LECTURE 10: AIR QUALITY MODELING

CE 433

Excerpts from Lecture notes of Professor M. Ashraf Ali, BUET.

Air Quality Modeling

- Air quality models use mathematical and numerical techniques to simulate the physical and chemical processes that affect air pollutants as they disperse and react in the atmosphere.
- Purposes
  - Establishing emission control legislation, i.e. determining the maximum allowable emission rates that will meet fixed air quality standards
  - Evaluating proposed emission control techniques and strategies i.e. evaluating the impacts of future control
  - Selecting locations of future sources of pollutants (e.g. industries), in order to minimize their environmental impacts
  - Planning the control of air pollution episodes, ie. Defining immediate intervention strategies.
  - Assessing responsibility for existing air pollution levels, ie, evaluating present source-receptor relationships.

Factors to be considered in modeling

- In air pollution dispersion modeling, 5 major physical processes are simulated:

i) Pollutant advection

ii) Diffusion

iii) Deposition

iv) Chemical reaction (ie, transformation)

v) Emission

Factors to be considered in modeling

- Important process to be simulated depend on transport seales of air pollution phenomena. Transport phenomena can be classified as follows:

i) Near-field phenomena (<1 km from source), e.g. downwash effect of plume caused by building aerodynamics.

ii) Short-range transport (<10 km from source), e.g. area in which maximum ground level impact of primary pollutants is generally felt.

iii) Intermediate range (between 10 and 100 km), e.g. area in which chemical reactions become important.

iv) Long-range (or regional) transport (>100 km) e.g. area in which large-scale meteorological effects and deposition and transformation rates play key roles.

v) Global effect, ie, phenomena affecting entire earth atmosphere such as CO_2 accumulation.

Mathematical Modeling Approaches

- Deterministic Model
  - Based on fundamental mathematical description of atmospheric processes, in which effects (ie, air pollution) are generated by causes (ie, emission).
  - Ex. Diffusion models (e.g. Gaussian Plume model)
- Statistical Model
  - Based upon semi-empirical statistical relationship among available data and measurements.
  - Ex. Forecast of the concentration in the next few hours as a statistical function of : (i) current measurements, and

(ii) Past correlation between there measurements and concentration trends

Types of Air Quality Models

- i) Dispersion/Diffusion Modeling: uses mathematical formulations to characterize atmospheric processes that disperse a pollutant emitted by a source.
- ii) Photochemical Modeling: Long-range air quality models that simulate the changes of pollutant concentrations in the atmosphere due to the chemical and physical processes in the atmosphere.
- Iii) Receptor Modeling: Mathematical or statistical procedure for identifying and quantifying the source of air pollutants at a receptor location.
- Example:- Chemical Mass Balance Method

Diffusion/Dispersion Models

- Behavior of gases and particles in turbulent flow (in the atmosphere) is referred to as atmospheric diffusion.
- Goal of diffusion models is to describe mathematically the spatial and temporal distribution of contaminants released into atmosphere.
- Two idealized source types:
  - i) Instantaneous point source (Puff)
  - ii) Continuous Point Source (Plume)
  - Other source types: Line source, Area source

