

1 Physical Properties of the Atmosphere and Meteorology

1.1 Stability Classification

Pasquill atmospheric stability classes: Atmospheric stability provides information on the degree of atmospheric turbulence. Pasquill depending on the temperature profile (i.e., dT/dZ) categorized the atmospheric turbulence into six **stability classes** and named as A, B, C, D, E and F (Table 1.1)

Table 1.1: Pasquill Stability classes

Pasquill Stability class	Atmospheric Stability	Temperature Gradient $\frac{dT}{dz}$ ($^{\circ}\text{C}/100\text{m}$)
A	Extremely Unstable	< -1.9
B	Moderately Unstable	-1.9 to -1.7
C	Slightly unstable	-1.7 to -1.5
D	Neutral	-1.5 to -0.5
E	Slightly Stable	-0.5 to 1.5
F	Stable	> 1.5

The hourly occurrence of various stability classes at a location should be determined for all the representative periods for which modelling is done. Three methods for determining atmospheric stability are generally recommended. These include insolation-based classification, vertical temperature profile measurements, and wind direction fluctuations.

1.1.1 Insolation-based classification

In principle, daytime stability can be determined from Table 1.2. If insolation (in coming solar radiation) data are not available in Table 1.2, these can be estimated using the method described at Sub-section 1.1.1.1 "Estimation of Insolation".

Table 1.2: Stability Classification

Surface Wind speed (at 10m), m/s	Day Time Insolation			Night Time Conditions	
	Strong	Moderate	Slight	Thin overcast or $\geq 4/8$ low cloud cover	$\leq 3/8$ cloud cover
< 2	A	A-B	B	-	-
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
> 6	C	D	D	D	D

To use Table 1.2, proper estimation of daytime insolation is essential. The following steps outline the procedure for using Table 1.2.

Step-1: For insolation categorization, refer to Table 1.3.

Step-2: For estimating insolation based on solar angle and cloudiness, refer to Table 1.4.

Step-3: Solar elevation angle may be obtained for a given date, time and latitude from astronomical

Step-4: Estimating of the solar insolation can calculated directly, and thereby Steps 2 & 3 can be avoided.

Step-5: Neutral class D should be assumed for overcast conditions during day or night. Night refers to a period from half hour before sunset to half hour after sunrise

Step-6: For A-B, use average of A and B. Proceed similarly, if estimated stability classes are B-C and C-D.

Example 1.1: State worst (most stable) atmospheric stability condition from Table 1.2, and discuss it with respect to air pollution impact.

Ans. Worst stability class always be F, and overcast nights and wind speeds are moderate at 2 – 5 m/s. , having pollution emission sources, because in such condition heavy inversion case pollution trap.

In practice, cloudiness data may not be available. At large airports, cloudiness is recorded every three hours, including night. However, at most meteorological stations, cloudiness is noted along with synoptic observations twice daily. Therefore, special efforts are to be made to record cloudiness if insolation data are not available. It can be seen from Table 1.2 that, during nighttime, cloudiness data are essential to distinguish between the two stability regimes E and F. Often, one has to interpolate between two observations separated by a few hours. Alternately, some other parameters must be found that can be continuously recorded. One such parameter is the temperature lapse rate. Another parameter is the wind direction fluctuations, which indicate the intensity of horizontal or lateral turbulence. Therefore, in principle Table 1.1 to Table 1.4 can be used for determining stability for horizontal or lateral dispersion.

Table 1.3: Insolation Category

Insolation Category	Insolation (Langley/hours)
Strong	$R > 50$
Moderate	$25 < R < 50$
Weak	$12.5 < R < 25$
Night	$R < 12.5$

R is the insolation (note: 1 langley = 1 caloric per square centimeter)

Table 1.4: Solar Angle and Cloud cover-based Insolation Category

Cloud Cover	Solar Elevation Angle > 60°	Solar Elevation Angle ≤ 60° but > 35°	Solar Elevation Angle ≤ 35° but > 15°
4/8 or less or any amount of high thin clouds (> 4800 m base)	Strong	Moderate	Slight
5/8 to 7/8, middle clouds (2100 to 4800 m base)	Moderate	Slight	Slight
5/8 to 7/8, middle clouds (< 2100 m base)	Slight	Slight	Slight

1.1.1.1 Estimation of solar angle and insolation

An approximate method for estimating insolation, the incoming solar radiation from the solar elevation, is discussed below. It consists of two steps (i) computation of solar elevation and (ii) computation of insolation. Before proceeding to elaborate on these two steps, it is necessary to understand the measurement principles of time.

Reckoning of Time

In each country, a reference meridian is used to define standard time. In India, the reference meridian is 82° 30' E. At any given location, the time the sun crosses the meridian is called the local noon. Obviously, the local noon is different from the noon based on the standard time. Local time is often needed in studies of local phenomena which depend on the sun's position. It may be obtained by adding to the standard time, a correction ΔT , given by

$$\Delta T = (M_{loc} - M_{std})/15, \text{ in hours} \quad \text{Equation 1.1}$$

Where, M_{loc} and M_{std} are the local and standard reference meridians, respectively.

Apparent Time

In the study of solar radiation, the sun's apparent position (i.e. position as it actually appears) is required. Using calendar time based on the mean solar time is equivalent to using the average rate of movement of the sun in the sky, thus giving an incorrect position. In this case, it is necessary to use the apparent solar time. The difference between the mean solar time and apparent solar time is called the Equation of Time (EQT). It changes from day to day and passes through an annual cycle. In India, EQT changes from a minimum of -14.4 minutes on February 11, to a maximum of +3.8 minutes on May 15. EQT is zero on April 15, June 14, September 1 and December 25. It can be approximately calculated (in minutes) for any date using the following relation

$$EQT = -7.7 \sin[(360/N). (n - 3)] + 9.5 \sin[2(360/N). (n - 80)] \quad \text{Equation 1.2}$$

Where, n is the number of days reckoned from January 1 as the first day and N is the number of days in a year (365 or 366).

Apparent Local Time

The apparent local time, t_a , in hours is obtained from the calendar time, t_c , using the combination of local time and EQT corrections as presented below

$$t_a = t_c + (M_{loc} - M_{std})/15 + EQT/60 \quad \text{Equation 1.3}$$

Computation of Solar Elevation

Solar elevation, (h), is calculated from the following equation

$$\sin(h) = \sin L \cdot \sin d + \cos L \cdot \cos d \cdot \cos t \quad \text{Equation 1.4}$$

Where, L is the location's latitude, and parameters t and d are explained below.

The parameter, t , the hour angle of the sun, is defined as the arc of the circle along the celestial equator measured from the upper meridian of the observer to that of the sun. The hour angle, t , may be expressed in terms of the angle measured east and westwards. It has a range of up to ± 180 degrees. Since the sun traverses 15 degrees in one hour, t may be obtained from the following relation

$$t = 15 \cdot (12 - ta), \text{ degree} \quad \text{Equation 1.5}$$

Where, ta is the apparent (i.e. actual, see Equation 1.3) local solar time in hours. The hour angle occurs in the cosine term; hence the algebraic sign of the hour angle does not matter.

The term, d (in Equation 1.4), is the solar declination of the sun's position concerning the celestial equator. Over the year, declination changes from 23.5° north to 23.5° south. Daily values of sun's declination are tabulated in the almanacs but can also be obtained with sufficient accuracy from the following relation

$$d = 23.45 \sin[(360/N) \cdot (n + 284)] \quad \text{Equation 1.6}$$

The sun's elevation can be computed using Equation 1.4 Equation 1.5 and Equation 1.6 for a given date & time and latitude & longitude of a place.

Sunrise and sunset times may be determined from the values of the apparent local time corresponding to $(h) = 0$. Solar elevations and sunrise and sunset times are used for determining the atmospheric stability class.

Computation of Incoming Solar Radiation

The insolation, R , may be estimated from the following approximate relation given by Briggs (1988)

$$R = (2/3) \cdot S \cdot (1 - 0.8C) \sin(h) \quad \text{Equation 1.7}$$

Where, S is the solar constant = 2 cal/sqcm/min and C is the cloudiness fraction. Note that even when the sky is completely cloudy, the radiation received by the ground is about 20% of the clear sky value. However, this depends upon the type of clouds. When the cloud cover is thick stratus clouds, the value of R is almost zero.

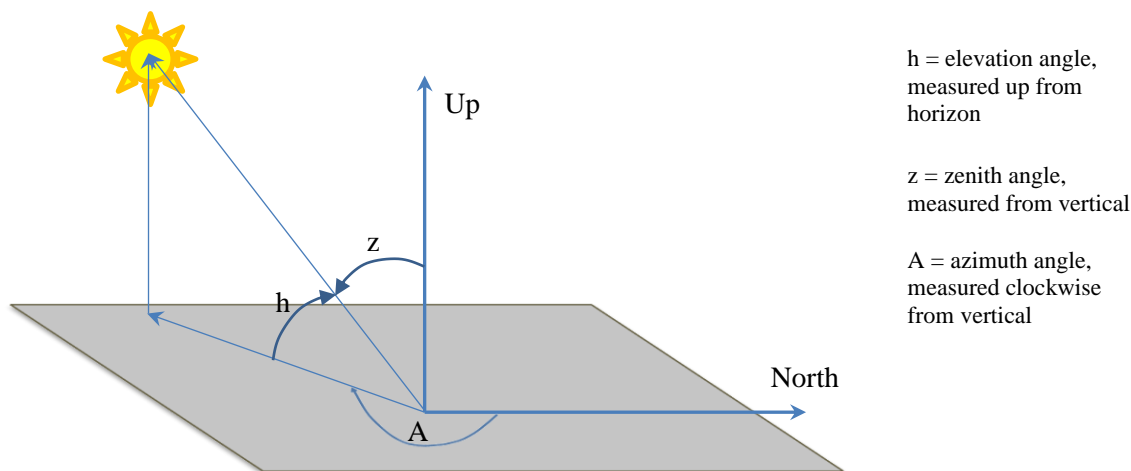
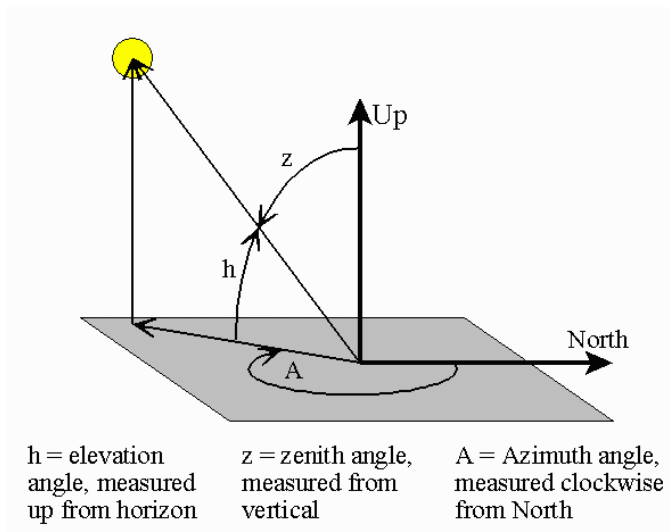


Figure 1.1: Different angles for solar radiation calculations

Q. Calculate average incoming solar radiation at your home on March 1.

1.1.2 Wind Direction Fluctuation Method

Since wind direction can be recorded continuously, σ_θ The standard deviation of wind direction fluctuations can be valuable for obtaining stability. If an online data acquisition system is used, computing of σ_θ may be quite easy. However, if it has to be obtained from the wind direction charts, exact computations shall be rather cumbersome and impractical. In such cases, one generally resorts to a crude approximation given by

$$\sigma_\theta = Wd_r/6 \quad \text{Equation 1.8}$$

Where, Wd_r is the overall range of the wind direction fluctuations or the width of the wind direction chart in degrees, over the averaging period. Relationship between σ_θ and stability class as suggested by (Slade, 1965) is given in Table 1.5

There are some differences in the stability class determined using σ_θ and that using other criteria, because σ_θ essentially measures lateral turbulence while the other criteria primarily relate to vertical turbulence.

Turbulence depends upon the roughness of the site in the upwind direction. The roughness can change seasonally because of the seasonal growth of grass and shrubs or permanently due to the construction of structures. In general, roughness at a site may

Table 1.5: Slades Stability Classification

Stability class	σ_θ (degree)
A	> 22.5
B	22.4 – 17.5
C	17.4 – 12.5
D	12.4 – 7.5
E	7.4 – 3.5
F	< 3.5

be different in different directions. Also, activities, like afforestation or construction of buildings and structures, change the site roughness. The calibration of σ_θ as an indicator of stability should, therefore, be done frequently.

Question: Consider in a certain area air is stagnant (i.e., no winds) and there is no emissions. However, the area has a background 24 hour average concentration of PM10 as $120 \mu\text{g}/\text{m}^3$. Assume that the entire quantity of the pollutant is mixed fully in the mixing height all the time. The concentration is proportional to the inverse of mixing height of the hour. The mixing height (Z) in the city with respect to time varies as per the following:

$$Z = \left(\frac{950}{12}t + 50\right) \text{ meter; for } t \in (0,12]$$

$$Z = \left(\frac{-950}{12}t + 1950\right) \text{ meter; for } t \in (12,24]$$

Question: Draw a windrose,

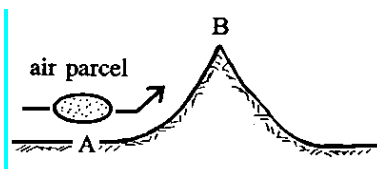
Direction	≤ 0.5	0.5 – 1.5	1.5 – 3.5	3.5 – 5	5 – 7.5	> 7.5
N						
NE						
E						
SE						
S						
SW						
W						
NW						

The joint frequency of wind speed range and direction are given for 72 hours. Draw the wind rose from in the above data. What is the % calm condition, and the most prevalent wind direction. What are the two directions in which a factory can locate its residential colony for workers.

Q2. Is dry adiabatic lapse rate function of temperature and pressure; justify your answer. Why does the atmosphere seldom behave adiabatically? Explain the diurnal variation of atmospheric stability on the surface of the earth. How will the stability change on the sea surface (ignore moisture, but remember specific heat capacity of water is much larger than earth's surface) as you may like to model the engine emission from a ship.

Q.3 On a cycle of 24 hours, at what time, you will expect maximum ground level concentration from an elevated source of effective stack height of H m. You can assume that mixing height on 24 hours ranges from 0.25 H and 2.5 H. Explain your answer with the help of figures so that one can see the concentration with time of day rising, then peaking and then decreasing.

As in the figure below, an unsaturated air parcel moves from A to B, how will its volume and its temperature change concurrently?



Q.8 Write step wise procedure with explanation of your understanding of estimating the atmospheric stability class using the method of solar insolation based data available at any airport. You need not write any equation or formulae but stepwise explanation of what are you doing and why are you doing is important.

- a) As seen the temperature and pressure rapidly decrease with altitude. If the atmosphere is behaving adiabatically, estimate the temperature at the tip of mount Everest at 8900 m (the height of the summit). Using the hydrostatic equation $dP = -\rho g dz$ derive an expression for atmospheric pressure at two different heights.
- b) In above question, find the pressure on the mount Everest considering the pressure at MSL is 100 kPa. The fall in atmospheric pressure at higher altitude decreases the partial pressure of inspired oxygen and hence the driving pressure for gas exchange in the lungs.

- c) Atmospheric pressure and inspired oxygen pressure fall roughly linearly with altitude. Find the inspired pressure of oxygen at MSL and at the mount Everest. Discuss why is it extremely difficult to scale mount Everest without oxygen.

2 Atmospheric Dispersion and Air Pollutant Concentration Models

Content:

Fick's Law

Dispersion, diffusion, turbulent

3D Advection derivation

Gaussian Model

The air pollution problem can be shown as a system having three essential components (Figure 2.1): (i) emission sources, (ii) atmospheric processes, and (iii) receptors.

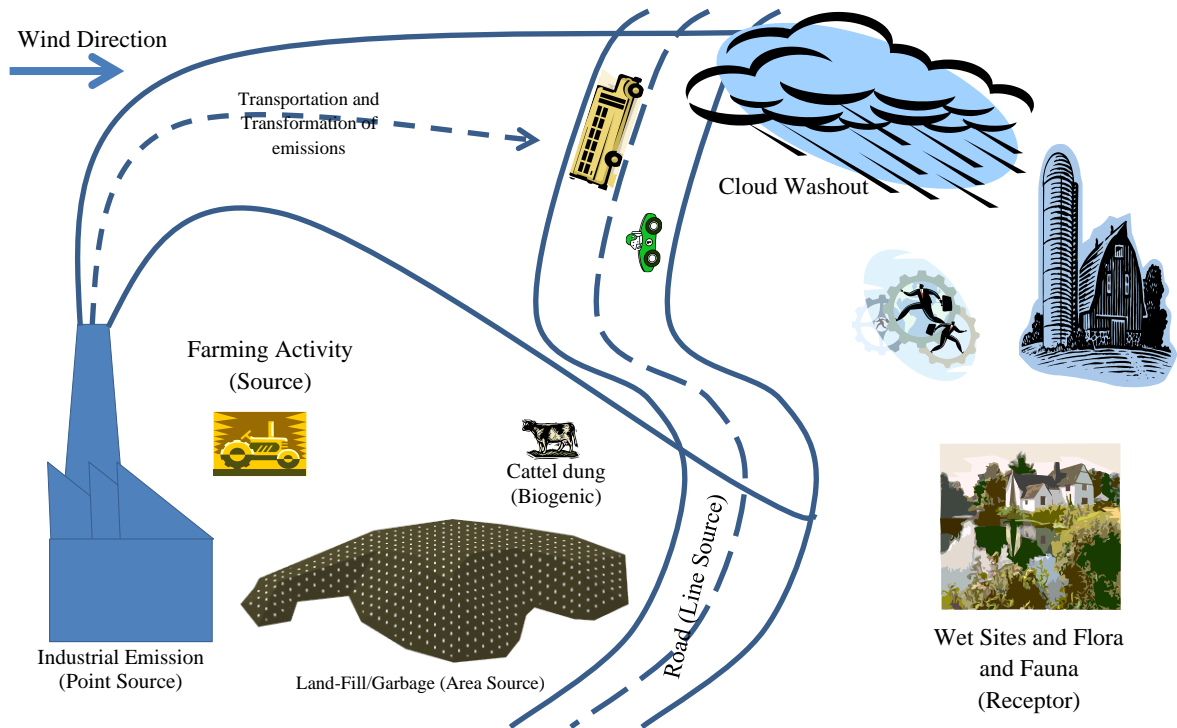


Figure 2.1: Three basic components of air pollution system

Emission sources: The air pollution problem begins with emission sources, anthropogenic or natural. Anthropogenic sources include industrial establishments, household cooking, automobiles, etc. Natural sources of air pollution include volcanic eruption, forest fires, desert storms, biogenic emissions, etc. The important aspect of these sources is their strengths in emission quantities, toxicity, release height, and proximity to the receptor.

Atmospheric processes: Atmospheric chemistry is driven mainly by solar energy reaching the earth's surface and air movements determine the transport, mixing, physical and chemical transformation of pollutants. The wind speed and direction determine the extent and direction of impact. The vertical temperature profile of the atmosphere decides the atmospheric vertical mixing.

Receptors: The third component, receptors, receives the harmful impacts of air pollution. The receptors can be human beings, wildlife, ecology, or buildings. The impact on receptors can be from short-term to life-threatening, whereas other impacts could be in terms of economic losses.

The ultimate aim of a study of this system is to answer the question: what are the optimum ways to prevent/minimize the impact of air pollution on the receptor? This answer can be accomplished by air quality modelling and management. In the simplest term, air quality modelling is a systematic approach that attempts to link the source emission strength (i.e., emission rate) through atmospheric processes to assess the extent of the impact on the receptors in terms of pollutant concentrations. Once such linkages are established between source emission rates and impact, the required reductions in emissions at sources can be planned in a cost-effective way to attain safe air quality levels at the receptors. We will discuss some fundamental laws that help establish the linkage between emission source and impact on the receptor.

2.1 Fick's Law:

Meteorology studies the atmosphere, its motion, and its phenomena like weather and climate. The word meteorology comes from the Greek word meteors, meaning “suspended in the air” (Seinfeld et al., 1998). One important phenomenon is diffusion. Diffusion is the movement of suspended particles, molecules, atoms, etc., in fluid, from high to low concentration; it is a macroscopic observation. One of well-accepted laws is Fick's Law (more precisely mass balance of solute within inhomogeneous solvent/fluid), which explains the diffusion in certain conditions.

