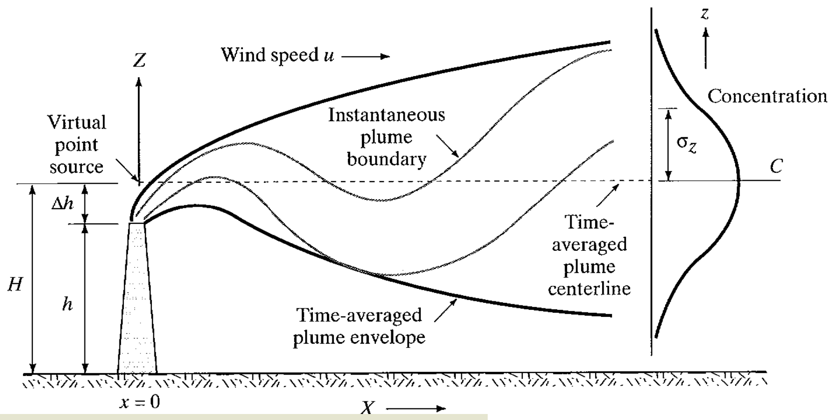

$$C(x,y,0)=\left[\frac{Q}{\pi\sigma_y\sigma_z u_H}\right]\left[\exp\left[-\frac{1}{2}\left(\frac{y}{s_y}\right)^2\right]\right]\left[\exp\left[-\frac{1}{2}\left(\frac{H}{s_z}\right)^2\right]\right]$$

Lecture 6

Air Quality:

Air Pollution Modeling

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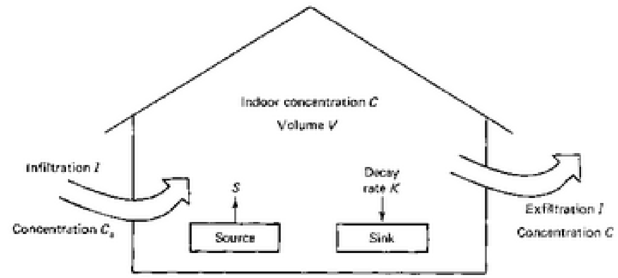


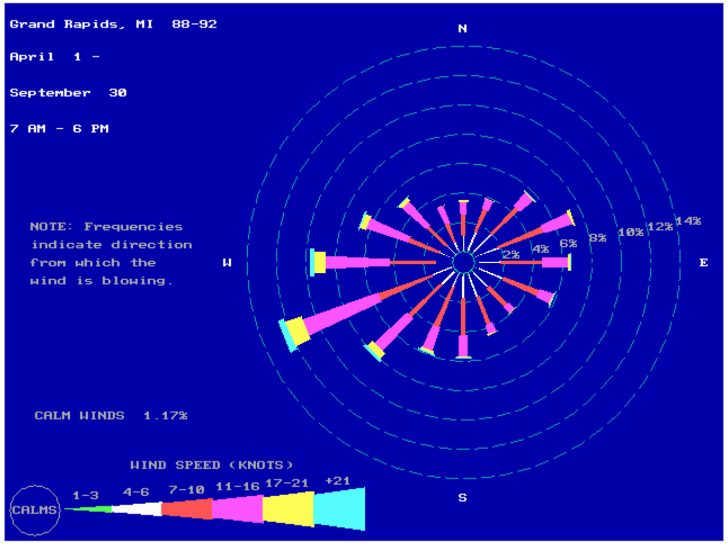
accumulation rate = input rate +sources – output rate – decay