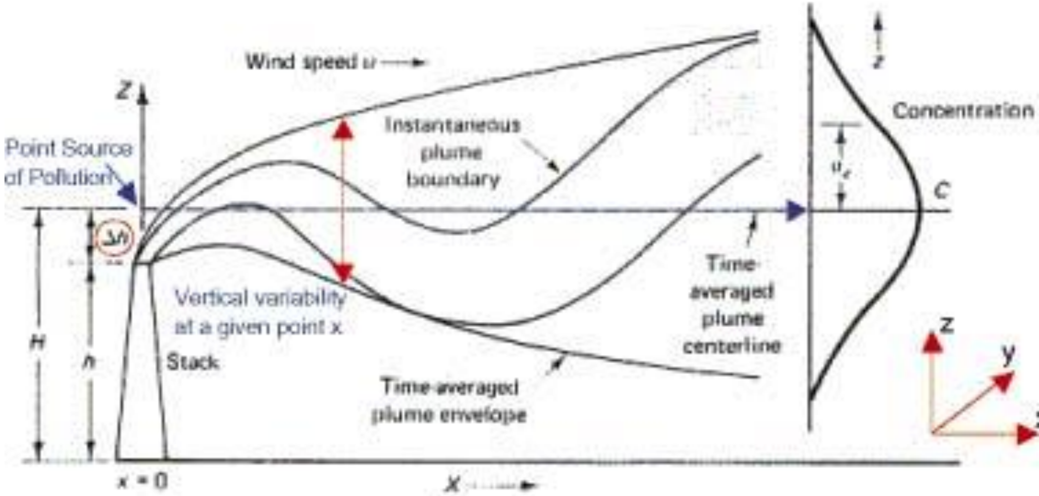
Atmospheric Diffusion Theories

Goal: To be able to describe mathematically the spatial and temporal distribution of contaminants released into the atmosphere

Point Source Gaussian Plume Model

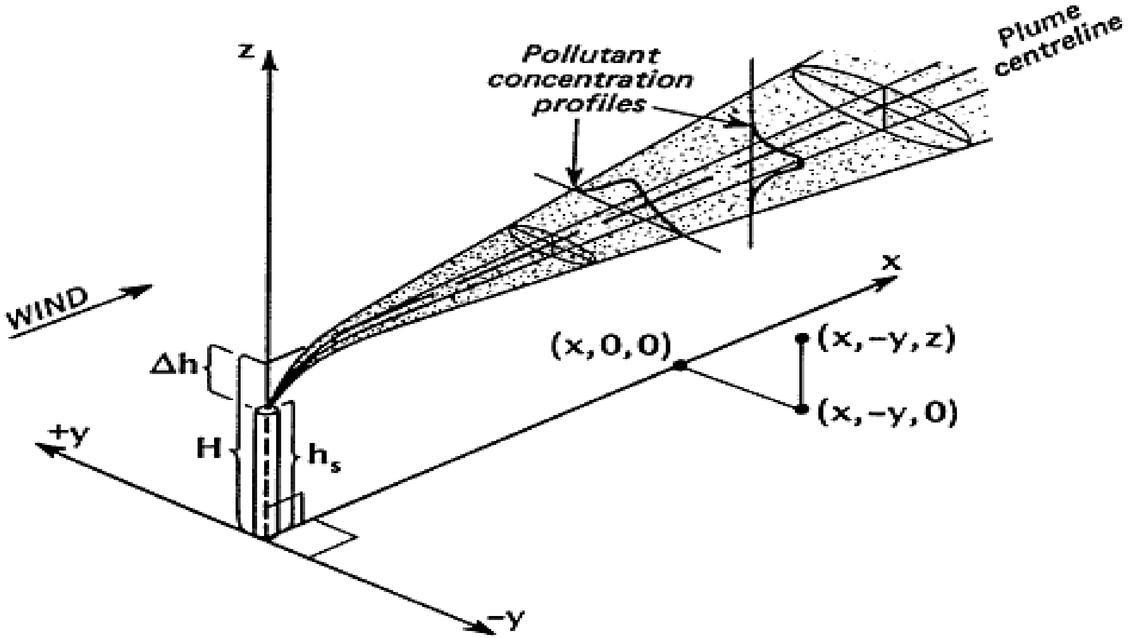
Assumptions:

- Pollutant material takes on Gaussian distribution in both y and z directions
- Steady-state condition
- Ideal gas
- Uniform continuous emission rate
- No diffusion in x-direction
- Homogenous, horizontal wind field. Wind speed constant
- Flat terrain



Gaussian Plume Equations

- The basic Gaussian model applies to a single “point source” (e.g. a smokestack), but it can be modified to account for “line source” (e.g. emission from motor vehicles along a highway) or “area source”.
- (1) Point Source:



Gaussian Plume Equations

- (a) No ground reflection (particles, nitric acid vapor)

$$c\left(x,y,z\right)=\frac{Q}{2\pi\sigma_y\sigma_z u}\exp\left(\frac{-y^2}{2\sigma_y{}^2}\right)\left(\exp\left(\frac{-\left(z-h\right)^2}{2\sigma_z{}^2}\right)\right)$$