Fick's diffusion is also termed as the classical diffusion controlled by thermodynamic forces (by the gradient of differences of concentrations and/or chemical/nuclear potential) with the constant (or even pseudo-constant) diffusion coefficients.

Figure 2.2 shows three views of diffusion phenomenon (a) as single solute molecule randomly moving, (b) microscopic movement of solute molecules from high to low concentration and (c) macroscopic aggregated movement of solute from high concentration to low concentration. Concentration changes as time go by; one can see a clear trend of solute molecules' movement until solute molecules' concentration becomes uniform or does not vary as a function of space. Fick's law explains such a smooth flow of solute molecules.

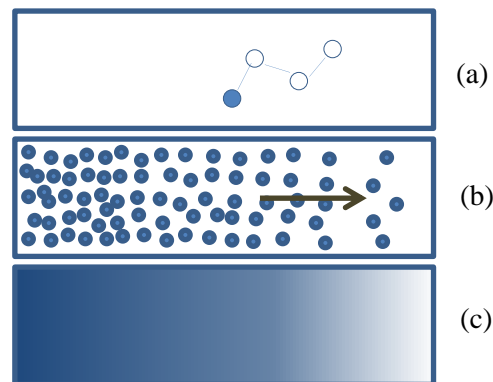


Figure 2.2: Diffusion of molecules in a fluid

Before solute molecules achieve homogeneous distribution within fluid/solvent, one must understand the inhomogeneous solute and solvent interaction system. Consider the one-dimensional concentration gradient of some molecules of a compound in a fluid (Figure 2.3).

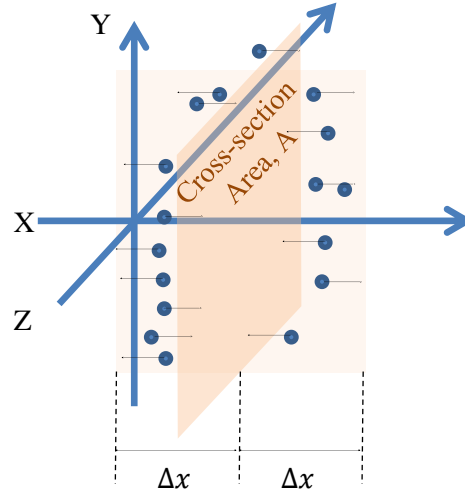


Figure 2.3: Molecule randomly moving along one-dimension crossing an area A

Consider inhomogeneous solute molecules near arbitrary plane having area A . There are $N(x)$ molecules on the left side of the plane having infinitesimal volume $A\Delta x$ and $N(x + \Delta x)$ molecules within a similar volume on the right side. Consider molecules randomly moving right or left in a 1-dimensional direction only. Due to inhomogeneous distribution and random movement of molecules, at given instance, a molecule has a probability p to move towards the right-side and $q = (1 - p)$ towards the left-side. Near plane (within a distance of Δx), one can consider the equal probability of movement of molecules through the plane, that is $p = q = 1/2$. For an infinitesimal/short time Δt it is assumed that molecule moves Δx distance in time Δt , the flux of molecules J can be written as Equation 2.1.

$$J = \frac{\frac{1}{2} [N(x) - N(x + \Delta x)]}{A\Delta t} \quad \text{Equation 2.1}$$

Here concentration can be written as $C(x) = \frac{N(x)}{A\Delta x}$ and substituting it in Equation 2.1

$$J = \frac{\frac{1}{2} A\Delta x [C(x) - C(x + \Delta x)]}{A\Delta t} = \frac{(\Delta x)^2 [C(x) - C(x + \Delta x)]}{2\Delta t \Delta x} \quad \text{Equation 2.2}$$

Equation 2.2 rewriting as below

$$J = - \left\{ \frac{(\Delta x)^2}{2\Delta t} \right\} \times \lim_{\Delta x \rightarrow 0} \frac{[C(x + \Delta x) - C(x)]}{\Delta x} \quad \text{Equation 2.3}$$

In Equation 2.3, limit $\Delta x \rightarrow 0$ can be written as gradient of concentration.

$$J = -D \frac{\partial C(x)}{\partial x} \quad \text{Equation 2.4}$$

in Equation 2.4, we can see flux J is proportional to gradient of concentration and $\left\{\frac{(\Delta x)^2}{2\Delta t}\right\}$. Here the term $\left\{\frac{(\Delta x)^2}{2\Delta t}\right\}$ written as diffusion coefficient D which is a constant for a given continuum under constant physical properties. The term, $\left\{\frac{(\Delta x)^2}{2\Delta t}\right\}$ is derived from random walk assumptions that variance of molecular movement is proportional to **the** total time of observation and D (Einstein, 1906, 1956; Smoluchowski, 1906). Equation 2.4 is often known as **Fick's First Law**.

In general, Fick's First Law of diffusion in three dimensions can be written as vector form (Equation 2.5).

$$J(x, y, z; t) = -D \left(\left[\frac{\partial C}{\partial x} \right], \left[\frac{\partial C}{\partial y} \right], \left[\frac{\partial C}{\partial z} \right] \right) = -D \nabla C(x, y, z; t) \quad \text{Equation 2.5}$$

In classical diffusion, it is considered that there is no change (or transformation) in solute molecules during diffusion process (Figure 2.4).

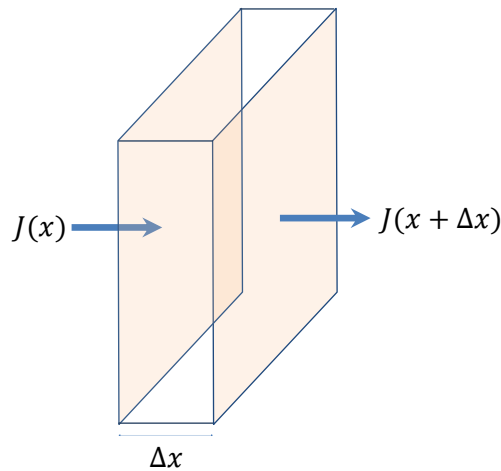


Figure 2.4: Derivation of Fick's second law

For a arbitrary infinitesimal box $A\Delta x$; $J(x)$ flux is entering from left-side wall of box and $J(x + \Delta x)$ flux leaving from right-side wall of box, then change in concentration inside of box for infinitesimal time Δt after time t can be written as

$$\frac{[C(t + \Delta t) - C(t)]}{\Delta t} = \frac{[J(x) - J(x + \Delta x)]}{\Delta x} \quad \text{Equation 2.6}$$

When limits are $\Delta x \rightarrow 0$ and $\Delta t \rightarrow 0$ then rearranging Equation 2.6

$$\lim_{\Delta t \rightarrow 0} \frac{[C(t + \Delta t) - C(t)]}{\Delta t} = \lim_{\Delta x \rightarrow 0} \frac{-[J(x + \Delta x) - J(x)]}{\Delta x} \quad \text{Equation 2.7}$$

Equation 2.7 becomes

$$\frac{\partial C(x)}{\partial t} = -\frac{\partial J(x)}{\partial x} \quad \text{Equation 2.8}$$

Now from Equation 2.4 and Equation 2.8

$$\frac{\partial C(x, t)}{\partial t} = D \frac{\partial^2 C(x, t)}{\partial x^2} \quad \text{Equation 2.9}$$

Equation 2.9 is known as **Fick's Second Law**, which states that the rate of change of concentration is proportional to second derivative of concentration profile at a given time and space.

Example 2.1: Find out relation between variance of molecular movement (displacement) and time in three dimensions.

Ans. The overall variance in 3d will be $(\sqrt{(\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2})^2$

If diffusion is even in all directions the variance will be $6D(\Delta t)$

2.2 Dispersion

Only advection does not dilute effluent if winds are steady in one direction. Typical thermal diffusion occurs at 10^{-9} m^2 spread in one second, so it will take 10^9 seconds (~ 31 years) to spread 1 m^2 cross-section of effluent plume under advection only (Nazaroff & Alvarez-Cohen, 2000). Life cannot exist if thermal diffusion is the only way to spread effluent in the atmosphere.

A common observation is that when a pollutant releases into the atmosphere, it dilutes due to uneven/non-uniform wind flow. The non-uniform wind flow could be due to thermal gradients, mechanical turbulence, uneven air density, etc. Due to non-uniform fluid flow, dispersal of pollutant concentration happens in advection, and all processes that add to diffusion are known as dispersion.

A significant dispersion happens when atmospheric air is highly turbulent or/and non-uniform, and vice-versa. Under effective dispersion, effluent dilution occurs because concentration spreads rapidly in space. Such phenomena are difficult to model mathematically because fluid velocities are hard to express as a function of time and space. Suppose there is no physical and chemical transformation of effluent/pollutant in turbulent and non-uniform air. In that case, one can use Fick's first law as analogous to define turbulence mixing. It can be stated that the flux of material being mixed across any surface (herein one dimension) is given by Equation 2.10.

$$J_x = -\varepsilon_x \frac{\partial C}{\partial x} \quad \text{Equation 2.10}$$

A few texts (Nevers, 1999) replace ε with K , and refer it as gradient transport K -theory. In Equation 2.10 J_x is dispersion flux and ε is dispersion coefficient. Here it should be remembered that dispersion flux depends on the fluid flow field. The above model is not precise enough to represent the atmospheric state in transport. Dispersion coefficient may be calculated from observations, empirical data, and theoretical basis (Pasquill, 1974; Turner, 1969).

ε represent the dispersion coefficient mainly depends on shear-flow dispersion and turbulent dispersion; these two dispersion phenomena are described below.

2.2.1 Shear-flow Dispersion

When fluid flows over a non-moving surface, the fluid velocity varies from a non-moving surface (low velocity) to away from the surface (high velocity). There is friction between moving fluid layers. Due to this friction, a shear force occurs between fluid layers and produces a velocity gradient. The concentration varies in the cross-sectional direction perpendicular to the mean flow. Due to the concentration gradient, pollutant transports from high to low concentration referred to as shear-flow dispersion.

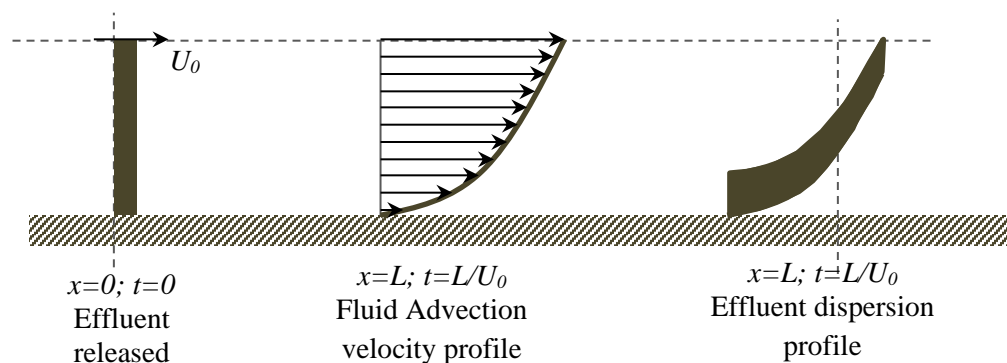


Figure 2.5: Model schematic of Shear-flow dispersion

As shown in Figure 2.5, a certain quantity of pollutant is released at time $t = 0$ and $x = 0$. In x direction, fluid speed at the top of effluent release is U_0 . After travelling $x = L$ distance due to shear forces on fluid, a concentration gradient profile occurs. Due to such variation in concentration, effluent spreads through air layers as shown in the schematic. Two things are happening first is concentration decrease from non-moving surface to open atmosphere, and second shear-flow dispersion happen due to change in concentration layer-wise. These phenomena can be represented as Equation 2.11.

$$J_{sd_x} = -\varepsilon_{sd_x} \frac{\partial C(x)}{\partial x} \quad \text{Equation 2.11}$$

Here, $C(x)$ cross-section averaged concentration at x and ε_{sd_x} is the shear-flow dispersion coefficient.

2.2.2 Turbulent Diffusion/Dispersion

When fluid flows in a laminar fashion, one can easily apply a continuity equation to predict concentration and velocity profile precisely, but in turbulent situations, it is not easy to calculate these profiles in time and space. In actual environmental fluid motions, either air or water, fluid-flows occur in a turbulent manner.

One can use statistics to estimate fluid properties in turbulent situations because it is a stochastic/chaotic phenomenon.

Analogous to first Fick's law, in turbulent motion also a concentration gradient exists. One can assume mean fluid properties (like velocity in a certain direction, plane concentration, spread of pollutant in certain meteorological conditions, etc.). Accordingly, Equation 2.12 represents turbulent dispersion flux J_{td} having turbulent dispersion coefficient or eddy diffusivity ε_{td} . Equation 2.13 represents 3D turbulent dispersion flux having eddy diffusivities in respected directions. One can define the Cartesian plane according to ease of calculations. In real atmospheric conditions, vertical turbulent diffusion/dispersion coefficient ε_{tdz} differs from xy plane and varies with height. Turbulent diffusion/dispersion coefficients are considered nearly the same ($\varepsilon_{tdx} = \varepsilon_{tdy}$), if meteorology is similar in xy plane.

$$J_{tdx} = -\varepsilon_{tdx} \frac{\partial C(x, y, z, t)}{\partial x} \quad \text{Equation 2.12}$$

$$\vec{J}_{td} = -\left(\varepsilon_{tdx} \frac{\partial C}{\partial x} \cdot \hat{i} + \varepsilon_{tdy} \frac{\partial C}{\partial y} \cdot \hat{j} + \varepsilon_{tdz} \frac{\partial C}{\partial z} \cdot \hat{k} \right) \quad \text{Equation 2.13}$$

One can take fuming incense stick example, as shown in Figure 2.6, which is fuming in almost still air, so buoyancy will be the only way to transport hot gases. Initially, gases are too hot to partition into particulate matter, so nothing is visible. After a certain distance, gases get partitioned, and the plume becomes visible as a narrow plume flow. The narrow plume rises steadily for a certain distance (around 10-30 cm) (Nazaroff & Alvarez-Cohen, 2000), and the laminar flow breaks to turbulent dispersion. Because we know that gaseous fumigation is almost constant, smoke concentration can be determined by taking time-averaged concentration. Turbulent air motion is the main reason for smoke dispersion and spread. This dispersion happens parallel to the earth's surface.

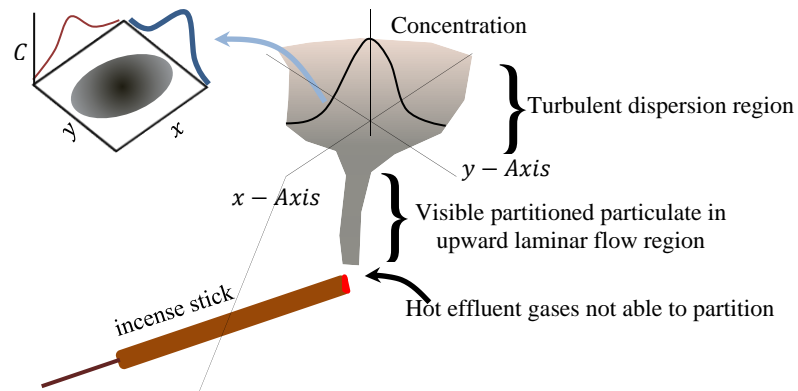


Figure 2.6: Schematic representation of time-averaged smoke plume rising from a fuming incense stick and turbulent dispersion

It is assumed that pollutant emission rate is almost constant and continuity mass balance equation is valid; that is, mean continuum velocity is independent of time and space. As shown in Figure 2.6, an average concentration profile is plotted for a certain period. It can be seen that in the direction of the plume, the highest concentration occurs in the centreline and gradually decrease horizontally (parallel to earth surface or perpendicular to earth gravity) evenly. This spread happens due to turbulent dispersion.

The mathematical analogy of turbulent dispersion challenges achieving precise turbulent dispersion coefficients or diffusivities. These coefficients depend on meteorological parameters (e.g., temperature, insolation, pressure, humidity, wind speed, etc.). A robust experimental database, theoretical basis, and logical reasoning are needed to calculate dispersion coefficients in real modelling/simulation scenarios.

2.3 Advection Diffusion/Dispersion

Advection is defined as the movement of solute (e.g., pollutant) mass entrained in the solvent fluid flow. Figure 2.7 show an arbitrary infinitesimal strip of solute (having concentration C) under fluid flow velocity $(U\hat{i} + V\hat{j} + W\hat{k})$. Under fluid (e.g. air) movement, the strip of pollutant also flows as a transport flux UC in x axis. Simultaneously along air flow pollutant disperse due to concentration gradient. A 4D mass balance can be written as Equation 2.14, here $r(x, y, z, t)$ represents transformation rate kinetics of pollutant. The term, which represents concentration change in time, $[\partial C(x, y, z, t)/\partial t]$ is known as accumulation term in a unit volume.

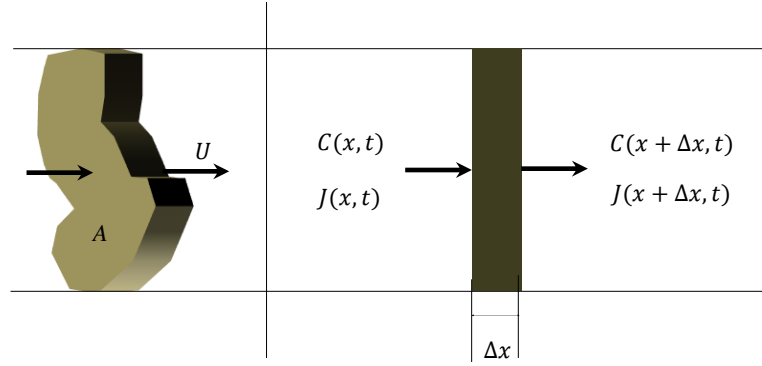


Figure 2.7: Arbitrary infinitesimal strip of Solute under fluid flow

$$\frac{\partial C(x, y, z, t)}{\partial t} = - \left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} \right) + r(x, y, z, t) \quad \text{Equation 2.14}$$

Eulerian advection–dispersion transport flux vector can be written as Equation 2.15.

$$\vec{j} = \left(\left[UC - \varepsilon_x \frac{\partial C}{\partial x} \right] \cdot \hat{i} + \left[VC - \varepsilon_y \frac{\partial C}{\partial y} \right] \cdot \hat{j} + \left[WC - \varepsilon_z \frac{\partial C}{\partial z} \right] \cdot \hat{k} \right) \quad \text{Equation 2.15}$$

Combining Equation 2.14 and Equation 2.15 gives the classic advection-diffusion model/equation for a given system of fluid (like air etc.) and solute (like pollutant etc.). In real atmospheric conditions for easy modelling/calculation point of view, we take assumption that advection can be taken as zero in perpendicular to downwind directions (that is y and z axis) as Equation 2.16.

$$\frac{\partial C(x, y, z, t)}{\partial t} = - \left(\frac{\partial}{\partial x} \left[UC - \varepsilon_x \frac{\partial C}{\partial x} \right] + \frac{\partial}{\partial y} \left[- \varepsilon_y \frac{\partial C}{\partial y} \right] + \frac{\partial}{\partial z} \left[- \varepsilon_z \frac{\partial C}{\partial z} \right] \right) + r(x, y, z, t) \quad \text{Equation 2.16}$$

2.3.1 Derivation of Gaussian Plume Equations

To obtain an atypical solution for the advection diffusion equation (Equation 2.16) for concentration in space for a continuous point source, we make the following assumptions:

- The process is steady-state, that is, $\partial C / \partial t = 0$.
- The transport through advection in y and z-direction is negligible
- The wind speed U is constant (in space) and independent of time.
- The transport of pollutants due to the wind in the x-direction is dominant over the dispersion (i.e., $U (dC/dx) \gg \varepsilon_x \partial(\partial C/\partial x)/\partial x$. and thus, $\varepsilon_x \partial(\partial C/\partial x)/\partial x$ is relatively negligible

$$U \frac{\partial C}{\partial x} = \frac{\partial}{\partial y} \left(\varepsilon_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(\varepsilon_z \frac{\partial C}{\partial z} \right) \quad \text{Equation 2.17}$$

The solution of Equation 2.17 requires one boundary condition in the x direction, two boundary conditions in y direction and two boundary conditions in z direction.