$$\boxed{V\frac{dC}{dt} = S + C_a IV - CIV - KCV}$$

Recap 1

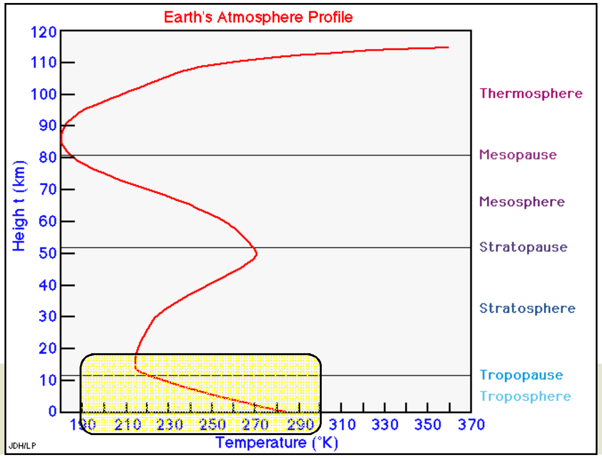
- Three type of sources: point, line, & area

- Atmospheric mixing and dispersion is governed by meteorology
  - Horizontal
    - o Wind speed and direction
  - Vertical
    - o Temperature



- Atmosphere cools with height
  - o Dry (adiabatic) lapse rate

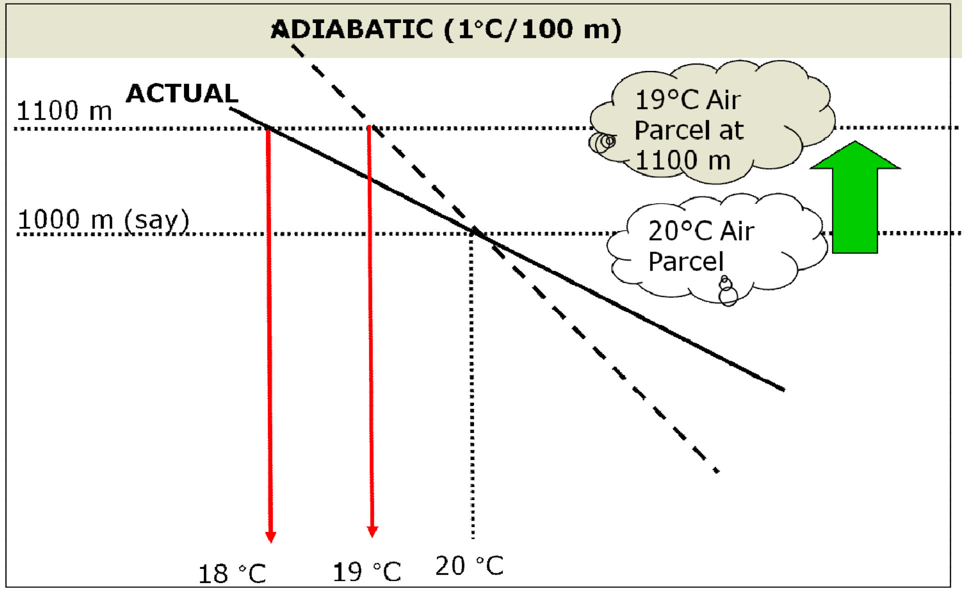
$$\Gamma = -\frac{dT}{dz} = -1.00\,°\mathrm{C}/100\ \mathrm{m}$$