- (b) Ground Reflection (CO, SO_2, NO_2)

$$c\left(x,y,z\right)=\frac{Q}{2\pi\sigma_y\sigma_z u}\exp\left(\frac{-y^2}{2\sigma_y{}^2}\right)\left(\exp\left(\frac{-\left(z-h\right)^2}{2\sigma_z{}^2}\right)+\exp\left(\frac{-\left(z+h\right)^2}{2\sigma_z{}^2}\right)\right)$$

Gaussian Plume Equations

- (c) Ground Reflection and Temperature Inversion
- Where,

C = Pollutant concentration (g/m^3, µg/m^3)

Q = Uniform continuous emission rate (g/s, µg/s)

u = mean wind speed at plume height (m/s)

σ_y = cross-wind dispersion parameter (m)

σ_z = vertical dispersion parameter (m)

x, y, z = location of receptor

H = effective stack height , m

(= stack ht + plume rise = $h_s + \Delta h$)

Simplifications of Gaussian Plume Equation under various conditions

- (1) Concentration at ground level (z = 0) (with ground reflection): c (x, y, 0)

$$c = \frac{Q}{\pi u \sigma_y \sigma_z} \exp -0.5\left(\frac{y}{\sigma_y}\right)^2 \left[\exp -0.5\left(\frac{H}{\sigma_z}\right)^2\right]$$

- (2) Concentration at ground level (z = 0) on centerline (y=0) (with ground reflection): c (x, 0, 0)

$$c = \frac{Q}{\pi u \sigma_y \sigma_z} \left[\exp -0.5\left(\frac{H}{\sigma_z}\right)^2\right]$$

- (3) Concentration at ground level (z = 0, y = 0, h = 0)(with ground reflection): c (x, 0, 0), h = 0

$$c = \frac{Q}{\pi u \sigma_y \sigma_z}$$

Determination/Estimation of Different parameters of Gaussian Plume Equation

- (1) Q = emission rate

Usually expressed in g/s

- (2) H = Effective stack height = $h_s + \Delta h$

= stack height + plume rise

Plume rise is caused primarily by buoyancy and momentum of exhaust gas and stability of atmosphere.

Buoyancy results when exhaust gases are hotter than the ambient and/or when the molecular weight of the exhaust is lower than that of air.

Momentum is caused by the mass and velocity of the gases as they leave the stack.

Problem 1: Estimation of Emission Rate

- A power plant consumes 250 tons of coal (containing 1% sulfur) each day. Assuming 10% of this sulfur is emitted as SO_2, estimate the emission rate of SO_2 (in g/sec) from the power plant.

Determination/Estimation of Different parameters of Gaussian Plume Equation

$$\Delta h = \frac{1.6 F^{1/3} x_f^{2/3}}{u}$$

- Difficult to estimate x_f. The following is sometimes used to estimate x_f:

  $x_f = 120\ F^{0.4}$ if $F \geq 55\ \mathrm{m^4/s^3}$

  $x_f = 50\ F^{5/8}$ if $F < 55\ \mathrm{m^4/s^3}$

$$F = g r^2 v_s (1 - \frac{T_a}{T_s})$$

Where, T_a = Ambient temperature

T_s = Exhaust temperature

Problem 2

- A power plant has a 100 m stack with an inside radius of 1m. The exhaust gases leave the stack with an exit velocity of 10 m/s at a temp. of 220°C. Ambient temp is 6°C, winds at the effective stack height are estimated to be 5 m/s, surface wind speed is 3 m/s, and it is a cloudy summer day. Estimate the effective height of this stack.