If we assume that ε_y and ε_z are constants at a point, then the general solution of partial differential Equation 2.17 is as

$$C = Kx^{-1} \exp \left[- \left\{ \left(\frac{y^2}{\varepsilon_y} \right) + \left(\frac{z^2}{\varepsilon_z} \right) \right\} \frac{U}{4x} \right] \quad \text{Equation 2.18}$$

Here K is an arbitrary constant, which can be determined based on specific atmospheric boundary conditions.

2.3.2 Point Source at ground level

An emitting source is called a *point source* if it can be approximated as a point in a mathematical sense. Figure 2.8 shows fluid/air flow with constant flow U at some point in x direction. Mass accumulation happens due to dispersion/diffusion and bulk motion in and out of infinitesimal fluid/air element

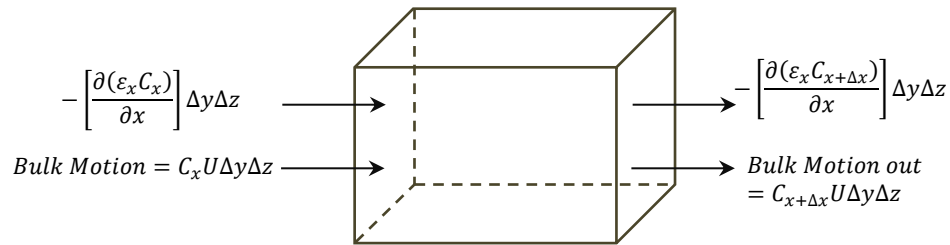


Figure 2.8: Schematic of advection-dispersion infinitesimal fluid element (Wark et al., 1998)

For point source at ground level, the solution of Equation 2.17 must fulfil boundary conditions as below

- i. $C(x, y, z) \rightarrow \lim_{(x,y,z \rightarrow 0)} \frac{Q}{(UA_{yz})} \rightarrow \infty$ (large concentration at the point source itself)
- ii. $C(x, y, z) \rightarrow 0$ as $x, y, z \rightarrow \infty$ (zero concentration at a great distance from the source)
- iii. $\left(\varepsilon_z \frac{\partial C}{\partial z} \right) \rightarrow 0$ as $z \rightarrow 0$ (no diffusion/dispersion into the surface as pollutant cannot penetrate the boundary layer at the ground)
- iv. For $x > 0$, $Q = \int_0^\infty \int_{-\infty}^\infty UC(x, y, z) dy dz$ (rate of transport of pollutant in x -direction equals to the pollutant emission rate Q at the source)

Then using Equation 2.18, calculating Q

$$Q = \int_0^\infty \int_{-\infty}^\infty KUx^{-1} \exp \left[- \left\{ \left(\frac{y^2}{\varepsilon_y} \right) + \left(\frac{z^2}{\varepsilon_z} \right) \right\} \frac{U}{4x} \right] dy dz \quad \text{Equation 2.19}$$

Now let $Y = y/(\varepsilon_y)^{1/2}$ and $Z = z/(\varepsilon_z)^{1/2}$, then the Equation 2.19 will become

$$Q = KUx^{-1}(\varepsilon_y)^{1/2}(\varepsilon_z)^{1/2} \int_0^\infty \exp\left[-\frac{Z^2U}{4x}\right] dZ \int_{-\infty}^\infty \exp\left[-\frac{Y^2U}{4x}\right] dY \quad \text{Equation 2.20}$$

Here we can use standard integration result

$$\int_0^\infty \exp(-a^2s^2) ds = \frac{(\pi)^{1/2}}{2a} \quad \text{Equation 2.21}$$

Using Equation 2.21 and integration identity Equation 2.20 gives the result

$$\begin{aligned} Q &= KUx^{-1}(\varepsilon_y)^{1/2}(\varepsilon_z)^{1/2} \left(\frac{\pi x}{U}\right)^{1/2} \left\{2\left(\frac{\pi x}{U}\right)^{1/2}\right\} \\ &= 2\pi K(\varepsilon_y)^{1/2}(\varepsilon_z)^{1/2} \\ \Rightarrow K &= \frac{Q}{2\pi(\varepsilon_y\varepsilon_z)^{1/2}} \end{aligned} \quad \text{Equation 2.22}$$

Then, Equation 2.18 represents ground-level concentration downwind from a continuous ground point source.

$$C(x, y, z) = \frac{Q}{2\pi x(\varepsilon_y\varepsilon_z)^{1/2}} \exp\left[-\left\{\left(\frac{y^2}{\varepsilon_y}\right) + \left(\frac{z^2}{\varepsilon_z}\right)\right\} \frac{U}{4x}\right] \quad \text{Equation 2.23}$$

We will briefly discuss the **Gaussian** or **normal distribution** to be used to derive of Gaussian like dispersion model.

Consider double Gaussian in two coordinate directions, y and z.

$$f(y, z) = \frac{1}{2\pi\sigma_y\sigma_z} \exp\left[-\left\{\left(\frac{(y - \mu_y)^2}{2\sigma_y^2}\right) + \left(\frac{(z - \mu_z)^2}{2\sigma_z^2}\right)\right\}\right] \quad \text{Equation 2.24}$$

In Equation 2.24, μ represents function's mean value and σ (standard deviation) represents position of inflection on either side of the Gaussian curve. μ and σ represent general position and shape of the Gaussian distribution function. Since the distribution occurs along the centre-lines of axes in the space, so for such physical level $\mu_y = \mu_z = 0$; then the Equation 2.24 reduce to

$$f(y, z) = \frac{1}{2\pi\sigma_y\sigma_z} \exp\left[-\left\{\left(\frac{y^2}{2\sigma_y^2}\right) + \left(\frac{z^2}{2\sigma_z^2}\right)\right\}\right] \quad \text{Equation 2.25}$$

Now comparing Equation 2.23 and Equation 2.25, a definition is introduced as below

$$\sigma_y^2 = \frac{2\varepsilon_y x}{U} \quad \text{and} \quad \sigma_z^2 = \frac{2\varepsilon_z x}{U} \quad \text{Equation 2.26}$$

Now substituting this definition to Equation 2.23

$$C(x, y, z) = \frac{Q}{\pi U \sigma_y \sigma_z} \exp \left[-\frac{1}{2} \left(\frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2} \right) \right] \quad \text{Equation 2.27}$$

One can rearrange Equation 2.23 to get the feel of the double Gaussian type. If we take y and z to zero, then Equation 2.27 becomes

$$C(x, 0, 0) = \frac{Q}{\pi U \sigma_y \sigma_z} \quad \text{Equation 2.28}$$

Equation 2.28 represents downwind, ground level, centre-line concentration from a point source at ground level.

2.3.2.1 Point Source at Elevation height H Above the Ground

If point source is above ground (Figure 2.9), then the limits of integration of z extend to $-\infty$ to $+\infty$, so the new K calculated as below

$$K = \frac{Q}{4\pi(\epsilon_y \epsilon_z)^{1/2}} \quad \text{Equation 2.29}$$

When we apply this K in Equation 2.26, we get mathematically much more tractable model with less error

$$C(x, y, z) = \frac{Q}{2\pi U \sigma_y \sigma_z} \exp \left[-\frac{1}{2} \left(\frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2} \right) \right] \quad \text{Equation 2.30}$$

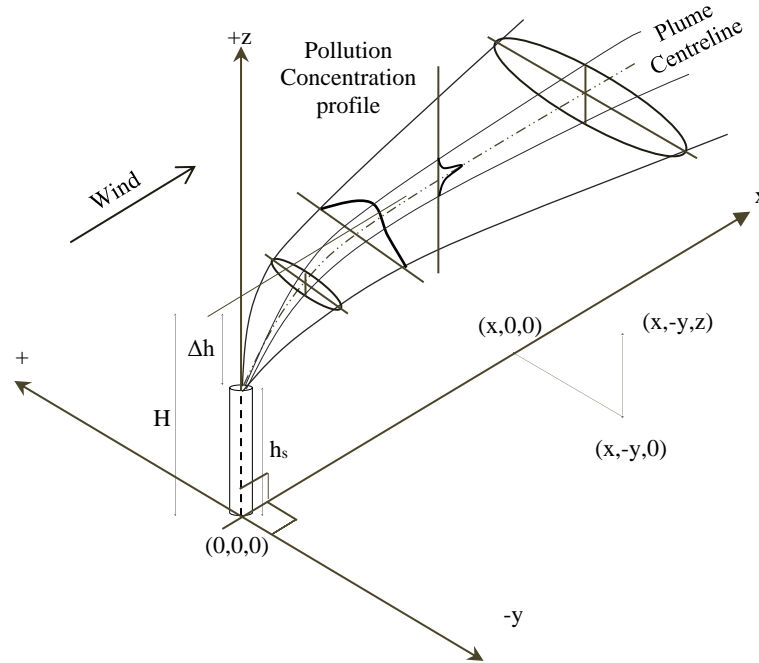


Figure 2.9: A typical plume from an elevated point source (Turner, 1969)

From Figure 2.9, we can see the effective elevated height of a point source is H , so we need to adjust Equation 2.30 for vertical axis as $(z - H)$, the new formulation become as below

$$C(x, y, z) = \frac{Q}{2\pi U \sigma_y \sigma_z} \exp \left[-\frac{1}{2} \left(\frac{y^2}{\sigma_y^2} + \frac{(z - H)^2}{\sigma_z^2} \right) \right] \quad \text{Equation 2.31}$$

Equation 2.31 is appropriate until concentration becomes significant at $(z = 0)$ in flow direction. Here it could be better to say no-reflection of concentration happens, and this equation is valid.

2.3.2.2 Point Source at Elevation height H Above the Ground with Reflection

Earlier we see that if the emission source is above ground, then there is a point after a certain length on the ground in the direction of downwind, where the pollutant contacts the ground, as shown in Figure 2.10. We consider ground is not a “sink” for pollutants, but the pollutants reflect from the ground. To model the reflection, now we can consider an imaginary mirror pollution source, as shown in Figure 2.10.

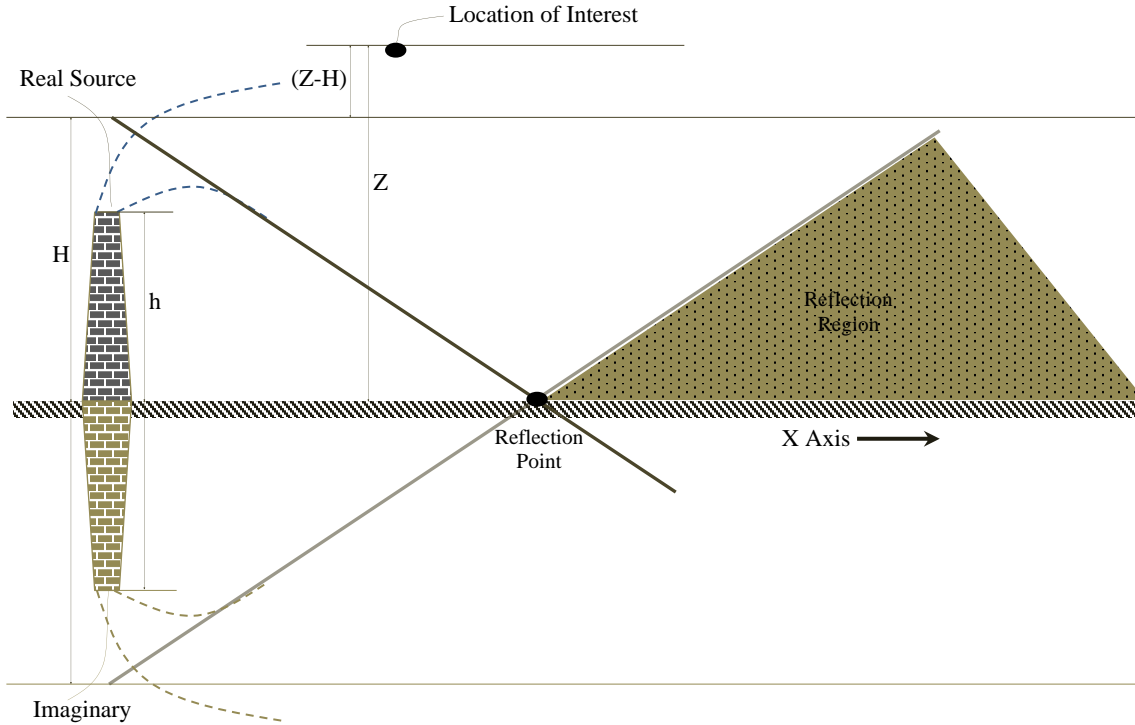


Figure 2.10: schematic to represent imaginary point source which acts as mirror contributor

Here it is clear that emission height is $-H$. We see that the imaginary emission source contributes similarly to the real source at the reflection point. The overall pollutant concentration will be calculated by linear superposition of two Gaussian-type concentration curves. So the total pollutant concentration with reflection becomes

$$C(x, y, z) = \frac{Q}{2\pi U \sigma_y \sigma_z} \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2}\right)\right] \left[\exp\left\{-\frac{(z-H)^2}{2\sigma_z^2}\right\} + \exp\left\{-\frac{(z+H)^2}{2\sigma_z^2}\right\} \right] \quad \text{Equation 2.32}$$

Equation 2.32 shows that in downwind after the reflection point, the overlap will become significant and increase as x increase. Equation 2.32 is widely used.

If we put $z = 0$ in Equation 2.32, then we will get ground-level concentration profile with reflection

$$C(x, y, 0) = \frac{Q}{\pi U \sigma_y \sigma_z} \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2}\right)\right] \left[\exp\left\{-\frac{1}{2}\left(\frac{H^2}{\sigma_z^2}\right)\right\} \right] \quad \text{Equation 2.33}$$

To obtain ground level central line concentration $y = 0$ thus Equation 2.33 takes the following form

$$C(x, 0, 0) = \left(\frac{Q}{U}\right) \frac{1}{\pi \sigma_y \sigma_z} \left[\exp\left\{-\frac{1}{2}\left(\frac{H^2}{\sigma_z^2}\right)\right\} \right] \quad \text{Equation 2.34}$$

Rearranging Equation 2.34 for ground-level, centerline concentration along x axis

$$\frac{C(x, 0, 0)U}{Q} = \frac{1}{\pi\sigma_y\sigma_z} \left[\exp \left\{ -\frac{1}{2} \left(\frac{H^2}{\sigma_z^2} \right) \right\} \right] \quad \text{Equation 2.35}$$

Here we see right side of Equation 2.35, becomes constant for given H , σ_y and σ_z , for a given stability class, in such a condition, one can obtain ground level concentration profile in downwind by just multiplying (Q/U) factor.

Example 2.2: A tracer study needs to be carried out to physically demonstrate the extent of contribution of pollutant from a source to a receptor. The tracer in question is fluorescent particles of very small size (1.8×10^8 particles per gram) that behave in a manner similar to gaseous pollutants. It is proposed to release a known quantity of the tracer from the source and measure the concentration at the receptor end located at 30 m height from the ground level. Sampling at the receptor end is at membrane filter through which $9 \times 10^{-3} \text{ m}^3$ of air is drawn every minute. A study involving 1-hour release of tracer from a source at ground level under slightly unstable (stability class C) meteorological conditions and wind speed of 5 m/s is to be carried out. The tracer concentration is to be measured at ground level 8 km from the source in down wind direction. It is desirable to obtain a particle count of at least 20 on the membrane filter for a sampling time of 1-hour. Determine at what time after the beginning of tracer release the sampling may commence and what would be the minimum total release the sampling may commence and what should be the minimum total release of tracer be (in gram) for this experiment. Assume no plume rise. The value of $\sigma_y=690 \text{ m}$ and $\sigma_z=310 \text{ m}$ at 8 km for stability class C,

Ans:

Total dose (say D_T) at the sampler is determined as

$$D_T = \frac{20}{1.8 \times 10^8 (\text{particles/gram})} \times \frac{60}{9 \times 10^{-3} (\text{m}^3/\text{min})} = 7.41 \times 10^{-4} (\text{gm} - \text{sec m}^{-3})$$

Given that $Y = 0, H = 0, Z = 30 \text{ m}, U = 5 \frac{\text{m}}{\text{s}}, \sigma_y = 690, \sigma_z = 310$ at $X = 8 \text{ km}$

From Equation 2.34 for total mass release (Q_T)

$$7.41 \times 10^{-4} = \frac{Q_T}{3.14 \times 5 \times 310 \times 690} \exp \left(-\frac{1}{2} \left(\frac{30}{310} \right)^2 \right)$$

$$Q_T \approx 2501 \text{ gm or } 2.501 \text{ kg}$$

$$\text{Now time to travel} = \frac{8000 (\text{m})}{5 (\text{m/s})} = 26.67 \text{ minutes}$$

So sampling should start after 26.67 minutes

It may seem that due to reflection, concentration with x , after touchdown of the plume, will always increase with x . However, this is not true beyond a certain point. As the x increases, both σ_y and σ_z increase causing an exponential decrease in concentration as x increases.

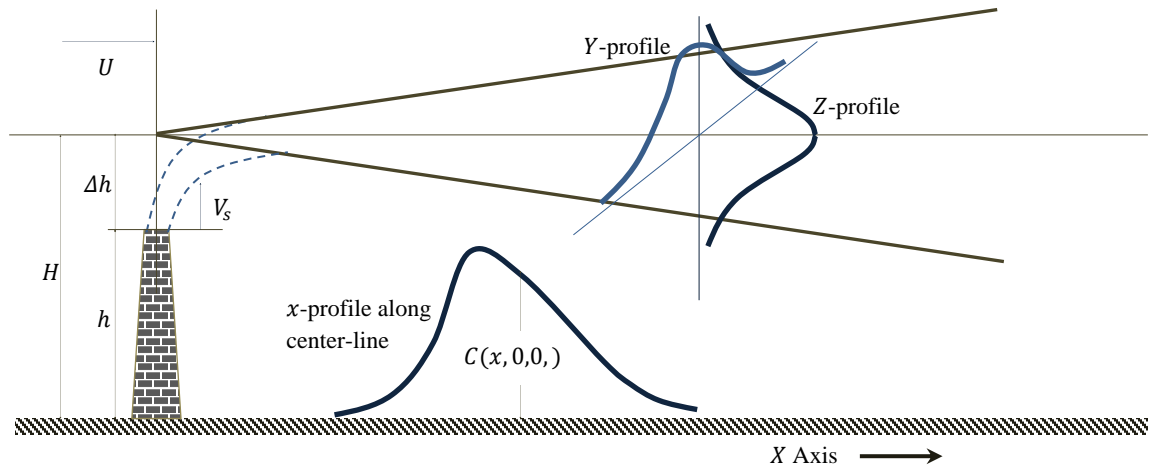


Figure 2.11: Concentration profile on ground-level and along center-line of downwind

A typical schematic diagram of concentration profiles in x , y and z direction shown in Figure 2.11. x -profile becomes maximum at certain distance than again reduce. y -profile and z -profile of concentration show Gaussian distribution in both (y and z) directions, but with different spreads.

2.4 Estimation of Standard Deviations σ_y and σ_z

It can be seen from Equation 2.26, that σ_y and σ_z are depend on diffusivities of pollutant in given two directions, downwind distance and stability class. Several models and equations were given to estimate proper and justified standard deviations. When using models, one should keep in mind that most models and equations do not work for variable rate emission and instantaneous puff like pollutant emissions. It should be remembered that velocity U , is always function of height. The best way to use velocity of flow is to use the mean value of velocity (Turner, 1969). Mean velocity is almost impossible to estimate because sufficient atmospheric data would not be available. To overcome this problem, average wind speed at the top of elevated height H is commonly used. If average wind speed is not available, then measured wind speed at $10m$ can be used to estimate velocity at elevated/stack height.

Several researchers provide methods and models to estimate σ_y and σ_z , based on the stability of the atmosphere. Most accepted work is done by (Turner, 1969), which is based on distinct stabilities that rarely co-occur. Charts are given in Figure 2.12 and Figure 2.13 prepared by (Turner, 1969).

