atmosphere. This is illustrated in Figure 6. In this plot, as you go from left to right on the x axis you are moving up in the atmosphere.





X = 1.5 km

Y = 1.5 m

Q_m = 20 g/Sec

$\bar{u}$ = 0.8 m/Sec

H_r = 30 m

∂_x = 298.2 m

∂_z = 1.071e3 m

Figure 6. Output from Fate© for a continuous release (plume) of pollutant into the atmosphere showing variations in plume concentration with changing vertical position in relation to the source.

Another useful function of Fate© is to evaluate the pollutant concentration as a function of distance from the point source. Fate can not plot this directly since dispersion in the x , y, and z directions are a function distance from the point source. In order to accomplish this we must repeatedly use Steps 5 and 6 in the plume model. Systematically change the x distance, increasing it incrementally, and record the pollutant concentration given in Step 6. A plot like the one shown in Figure 7 can be obtained. Note that the pollutant concentration decreases, as expected, as you move away from the point source.

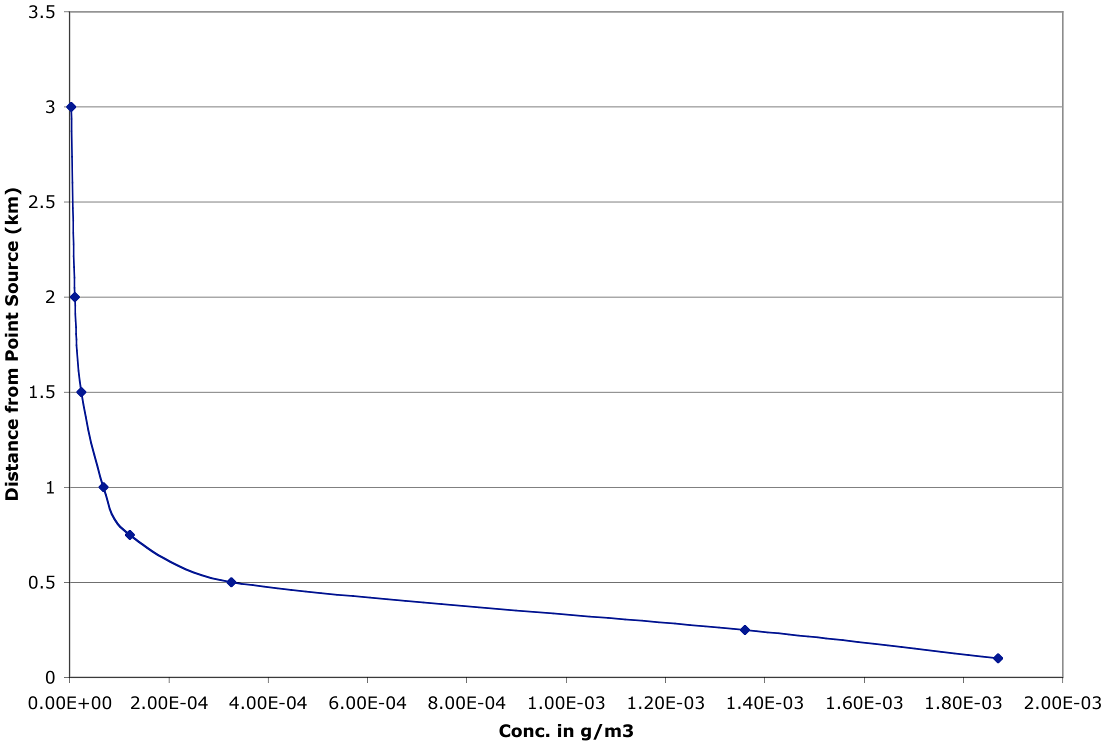


Figure 7. An evaluation of the pollutant concentration as you move away from the point source (plume model).

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