Determination/Estimation of Different parameters of Gaussian Plume Equation

u = mean wind speed at plume height

$$u = u_0 \left(\frac{z}{z_0}\right)^p$$

Where,

u (z) = wind speed at plume height, z

u_0 = wind speed at instrument ht

z = plume ht (m)

z_0 = instrument ht (m)

p = A factor which depends on stability condition of atmosphere

Table 2. Pasquill-Gifford stability classes

Class	Definition
A	Extremely unstable
B	Moderately unstable
C	Slightly unstable
D	Neutral
E	Slightly stable
F	Moderately stable

Table 3. Guidelines for determining Pasquill-Gifford stability classes

	Day with insolation			Night	
Surface wind speed (ms^{-1})	Strong	Moderate	Slight	Overcast or $\geq 4/8$ low low cloud	$\leq 3/8$ cloud
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

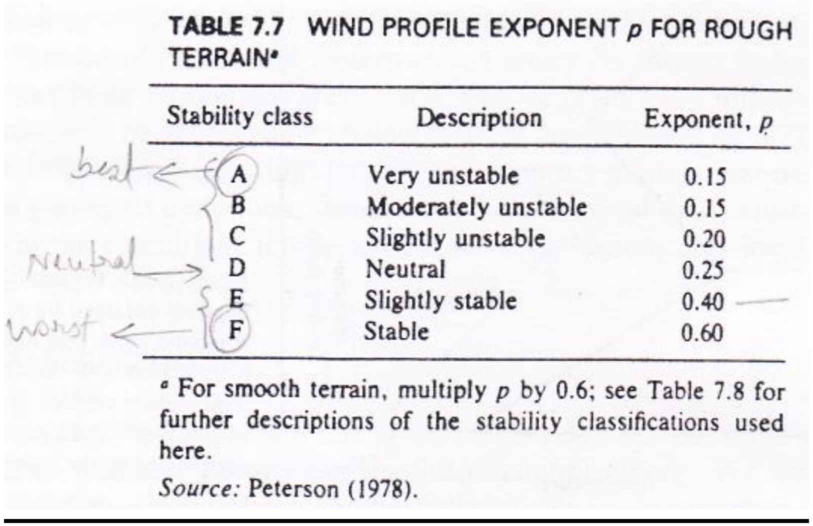


TABLE 7.7 WIND PROFILE EXPONENT *p* FOR ROUGH TERRAIN[a]

Stability class	Description	Exponent, *p*
A	Very unstable	0.15
B	Moderately unstable	0.15
C	Slightly unstable	0.20
D	Neutral	0.25
E	Slightly stable	0.40
F	Stable	0.60

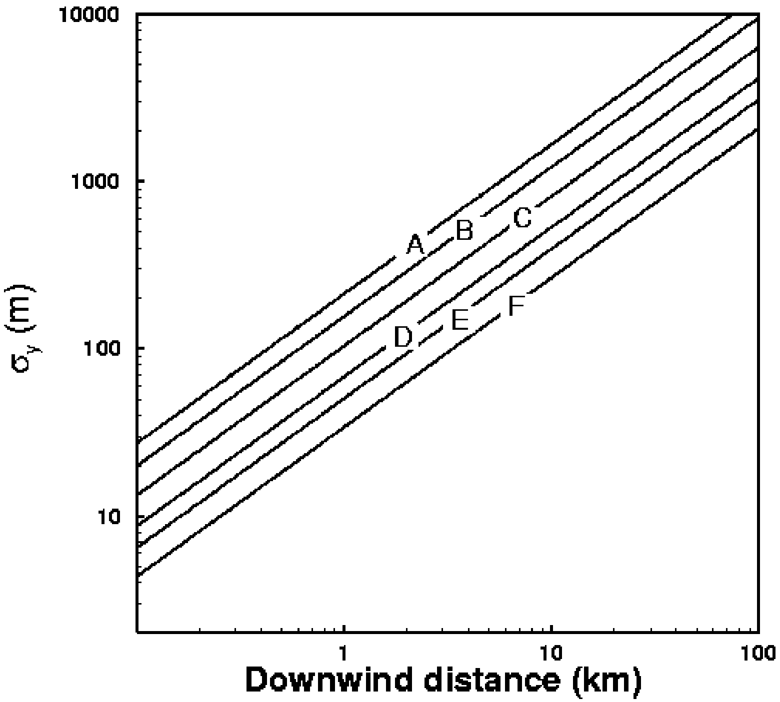
[a] For smooth terrain, multiply *p* by 0.6; see Table 7.8 for further descriptions of the stability classifications used here.