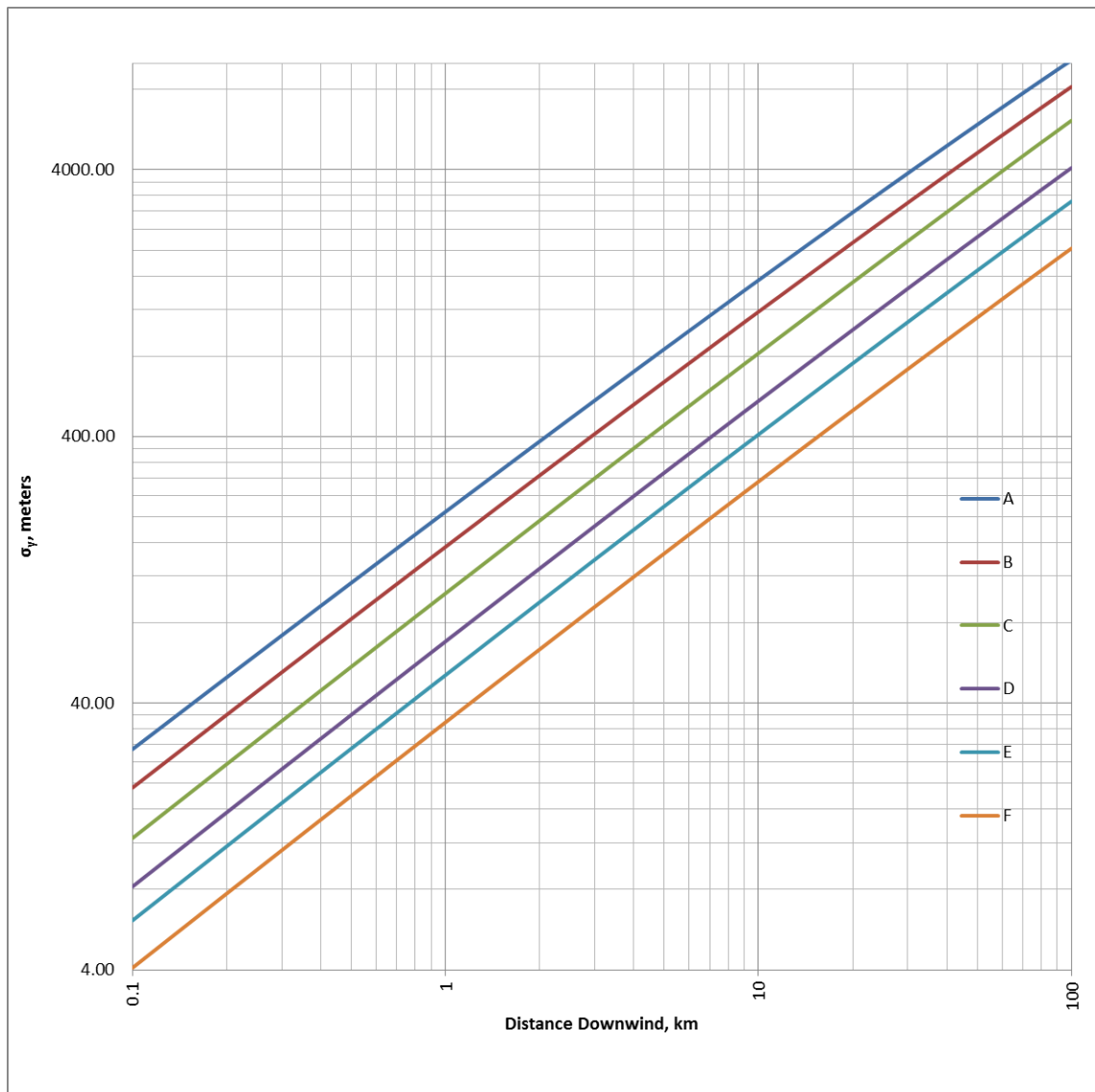


Figure 2.12: Standard deviation, σ_y , in the crosswind direction as a function of downwind x -axis

Charts values have restrictions as below-

1. The concentration estimated from these charts should correspond to a sampling time of approximately 10 minutes.
2. The horizontal and vertical deviations are based on a terrain representative of an open country.
3. The estimated concentrations more nearly represent only the lowest several hundred meters of the atmosphere.

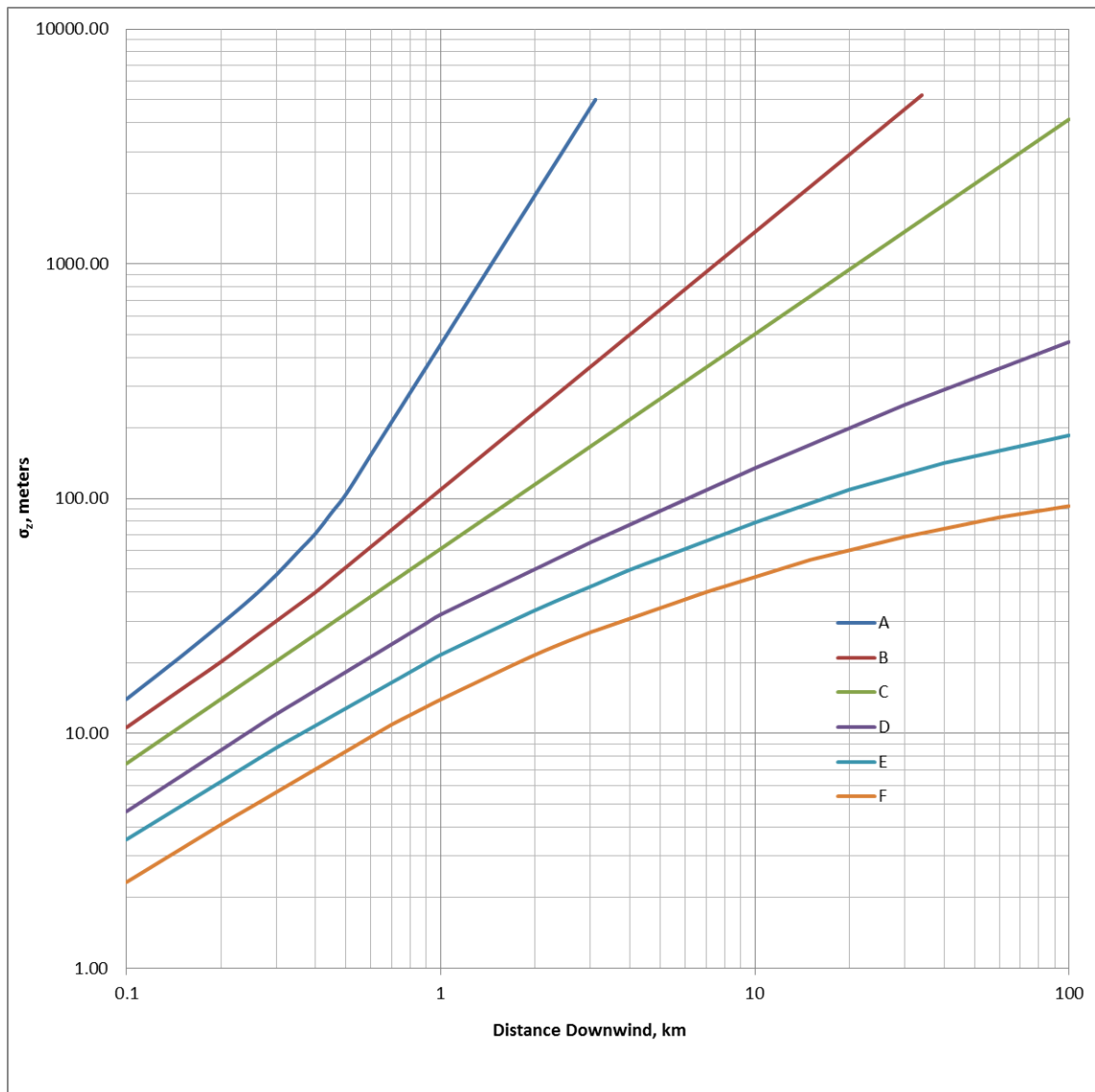


Figure 2.13: Standard deviation, σ_z , in the crosswind direction as a function of downwind x -axis

Table 2.1: Approximate values of σ_y and σ_z as a function of downwind distance for various stability classes (meters)

Distance (km)	Stability classes and σ_y values						Stability classes and σ_z values					
	A	B	C	D	E	F	A	B	C	D	E	F
0.1	27	19	13	8	6	4	14	11	7	5	4	2
0.2	50	36	23	15	11	8	29	20	14	8	6	4
0.4	94	67	44	29	21	14	72	40	26	15	11	7
0.7	155	112	74	48	36	24	215	73	43	24	17	11
1.0	215	155	105	68	51	34	455	110	61	32	21	14
2.0	390	295	200	130	96	64	1950	230	115	50	34	22
4.0		550	370	245	180	120		500	220	77	49	31
7.0		880	610	400	300	200		780	360	109	66	39
10.0		1190	840	550	420	275		1350	510	135	79	46
20.0		2150	1540	1000	760	500		2900	950	205	110	60

Source: (Turner, 1969)

The standard Pasquill-Gifford curves (Figure 2.12 and Figure 2.13) represent a sampling time of approximately 10 minutes. The estimation of σ_y and σ_z from Equation 2.37 represents one hour average sampling time. While the models are useful, one must be careful while sampling periods or required averaging time is bigger than a few minutes. For example, hypothetically, though mean meteorological conditions remain the same for 24 hour, the modelled concentrations (i.e. few minutes to one hour averaging) will be much higher than a 24 sampled concentration. This higher modelled concentration is primarily because the meandering of the plume and minor instant variations in the meteorology suggested that concentrations for a larger averaging time from modelled concentration can be estimated using Equation 2.36 (valid for less than 2 hours sampling).

$$C_2 = C_1 \left(\frac{t_1}{t_2} \right)^q \quad \text{Equation 2.36}$$

Here C_2 is Concentration to be calculated
 C_1 is Calculated concentration by dispersion model
 t_2 is Sampling time period in minutes
 t_1 is 10 minutes
 q is between 0.17 to 0.20

Table 2.1 lists σ_y and σ_z values for the six stability classes for some downwind distances. This table is shown here because the chart is difficult to read accurately. When this data is plotted, standard deviations reasonable curve fitted x distance as expression given by (Martin, 1976).

$$\sigma_y = ax^b \text{ and } \sigma_z = cx^d + f \quad \text{Equation 2.37}$$

Table 2.2: Values of constants to be used in Equation 2.37 as a function of downwind distance and stability condition

Stability	For all x	x ≤ 1 km			x ≥ 1 km		
	a	c	d	f	c	d	f
A	213	440.8	1.941	9.27	459.7	2.094	-9.6
B	156	106.6	1.149	3.3	108.2	1.098	2.0
C	104	61.0	0.911	0	61.0	0.911	0
D	68	33.2	0.725	-1.7	44.5	0.516	-13.0
E	50.5	22.8	0.678	-1.3	55.4	0.305	-34.0
F	34	14.35	0.740	-0.35	62.6	0.180	-48.6

Source: (Martin, 1976)

Values of stability-dependent constants are given in Table 2.2. the value of b is always 0.894, x must be expressed in kilometres (Martin, 1976). More information can found in (Bowne, 1974; Frenkiel & Munn, 1974; Slade, 1968; Stern, 1968, 1955).

Holland's formula can calculate the plume rise, Δh (meter)

$$\Delta h = \frac{V_s d}{U} \left[1.5 + 2.68 \times 10^{-3} P d \left(\frac{T_s - T_a}{T_s} \right) \right] \quad \text{Equation 2.38}$$

Here V_s is stack gas exit velocity in metres per second

d is stack exit diameter in metres

P atmospheric pressure in millibars

U wind velocity in meters per second at the tip of the stack

T_s is stack exit gas temperature in K

T_a is the atmospheric temperature at stack height in K

Holland's formula underestimates the plume rise. The obtained plume rise must be multiplied by 1.1 or 1.2 for stability A and B and stability D, E or F with 0.8 or 0.9. More precise results can be calculated using comparative studies by (Carson & Moses, 1969; Thomas et al., 1970; Carpenter et al., 1971).

Example 2.3: A consultant advised industry to enhance the plume rise by a factor of 1.3 and they will meet the air quality standards. What are the options for the industry to enhance the plume rise (mind that stack diameter cannot be changed). On the second examination, industry said that it is the only temperature of the exit gases that can be altered. What should be the rise/reduction in stack gas temperature to get the desired plume rise. Current parameter are: $d=2\text{m}$, $T_a=300\text{K}$, $T_s=400\text{K}$, $p=1000\text{mb}$, $V_s=20\text{m/s}$, U (at stack tip)= 4m/s .

Ans:

Typical three ways to increase plume rise are

- Increase stack diameter
- Increase stack temperature
- Increase exit velocity

Rewriting Equation 2.38

$$1.3\Delta h - \Delta h = \left[\frac{V_s d}{U} \left[1.5 + 2.68 \times 10^{-3} P d \left(\frac{T_s - T_a}{T_s} \right) \right] \right]_{T_{s1}}^{T_{s2}}$$

$$\Rightarrow T_{s2} = 507.575 \text{ K}$$

$$\text{So rise in temperature} = 507.575 - 400 = 107.57 \text{ K}$$

Table 2.3 presents a summary of widely used Briggs's formulation ((Briggs, 1969, 1971, 1974)) to estimate plume rise (in m) for plume dominated by buoyancy force and momentum force.

$$\Delta h = \frac{E x^\beta}{\bar{U}^\alpha} \quad \text{Equation 2.39}$$

Table 2.3: Summary of Several Plume Rise Formulae Expressed in the Form $\Delta h = Ex^\beta/\bar{U}^\alpha$

Atmospheric Stability	α	β	E	Conditions
Neutral and unstable	1	$\frac{2}{3}$	$1.6F^{1/3}$	$F < 55, x < 49F^{5/8}$
	1	0	$21.4F^{3/4}$	$F < 55, x > 49F^{5/8}$
	1	$\frac{2}{3}$	$1.6F^{1/3}$	$F \geq 55, x < 119F^{2/5}$
	1	0	$38.7F^{3/5}$	$F \geq 55, x \geq 119F^{2/5}$
Stable (use the formula which gives/predicts least plume rise)	$\frac{1}{3}$	0	$2.4(F/S_2)^{1/3}$	
	0	0	$5F^{1/4}S_2^{-3/8}$	
	1	$\frac{2}{3}$	$1.6F^{1/3}$	
Neutral (use the formula which gives/predicts least plume rise)	$\frac{2}{3}$	$\frac{1}{3}$	$1.44(dV_s)^{2/3}$	$V_s/\bar{U} \geq 4$
	1	0	$3dV_s$	$V_s/\bar{U} \geq 4$

Here;

g = acceleration due to gravity, 9.807 m s^{-2}

F = buoyancy flux parameter, $gd^2V_s(T_s - T_a)/4T_s, \text{ m}^4\text{s}^{-3}$

d = stack diameter, m

p = atmospheric pressure, kPa

$p_0 = 101.3 \text{ kPa}$

T_s is stack exit gas temperature in K

T_a is atmospheric temperature at stack height in K

$\Delta T = T_s - T_a$

V_s = stack exit velocity, m s^{-1}

$S_1 = (g\partial\theta/\partial z)(p/p_0)^{0.29}/T_a, \text{ s}^{-2}$

$S_2 = (g\partial\theta/\partial z)/T_a, \text{ s}^{-2}$

2.4.1.1 Elevated Inversion layer and pollutant concentration

In real atmospheric conditions, an elevated inversion layer causes a trap of pollutants in-between ground and inversion layer. In such a situation, the pollution concentration from a point source at elevated height H can be calculated by Equation 2.32. But if there is an elevated inversion layer at L height then analogy of virtual sources (described in section 2.3.2.2), infinite sources will contribute to pollutant concentration in downwind. Ground and elevated inversion layers act as mirrors, and the final simplified model can be written as Equation 2.40. Here $i = 0, 1, 2 \dots$

$$C(x, y, z) = \frac{Q}{2\pi U \sigma_y \sigma_z} \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2}\right)\right] \sum_{i=-\infty}^{i=+\infty} \left[\exp\left\{-\frac{(z-H+2iL)^2}{2\sigma_z^2}\right\} + \exp\left\{-\frac{(z+H+2iL)^2}{2\sigma_z^2}\right\} \right]$$

Equation 2.40

It can be imagined that for a stable inversion layer after a certain distance in downwind, the vertical dispersion (mixing) do not affect by an elevated inversion layer, say this distance x_L for which $\sigma_z = 0.47(L - H)$. For a given elevated inversion layer height L one can calculate x_L , because σ_z is a function of x axis/direction. It can be assumed that after a downwind distance $2x_L$, vertical mixing becomes uniform, then the following model can be used (ref??)

$$C(x > 2x_L, y, z) = \frac{Q}{(2\pi)^{1/2}LU\sigma_y} \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2}\right)\right] \quad \text{Equation 2.41}$$

Equation 2.41 has only two variables x and y , because the problem reduced to 2D dispersion of pollutant. To calculate concentration between x_L to $2x_L$, (Turner, 1969) suggests that center-line concentrations at ground-level can be calculated by drawing a straight line between the concentrations on a *log-log* plot of ground-level, center-line concentration versus distance x .

2.4.2 Area Source

If several small sources are at a site, it is mathematically simple to treat them as an area source. In such a situation, it is assumed that the area source has an initial horizontal standard deviation, σ_{y0} . For a square area having length s , the initial standard deviation is estimated as $\sigma_{y0} \cong s/4.3$ (Turner, 1969). For the obtained σ_{y0} and given stability class one can locate a virtual point source in the upwind direction of the area source that will produce exactly same σ_y as σ_{y0} at the centre of the area source. For the given σ_{y0} and stability class one can estimate the virtual distance x_y where the virtual point source is supposedly located (Figure 2.14). Now σ_y will be function of $(x + x_y)$. Then the point source gaussian model can be used for the virtual point source for estimating concentration in the downwind direction of the area sources. Calculation procedure: first, calculate $\sigma_{y0} \cong s/4.3$, then x_y from Figure 2.12, then for given x estimate σ_z from Figure 2.13, then for $(x + x_y)$ calculate σ_y , and use Equation 2.33 or Equation 2.34 for estimating the central line ground level concentration.

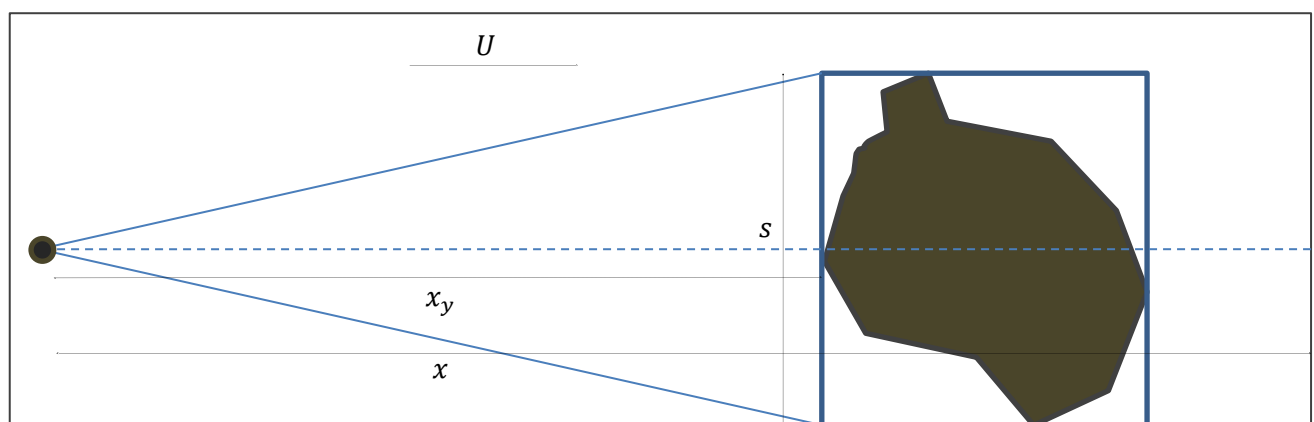


Figure 2.14: Illustration of Holland's method to

Similarly, effective elevation height H would be the mean effective height of that area source and σ_{z0} the standard deviation of the initial vertical distribution of sources. A virtual distance x_{z0} , can be calculated then can be used to calculate σ_z as a function of $(x + x_{z0})$.

2.4.3 Line Source

Downwind concentration of emissions from an infinite line source (e.g., several pollutions emitting vehicles on the road), when wind direction is φ angle to line source (Figure 2.15). To calculate modelled concentration at x , when line source emissions occur at elevation height of H from ground and having emission rate q per unit length.