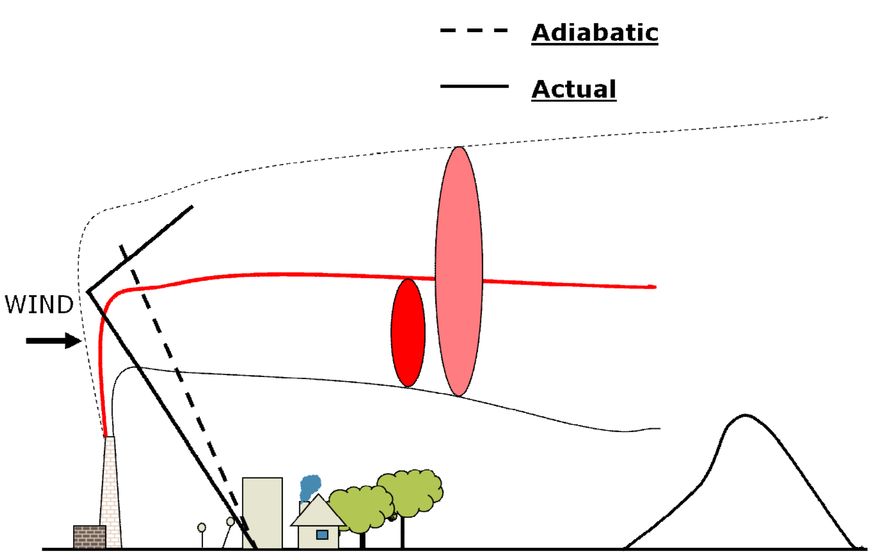


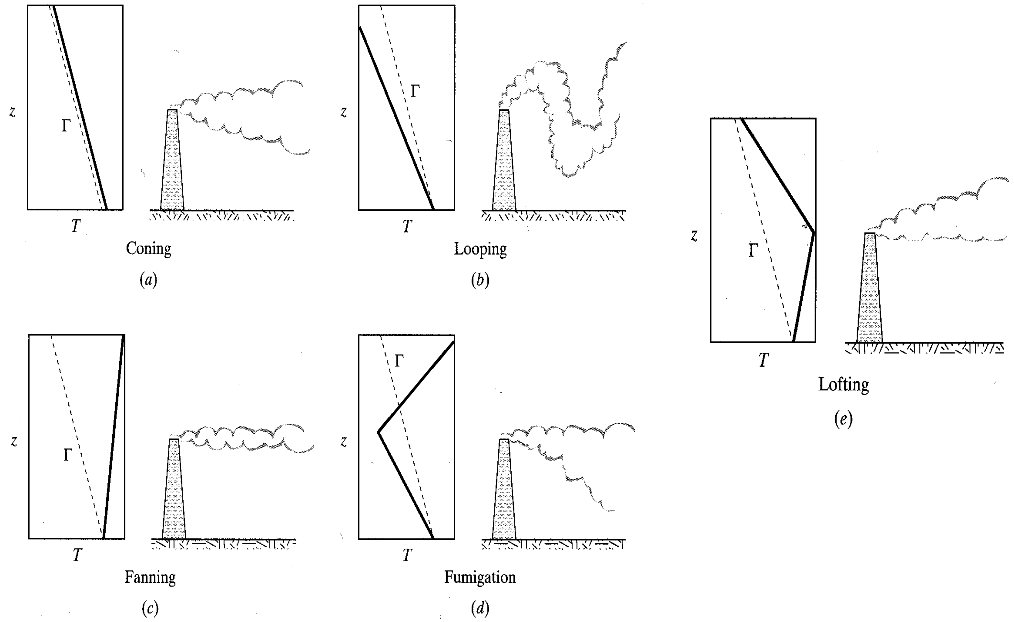
Recap 2

- Effect of actual lapse rate on vertical mixing

- Extreme case of stability when lapse rate is actually <u>positive</u>, leads to temperature inversion prevents nearly all upward mixing