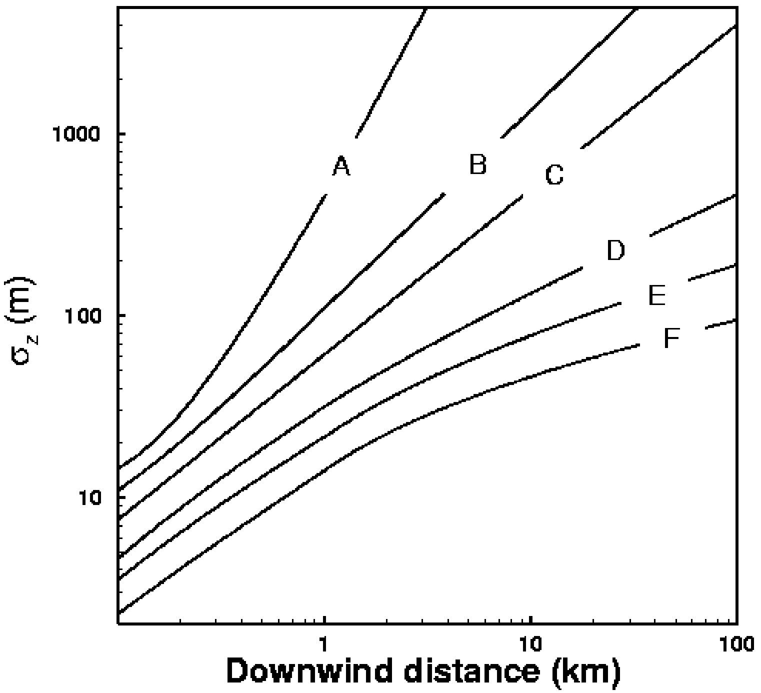
Source: Peterson (1978).

Determination/Estimation of Different Parameters of Gaussian Plume Equation

σ_y , σ_z = f (distance, stability conditions)

These are standard deviations. Can be obtained from plots of σ_y , σ_z versus distance downwind for different stability conditions.
There are number of other approaches for estimating σ_y , σ_z .