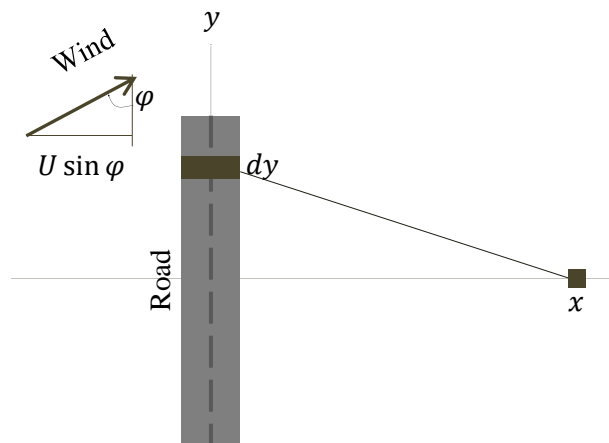


Figure 2.15: Schematic of line emission and its concentration at x distance

Now integrating Equation 2.33 w.r.t. y from $-\infty$ to $+\infty$, it reduces to

$$C(x, y, 0) = \int_{-\infty}^{+\infty} \frac{qdy}{\pi(U \sin \varphi)\sigma_y\sigma_z} \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2}\right)\right] \left[\exp\left\{-\frac{1}{2}\left(\frac{H^2}{\sigma_z^2}\right)\right\} \right]$$

On integration, the ground level concentration is estimated as

$$C(x, y, 0) = \frac{2q}{(2\pi)^{1/2}\sigma_z U \sin \varphi} \exp\left\{-\frac{1}{2}\left(\frac{H^2}{\sigma_z^2}\right)\right\} \quad \text{Equation 2.42}$$

Crosswind direction concentration in Equation 2.42 the value of φ should be less than 45° (Sutton, 1932; Turner, 1969).

One must account for a finite line source's “edge effects” caused by the end of the line source. For perpendicular crosswind through line source which passes through the point of interest in x direction can be written as for $y_1 < y_2$

$$C(x, y, 0) = \int_{y_1}^{y_2} \frac{qdy}{\pi U \sigma_y \sigma_z} \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2}\right)\right] \left[\exp\left\{-\frac{1}{2}\left(\frac{H^2}{\sigma_z^2}\right)\right\} \right]$$

Which can be written as

$$C(x, y, 0) = \frac{2q}{(2\pi)^{1/2} U \sigma_z} \left[\exp \left\{ -\frac{1}{2} \left(\frac{H^2}{\sigma_z^2} \right) \right\} \right] \int_{Y_1}^{Y_2} \frac{1}{(2\pi)^{1/2}} \exp \left[-\frac{1}{2} Y^2 \right] dY \quad \text{Equation 2.43}$$

$$\text{Where } Y_1 = \frac{y_1}{\sigma_y}, \text{ and } Y_2 = \frac{y_2}{\sigma_y}$$

The value of integral can be determined from statistical tables from any standard book on mathematical tables and formulas.

Example 2.4: (a) The general Gaussian air quality model is given. The pot-room emissions of fluoride from an aluminum smelter are to be modelled for ground level concentration. The length of pot-room is 'L'. The overall emission rate is 'Q' gm/sec from an effective height of 'H'. The wind direction is perpendicular to the pot-room. It is not correct to assume the pot-room as a point emission source as the length 'L' is large. Derive an expression to estimate the ground-level concentration (GLC) from the pot-room for the specified emissions in the downwind direction and geometry. You can assume that the emissions from the pot-room are uniform with respect to length.

(b) For a given Q of 30 gm/sec, estimate the ground-level concentration at 5 km from the pot-room of length 700 m in the downwind direction, however, the wind now is blowing from the 30 degree along the pot-room length. Take wind speed U as 3.5 m/s and H is 25 m. for the stability class C, $\sigma_y = 550$ m and $\sigma_z = 300$ m at 5 km.

Ans:

(a) Per unit length emission from line source can be written as $q = Q/L$, now rest of derivation as Equation 2.43

$$C(x, y, 0) = \frac{2(Q/L)}{(2\pi)^{1/2} U \sin \phi \sigma_z} \left[\exp \left\{ -\frac{1}{2} \left(\frac{H^2}{\sigma_z^2} \right) \right\} \right] \int_{Y_1}^{Y_2} \frac{1}{(2\pi)^{1/2}} \exp \left[-\frac{1}{2} Y^2 \right] dY$$

(b) Calculate at $x = 5000$ m, $Y = \frac{y}{\sigma_y} \Rightarrow$ Consider the point at mid line so, $Y_2 = \frac{350}{550} = 0.636 = -Y_1$

$$C(5000m, 0, 0) = 30.8 \mu g/m^3$$

2.5 Maximum ground-level in-line concentration and required stack height

It is shown in Figure 2.11 that concentration profile in downwind at $y = 0$, on ground-level center-line increase up to certain distance x , after that concentration diminishes. Equation 2.33 (Turner, 1969) used to make graphical representation and calculations of maximum concentration and distance of maximum concentration is plotted in Figure 2.16. Here stability class and the effective height are known.

The value of the parameter $(CU/Q)_{max}$ is plotted versus the distance x_{max} of the maximum concentration, the information on stability class and effective stack height are also incorporated within the diagram. In the typical

problem, the known data are the stability class and the effective height. With this information (value/data), a particular point on the figure can be obtained. From this point, we read downward and to the left to ascertain x_{max} and C_{max} , respectively (by $(CU/Q)_{max} \times (Q/U)$).

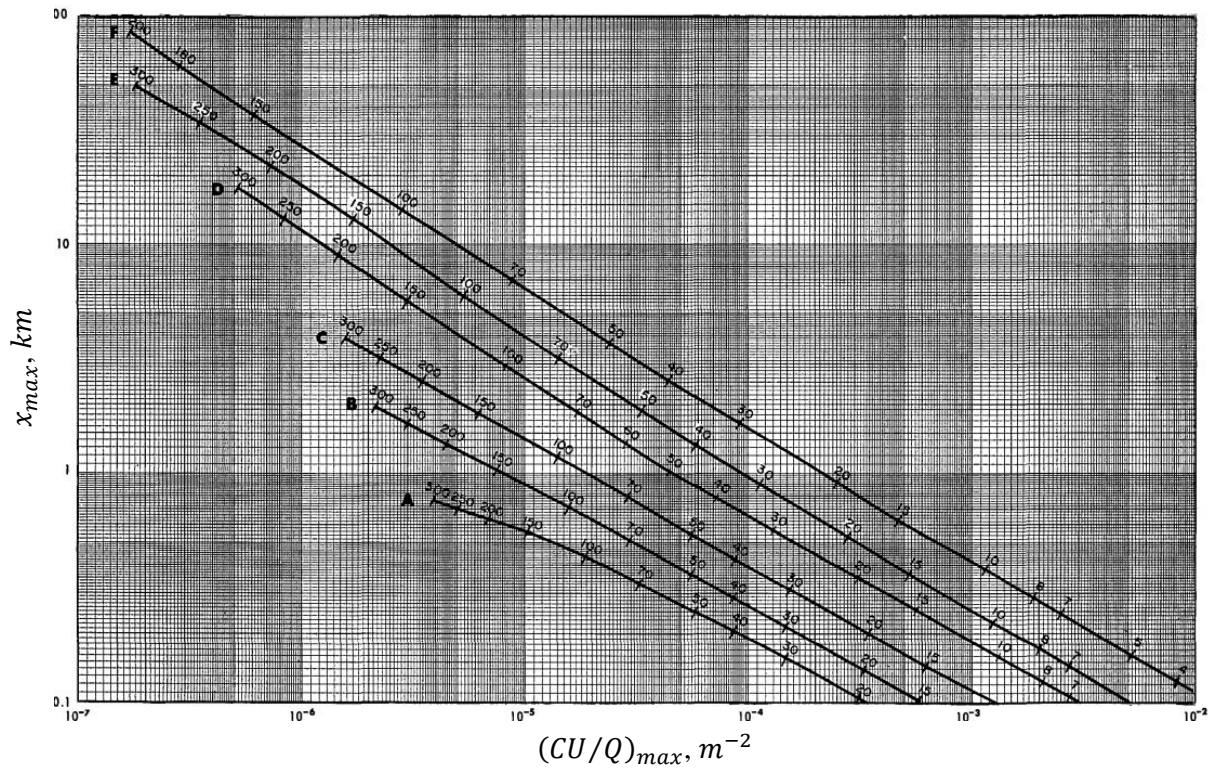


Figure 2.16: Maximum downwind concentration distance x_{max} and $(CU/Q)_{max}$ value as a function of stability class and effective height. (Turner, 1969)

To calculate $(CU/Q)_{max}$ one can use (Ranchoux, 1976) formula (Equation 2.44), by using effective height H .

$$\left(\frac{CU}{Q}\right)_{max} = \exp[a + b(\ln H) + c(\ln H)^2 + d(\ln H)^3] \quad \text{Equation 2.44}$$

Here H in meters
 CU/Q in m^{-2}

Table 2.4: Values of coefficients a , b , c , and d as a function of stability classes (Ranchoux, 1976)

Stability Class	Coefficients				Error
	a	b	c	d	
A	- 1.0563	- 2.7153	0.1261	0	< 2%
B	- 1.8060	- 2.1912	0.0389	0	
C	- 1.9748	- 1.9980	0	0	
D	- 2.5302	- 1.5610	- 0.0934	0	< 4.5%
E	- 1.4496	- 2.5910	0.2181	- 0.0343	
F	- 1.0488	- 3.2252	0.4977	- 0.0765	

The values for abscissa in Figure 2.16 can be calculated algebraically using Equation 2.44. Values of a , b , c , and d for each stability class are given in Table 2.4.

Alternatively, Equation 2.33 can be rewritten, with the assumption of, the ratio σ_y/σ_z is constant and $y = 0$ (under moderately unstable to neutral conditions). At the ground level centre-line the maximum concentration distance for an elevated source with effective stack height can be calculated from Equation 2.45 and the corresponding maximum concentration from Equation 2.46. These expressions are very well suited for unstable atmospheric conditions.

$$\sigma_z = \frac{H}{2^{1/2}} = 0.707H \quad \text{Equation 2.45}$$

$$C_{max} = \frac{0.1656Q}{U\sigma_y H} \quad \text{Equation 2.46}$$

Substituting σ_z value in Equation 2.46

$$C_{max, reflection} = \frac{0.1171Q}{U\sigma_y\sigma_z} \quad \text{Equation 2.47}$$

C_{max} from the first method and by Equation 2.47, do not always agree (remember this is 1-hour average). To compare with standard values (e.g., 24 hours average), one should multiply the hourly average by 0.4 to get 24 hours average.

2.6 Determination of Required Stack Height

For given stability, pollutant emission rate Q , typical general wind speed U and other meteorological parameters at a given location, one must ensure concentration C never goes above a certain level. To achieve this, one needs to calculate the required height H of the stack. Equation 2.47 can be rewritten as below

$$\sigma_y\sigma_z = \frac{0.1171Q}{UC_{max, regulatory}} \quad \text{Equation 2.48}$$

For given values right side of Equation 2.48, one can calculate the value of $\sigma_y\sigma_z$. A plot between $\sigma_y\sigma_z$ and downwind distance x can be estimated as Figure 2.17, because $\sigma_y\sigma_z$ is function of x and stability class. So from Figure 2.17 the downwind distance x_{max} can be calculated where concentration occurs maximum ($C_{max, regulatory}$) (Turner, 1969; Wark et al., 1998).

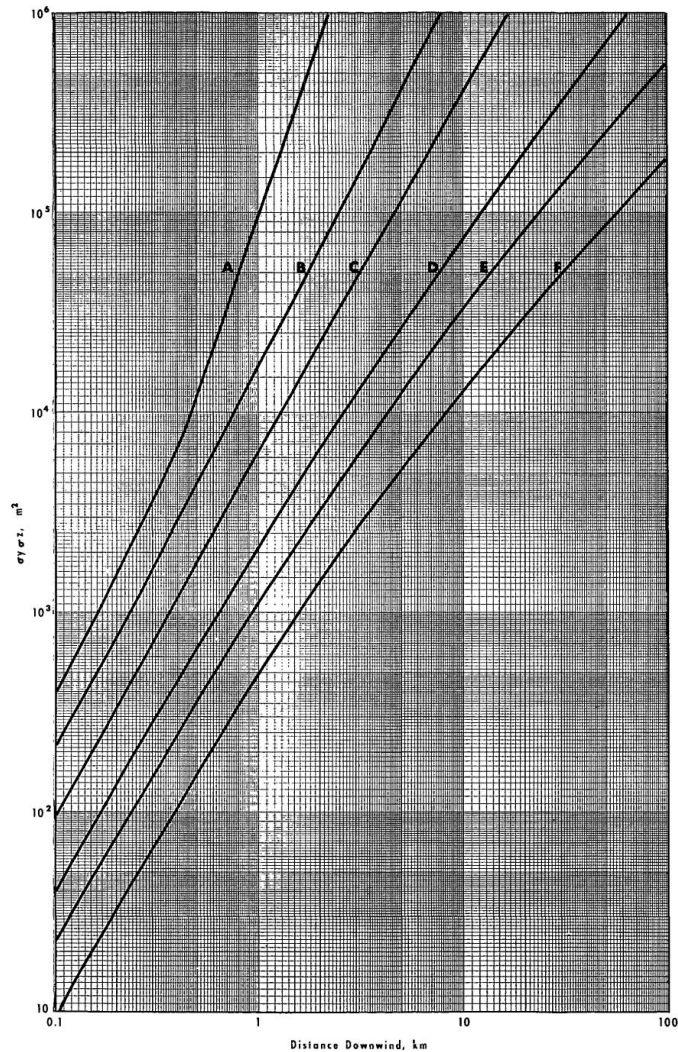


Figure 2.17: The product of $\sigma_y \sigma_z$, of the dispersion standard deviations as a function of downwind distance. (Turner, 1969)

Now for known x_{max} , from Figure 2.13 σ_z can be calculated, so the require stack height $H = (2)^{1/2} \sigma_z$ can be calculated. Here one should note that $H = h + \Delta h$, so the actual stack height h , become less.

The Equation 2.48 can rewrite as below

$$C_{max} = \frac{0.1171Q}{U\sigma_y\sigma_z} \left(\frac{\sigma_z^2}{\sigma_z^2} \right) = \frac{0.1171Q}{U\sigma_y\sigma_z} \left(\frac{2\sigma_z^2}{H^2} \right) = 0.2342Q \frac{\sigma_z}{\sigma_y} \left(\frac{1}{UH^2} \right) \quad \text{Equation 2.49}$$

It can be seen from σ_y vs x and σ_z vs x plots that σ_z/σ_y is constant for narrow ranges of downwind distances for a given stability class. So for given Q the maximum concentration becomes inversely proportional to the volume flux (UH^2) (π is skipped) at the point where plume reflect/touch the ground (Hanna, 1982). So the meaning of this is that as wind speed increases, the plume rise decreases, and the concentration decreases. At

a critical wind speed (U_c), C_{max} reaches a maximum. This occurs at a downwind distance x_c . For the neutral "breakup"¹ model, if we assume that $\sigma_z/\sigma_y = 0.707$, the critical wind speed occurs at $\Delta h/h = 1/3$.

$$U_c = 2.15 \left(\frac{U}{U_*} \right)^{2/3} \left(\frac{F_0}{h} \right)^{1/3} \quad \text{Equation 2.50}$$

$$x_c = 0.043 \left(\frac{U_*}{U} \right)^{2/3} \frac{Q}{F_0^{1/3} h^{5/3}} \quad \text{Equation 2.51}$$

Where, U_* is the friction velocity and U_*^2 is defined as the average of turbulent momentum flux $-\overline{U'W'}$

In Equation 2.50, the initial buoyancy flux F_0 is given by

$$F_0 = \frac{g}{T_{s0}} (T_{s0} - T_{a0}) W_{s0} R_0^2 \quad \text{Equation 2.52}$$

Where, R is plume radius in a plane perpendicular to the plume axis
Other abbreviations were already given before.

For the unstable model, the critical wind speed occurs at at $\Delta h/h = 5$

$$U_c = 0.43 F_0 H^{-2/3} h^{-5/3} \quad \text{Equation 2.53}$$

$$x_c = 0.015 \frac{QH^{2/3}}{F_0 h^{1/3}} \quad \text{Equation 2.54}$$

Find out maximum between Equation 2.50 and Equation 2.53. The dividing line for the neutral and unstable formulas is $U = 7 \text{ m/s}$ (Hanna & Pell, 1975; Moore, 1975).

¹ Briggs (1981) has developed the "breakup" model for the cases when rise is limited by ambient turbulence. In the "breakup" model the plume rise is assumed to terminate when the internal plume eddy dissipation rate just equals the ambient eddy dissipation rate. Theoretical estimate of plume rise at "breakup" in neutral conditions is $\Delta h = 3D \left(\frac{w_0}{U} - 1 \right)$, where w_0 is initial plume speed.

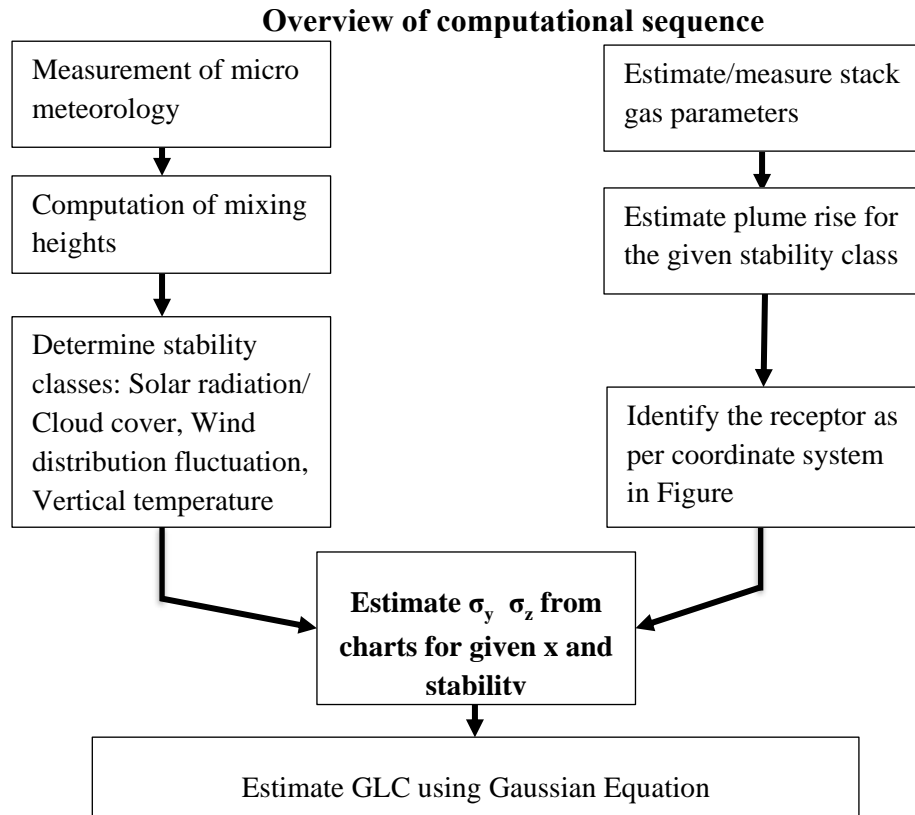


Figure 2.18: Overview of computational sequence

Questions.

Q1. A pile of waste is burning. Due to high temperature, NO_x is emitted at 11 gm/s from the ground. It is also seen that in cloudy night wind is flowing at 2 m/s. If there is a village is 1.5 km of downwind then calculate concentration of NO_x there.

Q2. Coal burning plant has 150 m effective height of SO_2 emissions at 105 gm/s. In the night wind is flowing at 0.5 m/s. Calculate SO_2 Concentration at downwind 100 m, 300 m and, 1500 m.

Q3. Calculate concentration at perpendicular to ground downwind 150 m, from last question.

Q4. A thermal power plant has 7 chimneys with 270 m height each has capacity to emit 6.75 tonnes/hour of burnt coal having 40% sulphur. One night the mixing height was reported to 1150 m and there was 2 m/s wind flow at 800 m. Calculate distance in downwind having maximum ground level concentration. Also find concentration 45° from plant to perpendicular to the maximum concentration point.