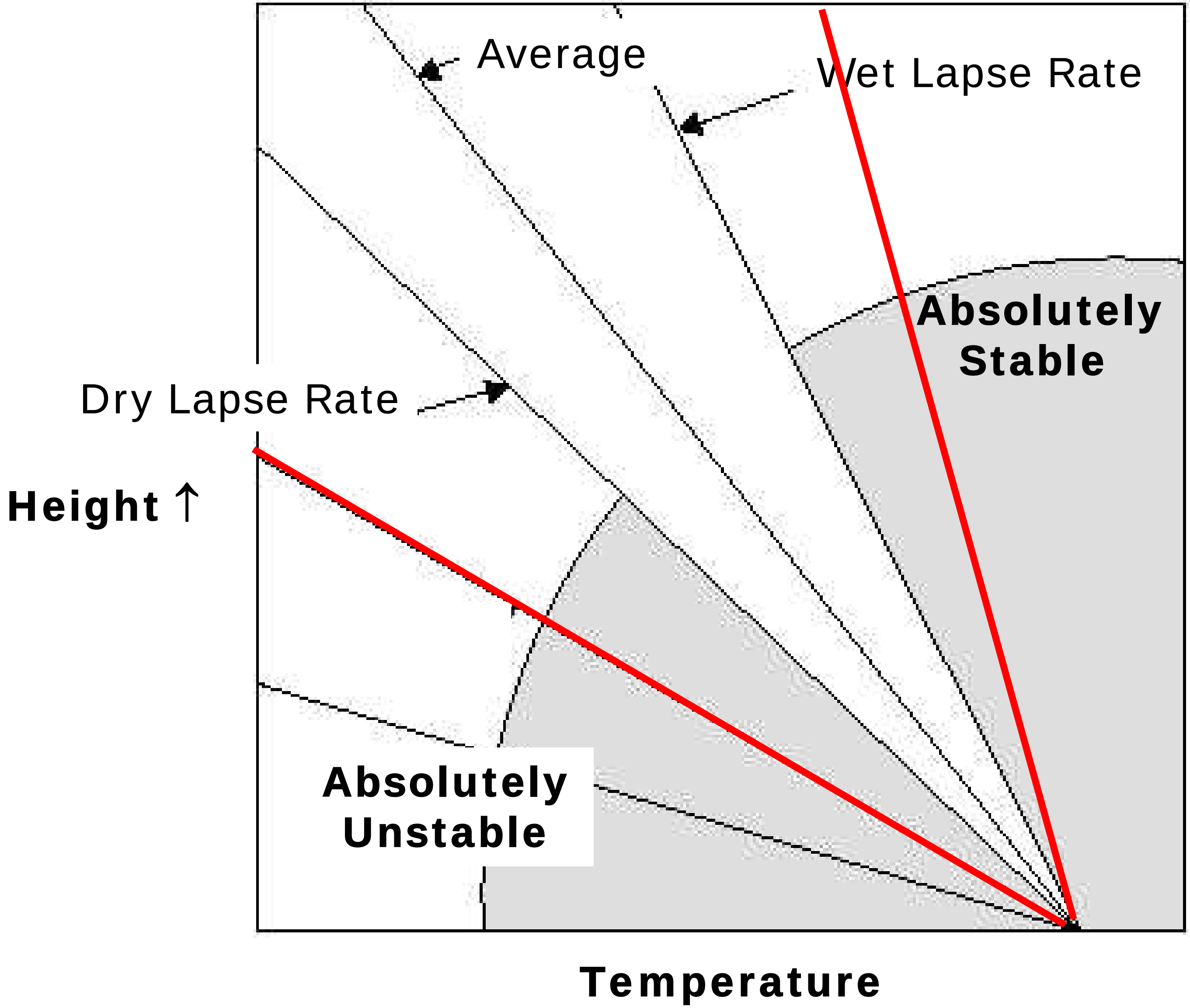






Coning (a)
Looping (b)
Fanning (c)
Fumigation (d)
Lofting (e)

Atmospheric Stability



http://www.tpub.com/content/aerographer/14312/css/14312_47.htm

Today’s Learning Objectives !

- To learn about air quality modeling methods

Why are we doing all of this ?

- If we want to set up a new industry, it implies adding a new source of pollutant(s)

- This source is PERMITTED to emit after it has applied the Best Available Control Technology (BACT) on their processes

- AFTER leaving the chimney, the concentrations on ground is determined by the meteorology

Why are we doing all of this ?