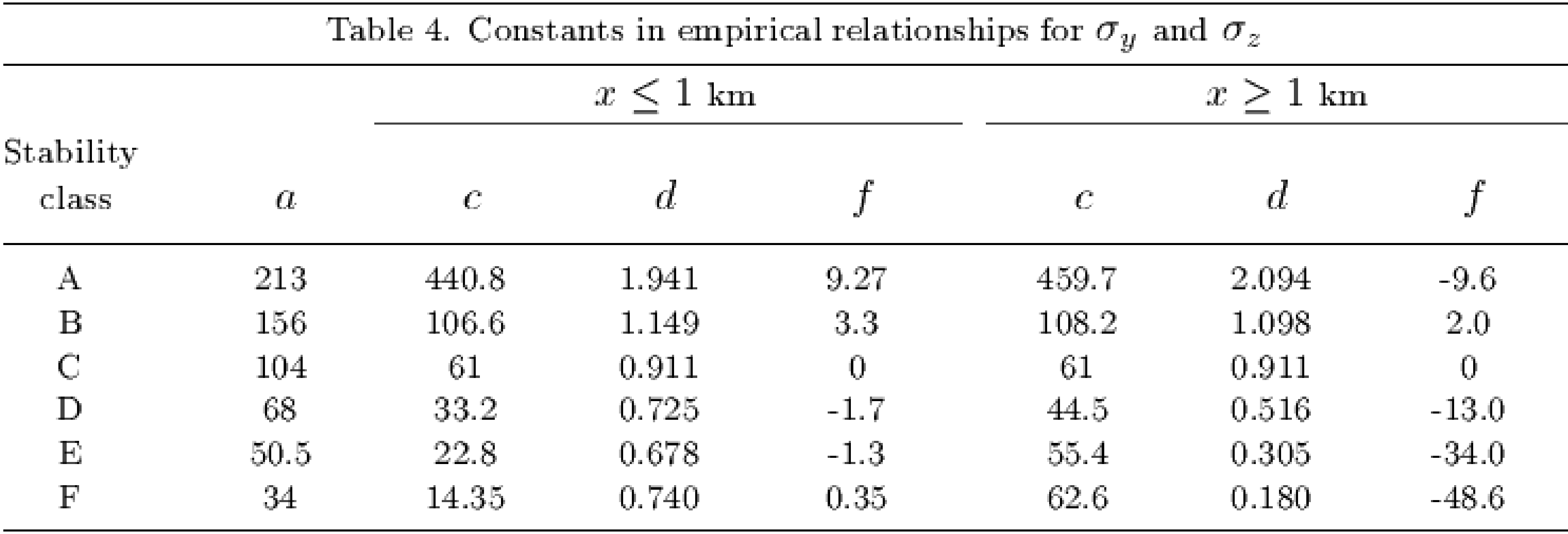


Table 4. Constants in empirical relationships for σ_y and σ_z

Stability class		$x \leq 1$ km			$x \geq 1$ 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	0.911	0	61	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

- $\sigma_y = a.x^{0.894}$
- $\sigma_z = c.x^d + f$

Estimating peak downwind concentration

- Simplest way: use a spreadsheet program to calculate C (x,0,0) as a function of x using,

$$c = \frac{Q}{\pi u \sigma_y \sigma_z}\left[\exp - 0.5\left(\frac{H}{\sigma_z}\right)^2\right]$$

- And find peak downwind concentration
- When a computer is not readily available, peak downwind concentration can be estimated using the chart

$$c_{\max} = \frac{Q}{u}\left(\frac{C_u}{Q}\right)_{\max}$$

- If stability class and H are known, can estimate
  - i) Distance to peak, ii) $(\frac{C_u}{Q})_{\max}$, from chart
  - Then use equation to estimate C_{max}

From stability class and H:
— find Xmax
— (Cu/Q) max.