Q5. Use last question, and calculate for a cloudy night having wind speed 7 m/s. (i) The distance of maximum concentration. (ii) Draw concentration at ground, on a *log-log* graph for 10 m to 100 km. (iii) Draw concentration profile perpendicular to wind direction (crosswind) at ground upto 2 km. (iv) Determine distance and area for concentration 10^{-6} gm/m³. (v) Determine concentration profile for (1500 m, 0 m, 350 m) and draw it with height. (vi) Find the condition, when ground level concentration equals the centreline concentration at 50 m. (vii) Calculate maximum concentration and distance for clear night. (viii) Calculate fumigation concentration at distance in (part vii) in the morning, when super-adiabatic lapse-rate extends to include most of plume.

Q6. On a clear day wind is blowing at 2 m/s at 45° . A Particulate Matter sampling site and cement plant are at 2 km at 215° of azimuth. PM10 emits at the rate of 3500 kg/hour from a 90 m chimney. Calculate concentration recorded by sampling site at 6 PM.

Q7. A plant emits SO_2 at 1250 kg/day, at a designed distance of 3 km for 15 ppb concentration. Town is 3.2 km away and frequency of wind towards town is 25-35 % with 2.5 m/s average wind. Calculate stack height.

Q8. For last question calculate ΔH at STP if stack diameter is 3 m and effluent temperature is 125°C and effluent velocity 15 m/s.

Q9. A tracer compound has size yield is 2×10^{10} particles/gm. Sampling is planned by high volume sampler (HVS) having 17000 liters/minute sampling rate. Detectable limit in lab is 30 particles on HVS filter. During a unstable day wind was flowing at 6 m/s. HVS is located at 1.5 km from centreline on ground with a sampling arc of 9 km. Calculate total tracer quantity to be release in 1 hour to detect it.

Q10. A railways material storage is complaining about corrosion of their material and they are accusing SO_2 emission from a nearby oil refinery for this problem. The oil refinery is vehemently opposed to this accusation that they are the polluters. As an expert, you recommended that refinery should do the tracer (material which is not emitted from any other source) release from the refinery to physically demonstrate the extent of contribution of pollutant from refinery. The tracer in question is fluorescent particles (1.8×10^8 particles per gram) of very small size that behave in a manner similar to gaseous pollutants. It is proposed to release a known quantity of the tracer from the refinery, and measure the concentration (c) at the railways storage facility (receptor). Sampling at the receptor end is at membrane filter through which $9 \times 10^{-3} \text{ m}^3$ of air is drawn every minute. A study involving 1-hour release of tracer from the refinery at ground level (height from MSL (mean sea level) 100 m) under slightly unstable (C) meteorological conditions and wind speed of 5 m/s is to be carried out. The tracer concentration is to be measured at storage facility (height from MSL 150 m) at 8 km (horizontal distance) from the refinery and 2 km from the plume centerline. It is desirable to obtain a particle count of at least 20 on the membrane filter for a sampling time of 1-hour. Determine at what time after the beginning of tracer release the sampling may commence and what should be the minimum total release of tracer be (in grams) for this experiment. Assume no plume rise.

Where the terms have their usual meanings and units. The values of $\sigma_y = 690 \text{ m}$ and $\sigma_z = 310 \text{ m}$ at 8 km for stability class C.

Now let us consider the issue of corrosion caused by SO_2 . Measured concentration of SO_2 at the storage is C_{SO_2} and emission rate from refinery is Q_{SO_2} . **Based on the concept of tracer study**, formulate model/procedure so that you can estimate ambient air SO_2 contribution at the storage facility caused by the refinery emission (i.e. $(C_{\text{SO}_2})_{\text{refinery}}$). Now you are given: Q_{SO_2} is 2000 kg/hr and overall measured C_{SO_2} at storage facility = $120 \mu\text{g}/\text{m}^3$. If the contribution of any source to ambient air level is more than 10% of ambient air level then the source can be considered corroding the material. Is the refinery really at fault and causing corrosion of railways material? Justify your answer.

3 Air Quality modelling in practice

In Chapter 2, the Gaussian Plume Model and the parameters required for using the model were described. This chapter, specifically, deals with the procedure that must be followed to obtain these parameters' values for carrying out the air quality modelling, especially for point sources.

Three seasons (winter, summer and post-monsoon) are suggested for modelling study. The representative months include December to February for winter, May for summer and October and November for post-monsoon season. Since winter is the critical season from an air pollution dispersion point of view, all three months, as suggested above, should be included for modelling work. All relevant data collection should refer to the above specified months.

3.1 Emission and Stack Details

For regulatory purposes, values of all parameters related to emission characteristics should correspond to full plant capacity (even if production is to be achieved in a phased manner). These parameters include:

- Quantities of raw materials (including fuels);
- Fuel analysis (e.g. ash, Sulphur & Nitrogen content and calorific value);
- For exit gases:
 - velocity;
 - temperature;
 - flow rate;
 - density (approximate);
 - specific heat (approximate); and
 - heat emission rate;
- For stack:
 - internal diameter at top; and
 - height from ground level
- Efficiencies of various proposed pollution control devices
- Ambient temperature and pressure

The emission rate (Q) for pollutants should either be measured or estimated from emission factors (see Chapter... on emission inventory) and duly accounted for the efficiency of control devices.

3.2 Meteorological Parameters

Surface meteorological data at the site of interest should be generated or taken from the nearest meteorological stations or airport. The meteorological parameters requiring data include

- Wind speed and direction (on a continuous basis);
- Ambient atmospheric temperature (daily mean);

- Cloud cover-(synoptic measurement atleast four times in 24 hours at regular intervals);
- Solar insolation (measurement/estimation); and
- Atmospheric pressure (daily mean)
- Vertical temperature profile (information desirable);
- Monthly precipitation (daily); and
- Number of rainy days (rainfall> 2.5mm)

3.3 Data Format

Before proceeding to the modelling procedure (Chapter 4), let us recapitulate the basic data requirements for modelling under ideal conditions. It may be recognized that the data required are very detailed for complex situations.as discussed in Chapter 4.

The objective here is to predict hourly concentration at several receptor locations (defined later in presentation of results). An input data file for a day of 24 hours may look as shown below in Table 3.1.

Table 3.1: Data Format

Parameter	Hour of Day (starting from 0000 hrs)					
	1	2	23	24
Emission rate (Q)						
Wind speed (U)						
Wind direction						
Stability						
Mixing height						
Ambient Temp. (T _a)						
Stack Temp. (T _s)						
Plume rise (Δh)						

Some of the parameters must be obtained from the site and some need to be derived from literature.

3.4 Receptor Location

Before describing the modelling procedure, it is necessary to specify the receptor locations. The receptor locations are defined relative to the absolute reference point of the plant. Generally, a receptor location is defined as x - y coordinates with reference to the absolute reference point. The approach adopted here is slightly different, as it is realized that a radial pattern of the receptor may be easier to implement for hourly calculation of concentration.

Absolute Reference Point (ARP)

The ARP for modelling purposes is considered as the point of release and not as the center point of an industrial complex. It implies that if there is more than one point of release, the ARP and relative receptor locations will also change.

Description of Location

The locations of receptors should be decided based on the modelling objectives and requirements. A general procedure could include 16 radial wind directions (N to NNW) and the radial distance from the ARP. Although the sixteen directions are kept constant, the radial distance of receptors should be a function of physical stack height. The receptor locations in each radial direction may be the following multiple of physical stack height 2.5, 5, 10, 15, 20, 25, 27.5, 30, 32.5, 35, 40, 45, 55, 70, 90, 110 and 140. The maximum distance could be 30 km; some Gaussian type models allow the estimation up to 50 km. The purpose of not having the fixed coordinates is that the concentration depends on stack height. Where concentration changes rapidly, a better resolution should be considered. For near-surface releases, include a set of receptors as close to the source as possible. These receptors should encircle the same. Any receptor of special significance, like national monuments, parks, wildlife reserves, etc., must be included as a receptor.

The Gaussian model described in **Chapter 2 is applicable** only under special conditions (see assumptions in model), which are not likely to exist in actual field conditions.

Some situations in the field that require different treatment are described below.

Plume Penetration

A buoyant plume, rising into a well-mixed layer trapped by stable air, may, partially or completely, penetrate the elevated stable layer. The fraction of the plume that penetrates the stable layer is first estimated. Then the emission rate, Q , and effective plume height, H , for the material remaining within the mixed layer, are modified.

The fraction P of the plume that penetrates the elevated stable layer is estimated as follows (Weil and Brower, 1934):

- 1) No penetration:

$$P = 0 \text{ if } z'_i / \Delta h \geq 1.5$$

Equation 3.1

- 2) Total penetration:

$$P = 1 \text{ if } z'_i/\Delta h \leq 0.5 \quad \text{Equation 3.2}$$

3) Partial penetration:

$$P = 1.5 - z'_i/\Delta h \text{ if } 0.5 < z'_i/\Delta h < 1.5 \quad \text{Equation 3.3}$$

Where, Δh is the predicated plum rise and $z'_i = z_i - h$, z_i is the height of the stable layer aloft, and h is the stack height.

The plume material remaining within the mixed layer is assumed to contribute to ground-level concentrations. The modified source strength, Q is then:

$$Q = Q_S(1 - P) \quad \text{Equation 3.4}$$

where, Q_S is the emission rate on top of the stack.

It is assumed that the plume rise due to penetration, Δh_p , is linearly varying between $0.62 z'_i$ for no penetration to z'_i for full penetration. Thus for partial penetration ($0 < P < 1$):

$$\Delta h_p = (0.62 + 0.38 P) z'_i \quad \text{Equation 3.5}$$

The modified plume height, h_m , to be used in further calculation, is:

$$h_m = \min(H, h_p); h_p = h + \Delta h_p \quad \text{Equation 3.6}$$

Q. Calculate modified source strength and modified plume height for stack having a 90 m height, 3.5 m diameter whose exit gas has a velocity of 25 m/s when the wind speed is 2.5 m/s, the pressure is 1 bar, and the stack temperature is 120°C and surrounding temperature is 25°C. The emission rate is given 10 kg/s. The stable layer aloft is at 350 m, 150 m and 280 m.

Terrain Characteristics and Downwash of Pollutants

If the release is located on or near a tall but narrow structure such that the height of release is less than $2H_B$ (H_B is the height of structure) but is equal or greater than $10 W_B$ (W_B is the width of structure) then the downwash related reduction in effective plume rise is estimated by (Vallero, 2014).

$$h_d = 2(v_s/u - 1.5)W_B \quad \text{Equation 3.7}$$

Downwash reduces the effective release height of the plume but is assumed not to reduce the efflux buoyancy or momentum.

Q. If height of building $H_B = 20 \text{ m}$ and building width $W_B = 6 \text{ m}$, then calculate plume rise, and than recalculate modified source strength and modified plume height, from above question.

Effect of Building Wake

If the height of release (modified for both types of downwash, if applicable) from building leaks or short stacks is less than $0.5H_B$ (or W_B), the emitted materials get mixed in the turbulent wake created by the air flow around the building or stack structure. This gives rise to a volume source. Based on the studies of experimental releases from buildings and on assumption of uniform mixing of the effluent in the building wake, the normal short term centerline concentration is given by

$$c(x, 0) = \frac{Q}{u(\pi\sigma_y\sigma_z + C_w A)} \tag{Equation 3.8}$$

where,

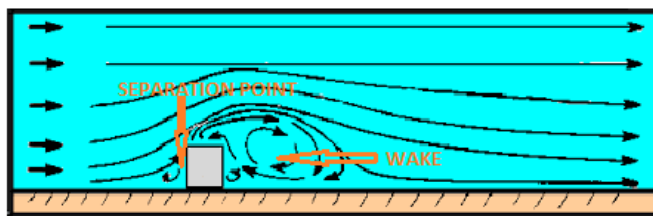
$A =$ Correctional area of the building normal to the wind, and

$C_w =$ fraction of A over which the plume is dispersed by the wake or more commonly known as building shape factor, conservatively estimated as 0.5.

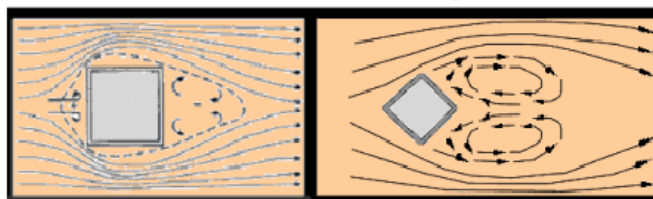
It would be seen from the expression that the effect of wake is to reduce the ground level concentrations in the downwind direction. However, if the corrected concentration value reduces to less than one third of the uncorrected value, then the concentration is taken to be equal to one-third the uncorrected concentration. The effect of wake becomes insignificant when

$$C_w A \ll \sigma_y \sigma_z$$

Q. A building has height and width are 25m and 20m respectively, it is located centerline of downstream of a emission stack having height of 70m. The emission is 0.28 ton/hours and Fluoride content is 0.07 kg/ton. Check if Concentration correction is needed (also calculate it) if the building is located at 0.5 km, and stability class is 'F', wind speed is 2 m/s and emission velocity is 20 m/s.



Flow Pattern: Side View Wind Against Face



Flow Pattern: Top View Wind Against Face

Flow Pattern: Top View Wind Against Edge

Aerodynamic Downwash

In atmospheric wind flow some times some big curvilinear structure (like mountains and aggregate down to up then down building trail of structures) comes in the path, the winds suddenly uplift, due to which low pressure created at the ground so the pollution emissions trap there, this phenomenon known as aerodynamic downwash.

In such situation Gaussian plume model cannot give right concentrations of pollutants.

Complex Terrain

A region having irregular topography, such as mountains or coastlines.

Complex terrain can also include variations in land use, such as urban, rural, irrigated, and unirrigated. Complex terrain often generates local circulations, or modifies ambient synoptic weather features, to create unique local weather characteristics such as katabatic winds, anabatic clouds, and sea breezes. In regions of complex terrain, weather forecast models must have high resolution to reproduce numerically the terrain-induced weather features (*Complex Terrain - Glossary of Meteorology*, n.d.).

- q. Consider that the vehicle emissions from the GT road to be infinite line source and that is causing an air pollution $C_0(x)$ and if an elevated flyover is made at the GT road of height H and the resultant concentration is $C(x)$. Plot the $\ln(C_0/C)$ with respect to x for stability class D.

4 Advection diffusion equations and numerical solutions

4.1 Box model

A box model is a simple way to model air pollution over a city or an area. The model's main assumption is to consider it a complete mixed flow system that suggests pollutant concentration is the same everywhere in the box. Figure 4.1 shows a schematic diagram of the box model. U (Assumed constant) is the prevailing wind speed along the x -direction and Q is the pollutant emission rate per unit area of the city.

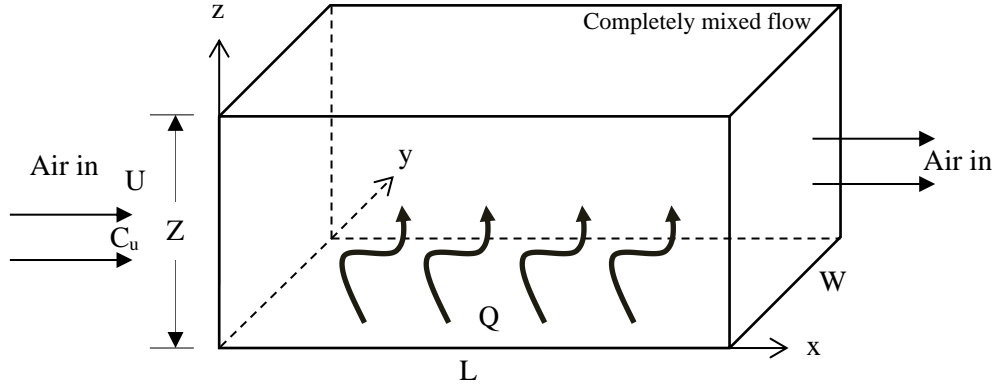


Figure 4.1: Rectangular city showing symbols used in the box model

The equation in the box model is based on the conservation of mass (in units mass/time) principle i.e.

$$\text{Input} - \text{Output} + \text{Generation} - \text{Consumption} = \text{Accumulation}$$

Applying the above principle, the pollutant concentration c inside the box is governed by the following equation

$$LWZ \frac{dC}{dt} = QLW + WZC_uU - WZCU \quad \text{Equation 4.1}$$

where C_u is the concentration in the inflowing air. Dividing by LWZ we get

$$\frac{dC}{dt} = \frac{U}{L} \left[\frac{QL + UZC_u}{UZ} - C \right] \quad \text{Equation 4.2}$$

This equation is of the form

$$\frac{dy}{dx} = a(b - x)$$

and its solution can easily be found as (assuming $C_0 = c$ at $t = 0$)

$$C(t) = \frac{QL + UZC_u}{UZ} \left[1 - \exp\left(-\frac{U}{L}t\right) \right] + C_0 \exp\left(-\frac{U}{L}t\right) \quad \text{Equation 4.3}$$

As t becomes large the concentration approaches the steady state value given by

$$C_u + \frac{QL}{UZ} \quad \text{Equation 4.4}$$

4.2 Addition of other processes

The process of dry and wet deposition can be added to box formula:

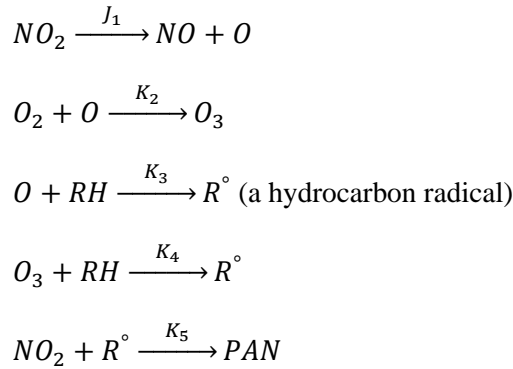
$$LWZ \frac{dC}{dt} = QLW + WZC_u U - WZCU - LWv_d C - LWH\Lambda C \quad \text{Equation 4.5}$$

where v_d represents the dry deposition velocity and Λ denotes the wet deposition coefficient. The solution of (Equation 4.5) is as before

$$C(t) = \frac{QL + UZC_u}{UZ + v_d L + LZ\Lambda} \left[1 - \exp\left(-\frac{UZ + v_d L + LZ\Lambda}{LZ} t\right) \right] + C_0 \exp\left(-\frac{UZ + v_d L + LZ\Lambda}{LZ} t\right) \quad \text{Equation 4.6}$$

4.3 Photochemical reactions

In all the above formulas, we have assumed constant emission generation. But this is no longer valid if generation/loss includes chemical reactions. For simplification, we assume that concentration in the inflowing air is zero and dry/wet deposition processes are absent. The primary pollutants are hydrocarbons (RH) and nitrogen dioxide (NO_2). The sunlight initiates photochemical reactions, which produce ozone (O_3) and peroxyacetyl nitrate (PAN). These compounds are harmful to human health, vegetation, etc. We consider the following simplified reactions



Further, we assume that the concentration of NO_2 , RH and O_2 are constant. Now using the box model, we write the equations for O , R° , and PAN as

$$\frac{d[O]}{dt} = J_1[NO_2] - \left\{ K_2[O_2] + K_3[RH] + \frac{U}{L} \right\} [O] \quad \text{Equation 4.7}$$

$$\frac{d[R^\circ]}{dt} = K_3[RH][O] + K_4[O_3][RH] - \left\{ K_5[NO_2] + \frac{U}{L} \right\} [R^\circ] \quad \text{Equation 4.8}$$

$$\frac{d[O_3]}{dt} = K_2[O_2][O] - \left\{ K_4[RH] + \frac{U}{L} \right\} [O_3] \quad \text{Equation 4.9}$$

$$\frac{d[PAN]}{dt} = K_5[NO_2][R^\circ] - \frac{U}{L} [PAN] \quad \text{Equation 4.10}$$

Thus the solution of the box model is reduced to a study of a set of four coupled ordinary differential equations (ODE). One practical method for the solution of the above system is the fourth-order Runge-Kutta method (Shampine et al., 1996).