Then Calculate:
$C_{max} = \frac{Q}{u}\left(\frac{Cu}{Q}\right)_{max}$

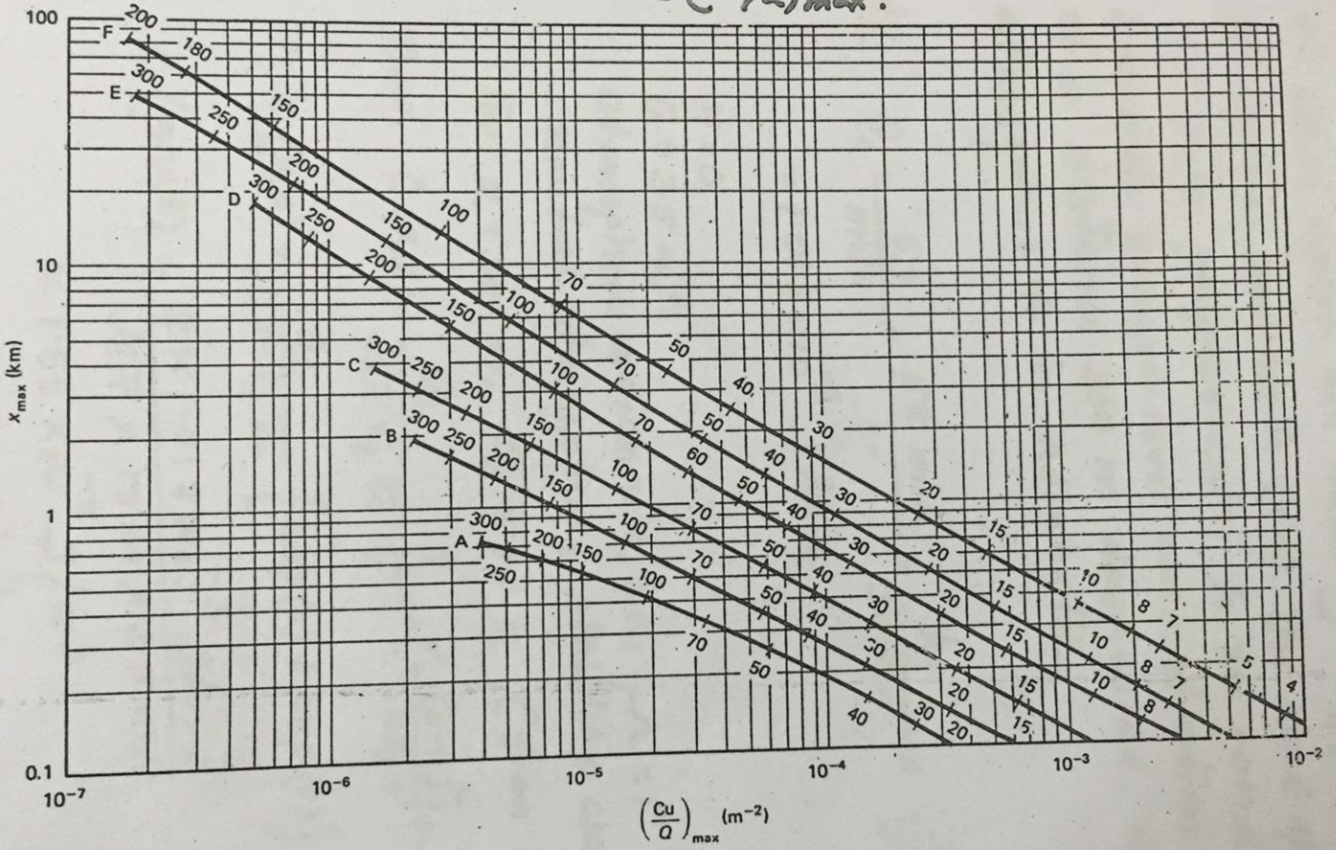


Figure 7.30 To determine the peak downwind plume concentration, enter the graph at the appropriate stability classification and effective stack height (numbers above the lines, in meters) and then move across to find the distance to the peak, and down, to find a parameter from which the peak concentration can be found (Turner, 1970).

Special Considerations

- Building Wakes
- A plume may get sucked into the low-pressure wake behind a building leading to a high level concentration
- The simple rule of thumb for avoiding this problem is to make the stack ht at least 2.5 times the height of the tallest nearby building
- Aerodynamic downwash

Aerodynamic downwash may significantly increase ground level concentration.

It is a major problem for any facility located near a mountain.

Problem 3

- Cars travelling at 55 mph speed at 75 m a part are emitting 5 g/mile of carbon monoxide. The wind speed is 3.5 m/s perpendicular to the road. Estimate ground level concentration of CO at a distance 300 m downwind. Consider atmosphere to be adiabatic.

Line Source (eg, a Road)

- For simplicity, consider: i) infinite length source of ground level, ii) Wind blowing perpendicular to the line
- Examples of Line Source :
  - Motor Vehicles travelling along a straight section of a highway
  - Agricultural burning along the edge of a field
  - A line of industrial sources on the bank of a river

(a) No Ground Reflection

$$C(x, 0,0) = \frac{Q_L}{\sqrt{(2\Pi)}u\sigma_z}\exp\left[-\frac{(z-H)^2}{2\sigma_z{}^2}\right]$$

(b) With Ground Reflection

$$C(x, z) = \frac{Q_L}{\sqrt{(2\Pi)}u\sigma_z}\left\{\exp\left[-\frac{(z-H)^2}{2\sigma_z{}^2}\right] + \exp\left[-\frac{(z+H)^2}{2\sigma_z{}^2}\right]\right\}$$

Where, Q_L = Source emission rate per unit length of road (g/sec-m)

Problem 4

- A stack emitting 80 g/s of NO has an effective stack height of 100 m. The wind speed is 4 m/s at 10 m, and it is a clear summer day with the sun nearly overhead. Estimate the ground level NO concentration:
  - (a) directly downwind at a distance of 2 km
  - (b) at a point downwind where NO is maximum
  - (c) at a point located 2 km downwind and 0.1 km off the downwind axis

Problem 5

- A 1000-MW coal fired power plant emits SO_2 at the rate of 6.47 X10^8 µg/s. If the atmosphere is slightly unstable and wind speed at the stack ht (=300m) is 4.9 m/s, estimate the peak downwind concentration and the distance to peak downwind concentration.

Problem 5

- Suppose a highway has 10 vehicles per second passing a given spot, each emitting 3.4 g/mile of CO. If the wind is perpendicular to the highway and blowing at 5 mph (2.2 m/s) on a heavy overcast day, estimate the ground level CO concentration 200 m from the highway.