4th order Runge–Kutta methods

An initial value problem of following type

$$\frac{dy}{dt} = f(t, y)$$

$$y(t_0) = y_0$$

$$y_{n+1} = y_n + \frac{1}{6}h(k_1 + 2k_2 + 2k_3 + k_4)$$

$$t_{n+1} = t_n + h$$

Here for $n = 0, 1, 2, 3, \dots$

$$k_1 = f(t_n, y_n),$$

$$k_2 = f\left(t_n + \frac{h}{2}, y_n + h\frac{k_1}{2}\right),$$

$$k_3 = f\left(t_n + \frac{h}{2}, y_n + h\frac{k_2}{2}\right),$$

$$k_4 = f(t_n + h, y_n + hk_3).$$

For a step-size $h > 0$ the variable y_{n+1} is 4th order Runge–Kutta approximation of $y(t_{n+1})$ using current value of y_n

k_1 is the increment based on the slope at the beginning of the interval, using y

k_2 is the increment based on the slope at the midpoint of the interval, using y and k_1 .

k_3 is again the increment based on the slope at the midpoint, using y and k_2 .

k_4 is the increment based on the slope at the end of the interval, using y and k_3 .

The meaning of a fourth-order method is that the local truncation error is on the order of $O(h^5)$, while the total accumulated error is order $O(h^4)$.

Example 4.1: The global CO₂ mean level was around 320 ppm in year 1960, it is increasing @0.525% each year and within a year the standard deviation is around 0.9%. Calculate the atmospheric water aerosol pH maximum difference in year 2022.

Ans.

Typical atmospheric water-Carbon dioxide chemistry (shown in) can be written as

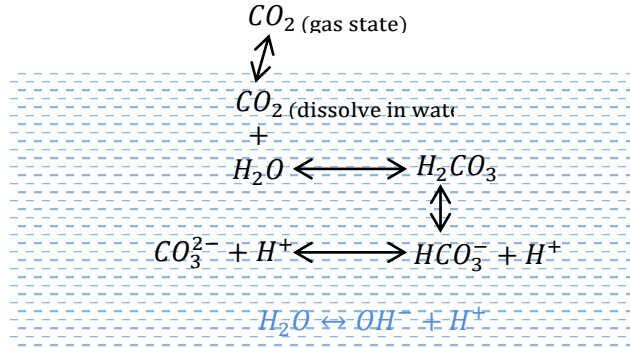


Figure 4.2: Typical atmospheric water-Carbon dioxide chemistry

$$K_w = [H^+][OH^-] \quad \text{Equation 4.11}$$

$$K_1 = 10^6 \frac{[H^+][HCO_3^-]}{K_H p_{CO_2}} \quad \text{Equation 4.12}$$

$$K_2 = \frac{[H^+][CO_3^{2-}]}{HCO_3^-} \quad \text{Equation 4.13}$$

$$C_T = \frac{K_H p_{CO_2}}{10^6} + [HCO_3^-] + [CO_3^{2-}] \quad \text{Equation 4.14}$$

$$0 = [HCO_3^-] + 2[CO_3^{2-}] + [OH^-] - [H^+] \quad \text{Equation 4.15}$$

At $25^\circ C$ consider typical values of $K_w = 10^{-14}$, $K_1 = 10^{-6.3}$, $K_2 = 10^{-10.3}$ and $K_H = 10^{-1.46}$.

Now calculate year 2022 CO_2 mean level = $320 + \frac{320 \cdot 0.525 \cdot 62}{100} = 424.16 \text{ ppm}$, so the *max* to *min* difference is 1.8% of 424.16 = 7.63ppm [420.34, 427.98] ppm

Solving Equation 4.11 to Equation 4.15

We get

$$\frac{K_1 [H^+]}{10^6} K_H p_{CO_2} + 2 \frac{K_1 K_2}{10^6} K_H p_{CO_2} + K_w [H^+] - [H^+]^3 = 0 \quad \text{Equation 4.16}$$

Equation 4.17 is cubic equation (third-order polynomial) and we know that typical *pH* value always within 2 and 12, so we can initiate from these initial guess. Now to get roots of Equation 4.17 one need to use some numerical method. Because we know the value is within 2 and 12 so using bisection method. If absolute error considers 0.001, then total iterations needed to calculate desired result will be = $\log_2(10 / 0.001) \approx 14$ iterations.

We get 32.55% rise in CO_2 level from year 1960 to year 2022, due to which *pH* rise by $\sim 1\%$. The variation in *pH* is calculated $\sim 0.036\%$ from mean.

4.4 Multiple box model

For this case, the conservation model in the i^{th} box is given by

$$LWZ \frac{dC_i}{dt} = Q_i LW + WZC_u U - WZC_i U \quad \text{Equation 4.17}$$

which shows that the concentration in the boxes are coupled with the concentration of the inflowing air in the i^{th} box depends on the upwind box and so on. Analytical solutions can be found in the cases where the processes on the right-hand side of (Equation 4.17) are linear.

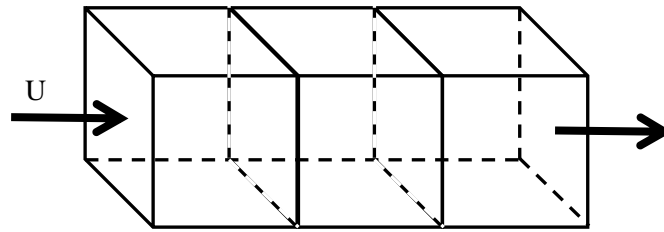


Figure 4.3: Multi box model

4.5 Numerical solution of advection-diffusion equation

The advection-diffusion equation with source term for a pollutant with concentration C is governed by the equation

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(uC) + \frac{\partial}{\partial y}(vC) + \frac{\partial}{\partial z}(wC) = \frac{\partial}{\partial x}\left(\epsilon_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\epsilon_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(\epsilon_z \frac{\partial C}{\partial z}\right) + S(C, t) \quad \text{Equation 4.18}$$

Here u, v, w are wind velocities, $\epsilon_x, \epsilon_y, \epsilon_z$ denote diffusivities and S is the source term. To solve the above advection-diffusion equation operator-splitting technique (MacNamara & Strang, 2016) is used. In this method, the original equation (Equation 4.12) (Equation 4.18) is split into three two-dimensional PDE and a single one-dimensional ODE. The split equations are

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(uC) = \frac{\partial}{\partial x}\left(\epsilon_x \frac{\partial C}{\partial x}\right) \quad \text{Equation 4.19}$$

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial y}(vC) = \frac{\partial}{\partial y}\left(\epsilon_y \frac{\partial C}{\partial y}\right) \quad \text{Equation 4.20}$$

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial z}(wC) = \frac{\partial}{\partial y} \left(\varepsilon_z \frac{\partial C}{\partial z} \right) \quad \text{Equation 4.21}$$

$$\frac{\partial C}{\partial t} = S(C, t) \quad \text{Equation 4.22}$$

The solution from (Equation 4.19) is used as input to the equation (Equation 4.20) and so on. The solution order of the equation may be reversed to improve the accuracy of the solution. Thus if the equations are solved in the order (Equation 4.19) to (Equation 4.22) during one-time interval, then they are solved in the order (Equation 4.22) to (Equation 4.19) during the next time interval. Due to operator-splitting, the advection-diffusion equation's solution reduces to the unidirectional advection-diffusion equation.

4.6 Finite difference approximation

The equation considered is

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(uC) = \frac{\partial}{\partial x} \left(\varepsilon_x \frac{\partial C}{\partial x} \right) \quad \text{Equation 4.23}$$

and the values are to be calculated at the grid points $1, 2, \dots, N$ (see figure 7.4).

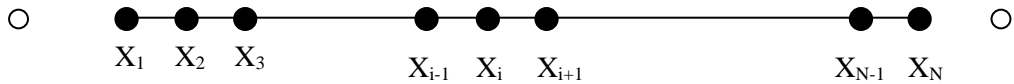


Figure 4.4: Grid in the x-direction

For simplicity we considered uniform grid spacing $\Delta x = x_{i+1} - x_i$ for $i = 1, 2, \dots, N - 1$. Let C^n denotes C evaluated at time $t^n = n\Delta t$.

Forward Euler scheme

We discretize (Equation 4.23) as

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \frac{(uC^n)_{i+1} - (uC^n)_{i-1}}{2\Delta x} + \varepsilon_x \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{\Delta x^2} \quad \text{Equation 4.24}$$

This scheme is called Forward Time Centered Space (FTCS), which is first-order in time and second-order in space. For all values of u this scheme is unconditionally stable for $\varepsilon_x = 0$ and for large value of ε_x and condition all stable for small values of ε_x . The solution at the boundaries i.e. at x_1 and x_n depends on the values beyond the domain which must be approximated.

Implicit scheme

In this case (Equation 4.24) is written as

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = -\frac{(uC^{n+1})_{i+1} - (uC^{n+1})_{i-1}}{2\Delta x} + \varepsilon_x \frac{C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}}{\Delta x^2} \quad \text{Equation 4.25}$$

where all the terms on the RHS are evaluated at $t = t^{n+1}$. The solution to (Equation 4.25) along $i = 1, 2, \dots, N$ is obtained by rearranging the equation as

$$A_i C_{i-1}^{n+1} + B_i C_i^{n+1} + D_i C_{i+1}^{n+1} = C_i^n \quad \text{Equation 4.26}$$

Where

$$A_i = -\Delta t \left(\frac{u}{2\Delta x} + \frac{\varepsilon_x}{\Delta x^2} \right)_{i-1}, B_i = 1 + \Delta t \left(\frac{2\varepsilon_x}{\Delta x^2} \right)_i, D_i = \Delta t \left(\frac{u}{2\Delta x} - \frac{\varepsilon_x}{\Delta x^2} \right)_{i+1}$$

These can be put in the tridiagonal matrix form as follows

$$\begin{bmatrix} B_1 & D_1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ A_2 & B_2 & D_2 & 0 & \cdots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdots & A_{N-1} & B_{N-1} & C_{N-1} \\ 0 & 0 & 0 & 0 & \cdots & 0 & A_N & B_N \end{bmatrix} \begin{bmatrix} C_1^{n+1} \\ C_2^{n+1} \\ \cdot \\ \cdot \\ \cdot \\ C_{N-1}^{n+1} \\ C_N^{n+1} \end{bmatrix} = \begin{bmatrix} C_1^n \\ C_2^n \\ \cdot \\ \cdot \\ \cdot \\ C_{N-1}^n \\ C_N^n \end{bmatrix} - \begin{bmatrix} A_1 C_0^{n+1} \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ D_N C_{N+1}^{n+1} \end{bmatrix}$$

where $A_1 C_0^{n+1}$ and $D_N C_{N+1}^{n+1}$ are outside values and assumed to be known in advance. The above tridiagonal system is solved by matrix decomposition and back substitution.

4.7 Air Quality Model evaluation

The performance of air quality must be checked before the model is proven adequate. The underlying idea to check the model adequacy is to compare the model predicted concentrations with observed concentrations in a statistical sense. The common methods used for model adequacy are briefly described here (see Table 4.1 for mathematical formulation). The large set always provides a better assessment of model performance.

(i) Fractional Bias (FB)

FB is a nonlinear operator that varies between -2 and +2 and has an ideal value of 0 for best model performance (Abdul-Wahab, 2004). A negative FB value indicates that a model over-predicts, and a positive value suggests under-predicts. FB value between -0.5 to +0.5 is considered acceptable (Chang & Hanna, 2004).

(ii) Normalized Mean Square Error (NMSE)

NMSE is an unbiased dimensionless statistic, and it measures the mean of squared error normalized with respect to the product of mean observed and predicted values (Kumar et al., 1999). A value of zero for NMSE is equivalent to a perfect modelling fit. Smaller values of NMSE indicate better model performance, and $NMSE \leq 0.5$ suggests reliability of model (Kumar et al., 1993).

(iv) Index of agreement (d)

The agreement (d) index measures the relative error in model estimates. It is a dimensionless number ranging from 0.0 to 1.0, where 0.0 describes complete disagreement between modelled and observed values and 1.0 indicates a perfect fit (Willmott, 1981).

(iii) Coefficient of correlation (r)

The coefficient of correlation measures the degree to which the magnitude of predictions increases linearly with the magnitude of the observations. The coefficient, however, is insensitive to the extent of the increase. If the predictions increase linearly at only 1/10 the rate of the observations, the correlation coefficient will still be one. The statistical significance of r can be examined by t-statistics (Brown & Beck, 1994).

Table 4.1: Statistical parameters for model evaluation

Parameter	Formula
FB	$FB = 2 * \frac{(\bar{C}_o - \bar{C}_p)}{(\bar{C}_o + \bar{C}_p)}$
NMSE	$NMSE = \frac{(\bar{C}_o - \bar{C}_p)^2}{\bar{C}_o * \bar{C}_p}$
r	$r = \frac{(\bar{C}_o - \bar{C}_o)(\bar{C}_p - \bar{C}_p)}{\sigma_{C_p} * \sigma_{C_o}}$
d	$d = 1 - \frac{\sum(C_o - C_p)^2}{\sum(C_p - \bar{C}_o + C_o - \bar{C}_o)^2}$

Where: C_p is the model predicted concentration; C_o is the observed concentration and σ is the standard deviation

Besides the above model evaluation tests, it is advisable to have the random plot of the observed and predicted data and visually examine the linear fit (Sivacoumar et al., 2001).

Q. A city has the following characteristics: $W=5$ km, $L = 10$ km, u (wind speed) = 2.5 m/s, H (mixing height) = 1000 m. the upwind, or background, concentration of nitrous oxide is $b = 10 \mu\text{g}/\text{m}^3$. The emission rate per unit area is $q = 4 \times 10^{-6} \text{ g}/\text{s} \cdot \text{m}^2$. What is the concentration of nitrous oxide over the city?

Q. In the potroom of aluminum plant, the workers complain about the high pollution level of fluoride. Your task is to design the ventilation system so that pollution level inside the potroom is within the acceptable level. You can consider the potroom to be completely mixed reactor at steady state condition. Other information: Volume of potroom = $V \text{ m}^3$, acceptable concentration (in the potroom) = $C_s \text{ mg}/\text{m}^3$, emission rate in the potroom = $E_0 \text{ g}/\text{sec}$. The outside potroom air is also polluted to the extent $C_0 \text{ mg}/\text{m}^3$. Derive an expression for required exhaust rate so that concentration is below acceptable level.

Using the derived expression, determine the Q (exhaust rate), if $C_s = 0.5 \text{ mg}/\text{m}^3$, $C_0 = 0.005 \text{ mg}/\text{m}^3$, $V = 1000 \text{ m}^3$ and emission rate, $E_0 = 5 \text{ g}/\text{sec}$.

5 Air Pollution Risk Assessment and Characterization

Risk is the probability that the presence of a substance or situation will produce harm under some specific conditions. The substance or situation that produces harm is known as a 'hazard.' The probability estimated from the likelihood of

occurrence/severity of hazard is indicative of the risk that a situation or substance poses. (Kaplan & Garrick, 1981) defines the risk as

$$R_i = \langle S_i, P_i, C_i \rangle \tag{Equation 5.1}$$

In Equation 5.1 where S_i is the scenario i (set of happening/conditions), P_i the probability of scenario i , and C_i the consequence (impact) of scenario i . It is safe to say that there is nothing like zero risk for a given situation.

Long-term exposure to pollutants impose life-threatening situation. This threat has probabilistic nature and can be modelled based on dose or exposure to pollutant and consequent body response referred to as Dose-Response analysis of the pollutant. The end result of such investigation comes as probabilities known as risk. The process is known as risk assessment, and the application of risk assessment is to apply this understanding for planning and managing air quality and taking control actions.

The basic framework of any air pollution health risk assessment is (a) exposure/dose assessment, (b) dose-response toxicity relationship, and (c) risk characterization. Apparent from the diversity of components, this basic framework is inherently interdisciplinary. The first part of the framework, exposure/dose assessment, is generally addressed by air pollution control engineers and scientists who specialize in air quality monitoring and modeling. The overall framework of the **air pollutant exposure/dose** assessment is illustrated in Figure 5.1.

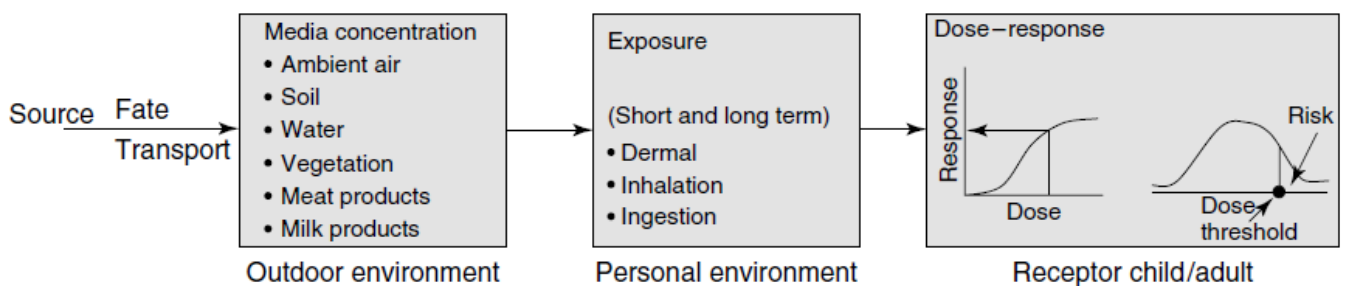


Figure 5.1: Conceptual framework for Source, Concentration, Exposure, Dose-response and Risk Assessment

Emission Source Characterization

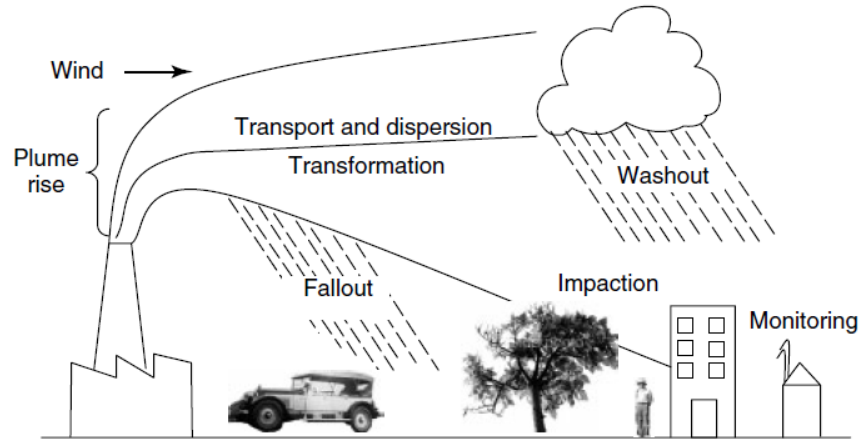
Source characterization begins with hazard identification in terms of releasing a chemical and/or multiple chemicals. The source includes industry, vehicles, households and nonpoint sources. Source emission monitoring or estimation represents comprehensive source characterization, including the location, contaminant release quantity, and emission frequency (e.g., continuous or intermittent). The **chapter ...** on emission inventory explains how to quantify the emissions from different source types.

Fate and Transport of Air Pollutants

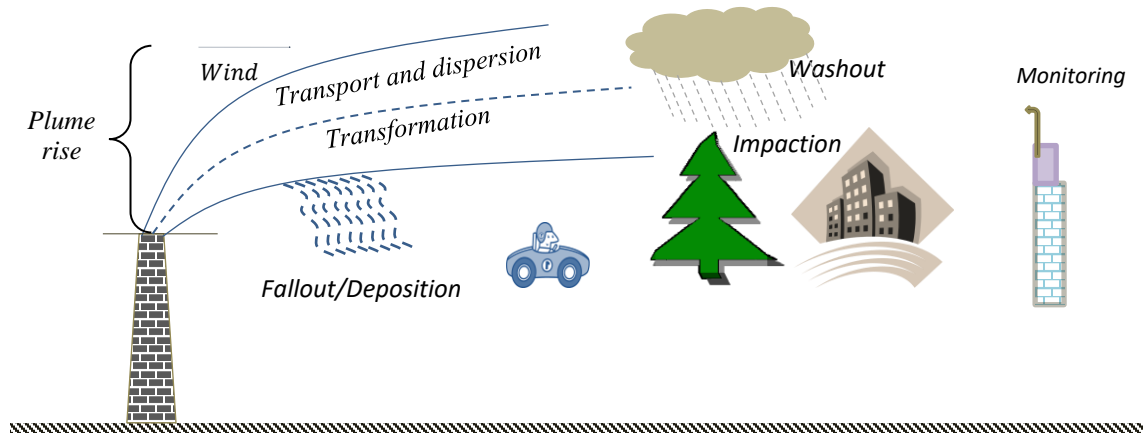
Once the source characteristics are established, fate and transport of contaminants through monitoring and/or mathematical modeling is essential to estimate the receptor's exposure and/or dose experienced by the receptor. The modeling of contaminants describes the pathways, phase transformation, and chemical

transformation. Most of the models are based on simple concepts of mass conservation. Figure 2, in a simplistic way, presents the air quality model concept to develop a linkage between emission and air quality impact. The aspect of modelling has been discussed in the chapter Atmospheric Dispersion and Air Pollutant Concentration Models. As apparent from Figure 2, the exposure concentrations of a contaminant depend on several factors, including:

- Dispersion by atmospheric advection and diffusion;
- Reduced by deposition, transfer to other media, and transformation reactions; and,
- Meteorological parameters
 - Wind parameters (direction, speed, and turbulence)
 - Thermal properties (stability).



Source	Transport	Receptor
Emissions time and duration	Wind speed and direction turbulence	Humans plants buildings
Characteristics height volume flow temperature	Physical and chemical transformations	Monitoring



Source:	Transport:	Receptor:
- Emission time and duration	- Wind speed and direction	- Humans, plants, buildings
- Characteristic height volume flow temperature	- turbulence	- Monitoring
	- Physical and chemical transformations	

Figure 5.2: Transport and transformation of air contaminants (after (Bouhel et al., 1994))

5.1 Air Concentration and Exposure and Human health

5.1.1 Dose response

Quantitative representation of risk starts with dose estimation and its adverse response/effect on receptors, especially in humans. The Dose-response analysis is the fundamental need of toxicology. Here 'Dose' is the quantification of air pollutants of interest and, 'Response' is the evidence of effect for that quantity. The dose is generally estimated as mg of pollutant per unit body weigh in kg per day or mg/kg-d. A typical relation between 'Dose' and 'Response'

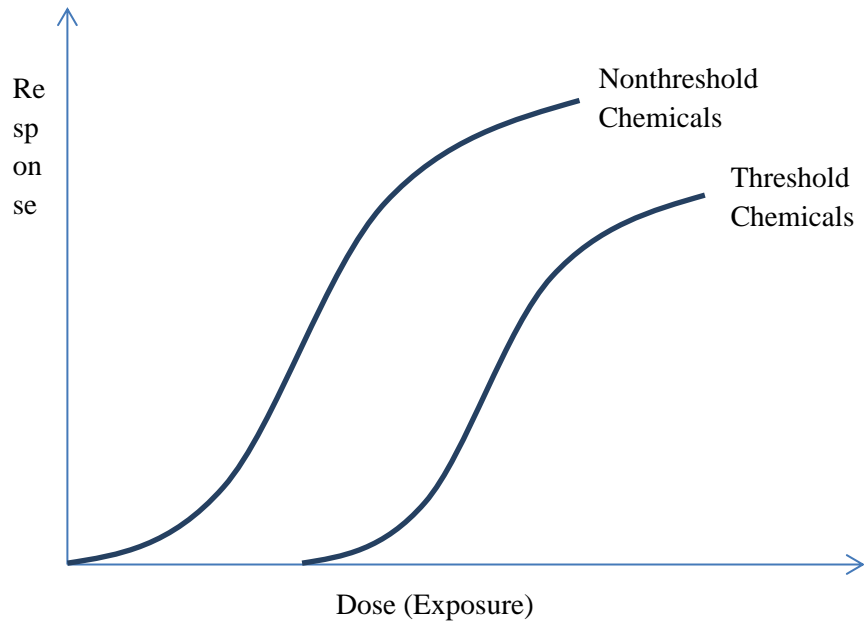


Figure 5.3: Typical Dose-response relationship

Dose-response curves can be seen in two general categories/groups (Figure 5.3). One in which no response is observed until some minimum (i.e., threshold) dose is exceeded, and second which has no threshold suggesting that response is expected at dose, no matter how small. A minimal dose causes no observable effects for some pollutants, whereas a higher dose will show toxicity (Figure 5.3). For other chemicals, such as most carcinogens, the threshold concept may not be applicable, in which case no minimum level is required to induce adverse health effects (Figure 5.3).

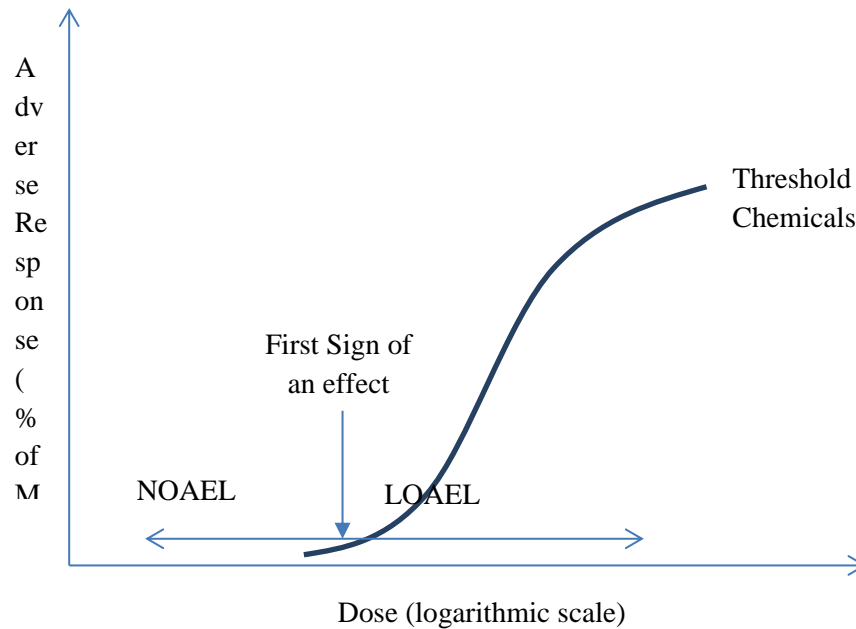


Figure 5.4: Illustrative relationship between 'toxicological endpoints' for a typical dose-response curve for 'threshold chemicals'

The most important part of the dose-response curve with a threshold chemical is the dose at which significant effects begin to occur (Figure 5.4). The highest dose which does not produce an observable adverse effect is the 'no-observed-adverse-effect level' (*NOAEL*), and the lowest dose that has an observable adverse effect is the 'lowest-observed-adverse-effect level' (*LOAEL*). For non-threshold chemicals, the dose-response curve behaves differently because no dose is free of risk.

Important parameters/factors to consider in toxicity assessments for air pollutants include

- Route of exposure. The toxicity of some chemicals depends on whether the route of exposure is by inhalation or dermal contact. Also, there may be local responses at the absorption site (i.e., lungs, skin, absorption/transfer in the blood stream).
- Frequency and duration of exposure. The toxicity of many chemicals depends not only on dose (i.e., the amount of chemical contacted or absorbed each day) but also on the length of exposure (i.e., number of days, weeks, or years).
- Toxicological endpoints represent the changes detected in test animals, which become an index of the chemical's toxicity. Some commonly measured endpoints are carcinogenicity, hepatotoxicity (i.e., liver toxicity), mutagenicity, neurotoxicity, renal toxicity, reproductive toxicity, teratogenicity, etc.

5.1.2 Dose- Response Assessment

Dose-response assessment is the process of quantitatively evaluating toxicity information and characterizing the relationship between the dose of the contaminant administered or received (i.e., exposure to an agent) and the incidence of adverse health effects in the exposed populations. The process consists of estimating the potency of the specific compounds by the use of dose-response relationships. For example, in the case of carcinogens, this involves estimating

the probability that an individual exposed to a given amount of chemical will contract cancer due to that exposure; potency estimates may be provided as 'unit risk factor' (expressed in mg/m^3 or ppb) or as 'potency slopes' (in units of $[mg/kg - day]^{-1}$). Data are generally derived from animal studies or, less frequently, from studies in exposed populations.

The dose-response assessment first addresses the dose relationship to the degree of response observed in an experiment or human study. When environmental exposures are outside the range of observations, extrapolations are necessary to estimate or characterize the dose relationship. The extrapolations will typically be made from: high to low doses, animal to human responses. For chemicals showing threshold concentration, the information on *NOAEL* and *LOAEL* is useful. The common dose-response quantification method for cancer is the linearized multistage model described later.

Physiologically-based pharmacokinetic (PBPK) models are used for environmental risk assessment. These models describe the uptake and accumulation of chemical substances and establish the relationships among critical biological processes for predicting the chemical's absorption, distribution, metabolism, and excretion in humans and animal species (Sharma & Reddy, 2012) Most PBPK models are multi-compartment (organs or tissues) for which the interconnections correspond to blood or lymph flow. For example, (Sharma & Reddy, 2012) have described the PBPK model for uptake, accumulation disposition of lead in organs and blood-stream.

10.3.3 Chronic versus Subchronic Exposures

Chronic daily intake (*CDI*) measures long-term (chronic) exposures from the number of events that are assumed to occur within an assumed lifetime for potential receptors. Subchronic daily intake (*SDI*), which represents projected receptor exposures over a short-term period, considers only a portion of a lifetime (USEPA, 1989 b). These air pollution risks are calculated by multiplying the average pollutant concentrations by the appropriate receptor exposure and body weight factors.

The *CDI* is calculated as per the following formulation

$$CDI = \frac{(CA \times IR \times f \times ABS_f \times ET \times EF \times ED)}{(BW \times AT)} \quad (3.2)$$

Where *CA*: Chemical/pollutant concentration in air (mg/m^3)

IR: Inhalation rate (m^3/h)

f is Fraction of intake from contaminated source/area (dimensionless)

ABS_f is Bioavailability or absorption factor (%)

EF is Exposure frequency (days/year)

ED is Exposure duration (years)

BW is Body weight, i.e., the average body weight over the exposure period (kg)

AT is Averaging time (period over which exposure is averaged - days)

= $ED \times 365 \text{ days/year}$, for noncarcinogenic effects of human exposure

= $LT \times 365 \text{ days/year} = 70 \text{ years} \times 365 \text{ days/year}$, for carcinogenic effects of human exposure (assuming an average lifetime, *LT*, of 70 years)

One should be careful with the units in the above formulation.

The major difference between *CDI* and *SDI* is the averaging time or *AT*; the exposure duration becomes lifetime in *CDI*, and it is the actual exposure duration in *SDI*.

SDIs are generally used to evaluate subchronic noncarcinogenic effects. The *CDIs* assess both carcinogenic risks and chronic noncarcinogenic effects. Short-term exposures can result when, for instance, a particular activity is performed for a limited number of years or when a chemical with a short half-life degrades to negligible concentrations within several months.

The levels or variables in the above equation for Children aged up to 6, Children aged 6-12 and Adult is given in Table 5.1.

Table 5.1: An example listing of case-specific exposure parameters (Asante-Duah, 1998)

Parameter	Children aged up to 6	Children aged 6-12	Adult	Reference sources
<i>Physical characteristics</i>				
Average body weight (kg)	16	29	70	(a,b,c)
Average lifetime (yrs)			70	(a,b,c,d)
Average lifetime exposure period (yrs)	5	6	58	(b,d)
<i>Activity characteristics</i>				
Inhalation rate (m ³ /h)	0.25	0.46	0.83	(b,d)
Retention rate of inhaled air (%)	100	100	100	(d)
Frequency of fugitive dust inhalation (365 days/yr)				
Off-site residents, schools and passers-by	365	365	365	(b,d)
Off-site workers	-	-	260	(b,d)
Duration of fugitive dust inhalation (outside) (h/day)				
Off-site residents,	12	12	12	(b,e)

schools and passers-by				
Off-site workers	-	-	8	(b,e)
<p>Note: The exposure factors represented here are for potential maximum exposures (for conservative estimates), and could be modified as appropriate to reflect the most reasonable exposure patterns anticipated. For instance, soil exposure will be reduced by snow cover and rainy days, thus reducing potential exposures for children playing in contaminated areas.</p> <p>(a) (USEPA, 1989 d); (b) (USEPA, 1989 a); (c) (USEPA, 1988); (d) Estimate based on site-specific conditions</p>				

The risk of exposure can be assessed through hazard index (*HI*) (Asante-Duah, 1998) and cancer risk. Specifically, the *HI* has been estimated for permanent staff (*PS*) who works in laboratory for 35 years.

3.1.1 Reference dose and reference concentration

The reference dose, *RfD* is a dose derived from the *NOAEL* or *LOAEL* by accounting for uncertainty factors (*UFs*) or safety factor. (Asante-Duah, 1998) suggests a modifying factor *MF* based on professional judgment.

RfDs are calculated by dividing a *NOAEL* or a *LOAEL* which are derived from human or animal toxicity studies, by one or more uncertainty and modifying factors.

$$RfD = \frac{NOAEL \text{ or } LOAEL}{(\prod_{i=1}^n UF_i \times MF)} \quad \text{Equation 5.2}$$

The UF_i present various uncertainty factors such as (i) vulnerability or immunity among the human beings (taken as 10 H) (ii) to account for toxicity is extrapolated from animal studies (taken as 10 A) and (iii) *NOAEL* is developed from subchronic studies like short animal studies with accelerated doses (taken as 10 S). In addition, there is a subjective adjustment modifying factor ($MF \leq 1$); default value is 1.

Example: A study made on 250 rats at an concentration of an air pollutant yielded a *NOAEL* dosage of 3.5 mg/kg-day. Take *MF* as 0.55. Find the *RfD* and *RfC* for an adult having an inhalation rate of 15 m³/d and the bodyweight of 70 kg.

$$UF = 10H \times 10A \times 10S = 1000 \quad \text{Equation 5.3}$$

$$MF = 0.55 \quad \text{Equation 5.4}$$

These factors then give $UF \times MF = 550$, so that

$$RfD = \frac{NOAEL}{(UF \times MF)} = \frac{3.5}{550} = 0.00636 \text{ (mg/kg-day)} \quad \text{Equation 5.5}$$

Now if *LOAEL* was used in place of *NOAEL* an additional *UF* of 10 would be advisable.

$$\begin{aligned}
 RfC &= RfD \text{ (mg/kg-d)} \times 1 / (\text{Inhalation rate (m}^3\text{/d)}) \times BW \text{ (kg)} \\
 &= 0.00636 \times (1/15) \times 70 \\
 &= 0.02968 \text{ mg/m}^3 \text{ or } 30 \text{ } \mu\text{g/m}^3
 \end{aligned}$$

We will use the concept of *RfD* and *RfC* later for assessment of risk.

13.3.2 Toxicity Parameters for Carcinogenic Effects

The slope factor (*SF*) represents the slope of the dose-response function in dose-related units (viz. [mg/kg-day]⁻¹), while the unit risk factor (*URF*) expresses the slope in concentration-based units (viz. [μg/m³]⁻¹); see above example to convert [mg/kg-day] into [mg/kg-day]⁻¹. Typically, *SFs* are used when evaluating risks from oral or dermal exposures, while *URFs* are used in evaluating risks from inhalation exposures as in the case of air pollution.

The *SF*, also called cancer potency factor or potency slope, measures cancer risk per unit of dose (i.e., risk per mg/kg-day) for a chemical/pollutant. The *SF* is the upper-bound estimate of the probability of a response per unit intake of a chemical over a lifetime. It is used in risk assessments to estimate an upper-bound lifetime probability of an individual developing cancer due to exposure to a particular level of potential carcinogen.

The USEPA (US EPA, 2014) follows the multistage model with a shape at low doses described by a polynomial function. To determine the additional risk above the background rate at dose, *d* the model takes the form:

$$P(d) = 1 - \exp [-(q_1d + q_2d^2 + \dots + q_kd^k)] \quad \text{Equation 5.6}$$

The one-hit model is achieved by ignoring higher terms in the above model

$$P(d) = 1 - \exp [-(q_1d)]$$

At low doses, the additional risk is approximated by:

$$P(d) = q_1d \quad \text{Equation 5.7}$$

In the above model slope *q*₁ of this line (formerly called the potency) is called the slope factor (described above) and generally represented as *SF*. The cancer probability can be stated as

$$P(d) = SF \times [DOSE] \quad \text{Equation 5.8}$$

Thus, the inhalation potency can be converted to an inhalation URF by applying the following conversion factor (assuming body weight 70 kg and inhalation rate $20 \text{ m}^3/\text{day}$ for an adult:

$$[(kg - day)/mg] \times [1/70 \text{ kg}] \times [20 \text{ m}^3/\text{day}] \times [1 \text{ mg}/1000 \mu\text{g}] = 2.86 \times 10^{-4} \quad \text{Equation 5.9}$$

Thus, the lifetime excess cancer risk from inhaling $1 \mu\text{g}/\text{m}^3$ concentration for a full life is:

$$URF_i(\mu\text{g}/\text{m}^3)^{-1} = (2.86 \times 10^{-4}) \times SF_i \quad \text{Equation 5.10}$$

Conversely, the SF_i can be derived from the URF_i as follows:

$$SF_i = (3.5 \times 10^3) \times URF_i \quad \text{Equation 5.11}$$

In the above conversions, The assumptions are 70-kg bodyweight, and an average inhalation rate of $20 \text{ m}^3/\text{day}$.

In reality, and for all practical purposes, the linear low-dose cancer risk model is valid only at low-risk levels (i.e., estimated risks <0.01). For situations where chemical intakes may be high (i.e., potential risks >0.01), the one-hit model represents the more appropriate algorithm to use.

As a rule-of-thumb, incremental risks of between 10^{-5} and lower are generally perceived as acceptable for the protection of humans the most common acceptable risk is 10^{-6} (implying one cancer per one million persons) or lower.

Example: A regulatory agency wants to propose the annual air quality standard for Ni with an acceptable risk of 10^{-6} . If the inhalation slope factor of risk is $0.955 \text{ (mg/kg-d)}^{-1}$, what should be the air quality standard for Ni.

$$\begin{aligned} \text{Acceptable dose} &= \text{Acceptable risk}/(\text{SF}) \\ &= 1 \times 10^{-6} \times 10^6 / (0.955) \text{ ng/kg-d} \\ &= 1.047 \text{ ng/kg-d} \\ \text{Proposed air quality standard} &= 1.047 \text{ (ng/kg-d)} \times 70 \text{ (kg)} / (20 \text{ (m}^3/\text{d)}) \\ &= 3.6645 \text{ ng/m}^3. \end{aligned}$$

13.4.4 Estimation of Noncarcinogenic Hazards to Human Health

The potential noncancer health effects of contaminants associated with air pollution are usually expressed as the hazard quotient (HQ) and/or the hazard index (HI). The HI is defined by the ratio of the estimated exposure level to the route-specific reference dose (RfD , represented as follows (USEPA, 1989 d):

$$HI = \frac{E}{RfD} \quad \text{Equation 5.12}$$

where E is the chemical exposure level or intake (mg/kg-day) and RfD is the reference dose (mg/kg-day).

For multiple air pollutant exposures to non- carcinogens and noncarcinogenic chronic effects, pollutants are grouped.

The total chronic hazard index (HI) for i pollutants can be calculated as

$$HI = \sum_{i=1}^n \frac{CDI_i}{RfD_i}$$

For any pollutants, hazard indices' interpretation may be potential for adverse health effects if the hazard index exceeds unity (1). the interpretation of the results from HI calculations, a reference value of less than or equal to unity (i.e., $HI \leq 1$) should be taken as acceptable (Asante-Duah, 1998).

Q. The 24-hr National Ambient Air Quality Standard of PM2.5 is $60 \mu\text{g}/\text{m}^3$ and the city is exactly compliant with the standard. What is the dose of PM2.5 (in gm/kg-d) to the population if average weight of person is 60 kg and one breathes in 20 m^3 of air per day?

Q. Kids below age 6 years, inhale indoor air @ $0.25 \text{ m}^3/\text{hr}$ for 12 hrs daily. Indoor air has average formaldehyde concentration of $5 \mu\text{g}/\text{m}^3$. Calculate chronic daily intake, and consider body absorb formaldehyde 100%.

Q. Drive relation between URF and SF due to inhalation for kids below/up to 6 year olds.

Q. Formaldehyde URF is $1.5 \times 10^{-5} (\mu\text{g}/\text{m}^3)^{-1}$, calculate cancer risk for SECOND above question.

Q. In THIRD above Question Calculate total risk when there is also 1 ppb Benzene ($SF = 2.9 \times 10^{-2} (\text{mg}/\text{kg} - \text{day})^{-1}$) and $90 \mu\text{g}/\text{m}^3$ PM10 ($F = 1.1 \times 10^{-2} (\text{mg}/\text{kg} - \text{day})^{-1}$) present in air on average.

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