Therefore,

- If we want to know WHERE to put the new industry

- If we want to know the pollution levels under the worst case scenario of STABLE conditions and low wind speeds

- If we want to know what height does the chimney need to be

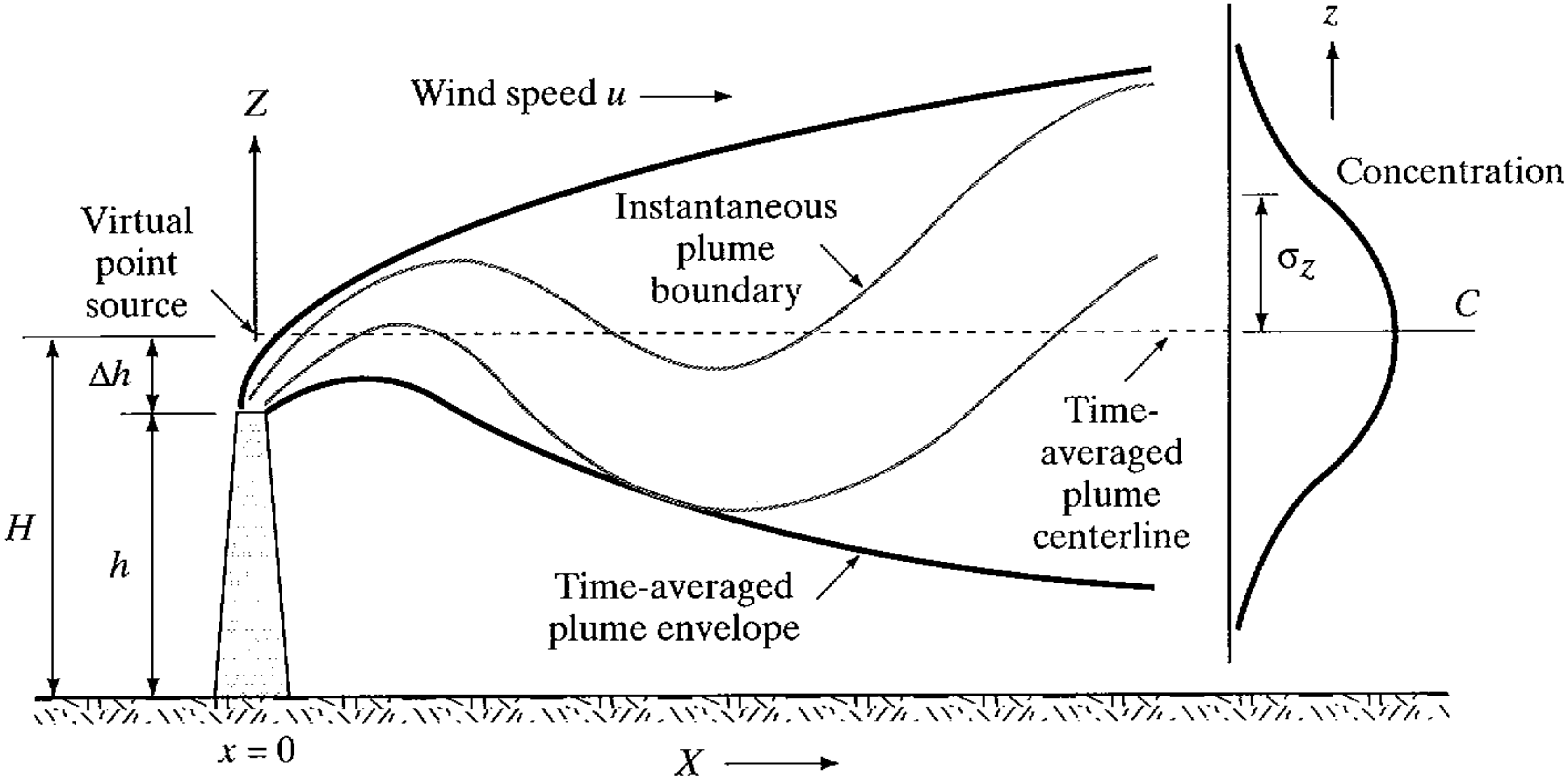
⇨ QUANTIFICATION of horizontal movement and vertical mixing becomes essential

Modeling air quality

- Gaussian Plume (Dispersion) Model (GPM) is used to estimate the ground level concentrations for pollutants coming from a chimney

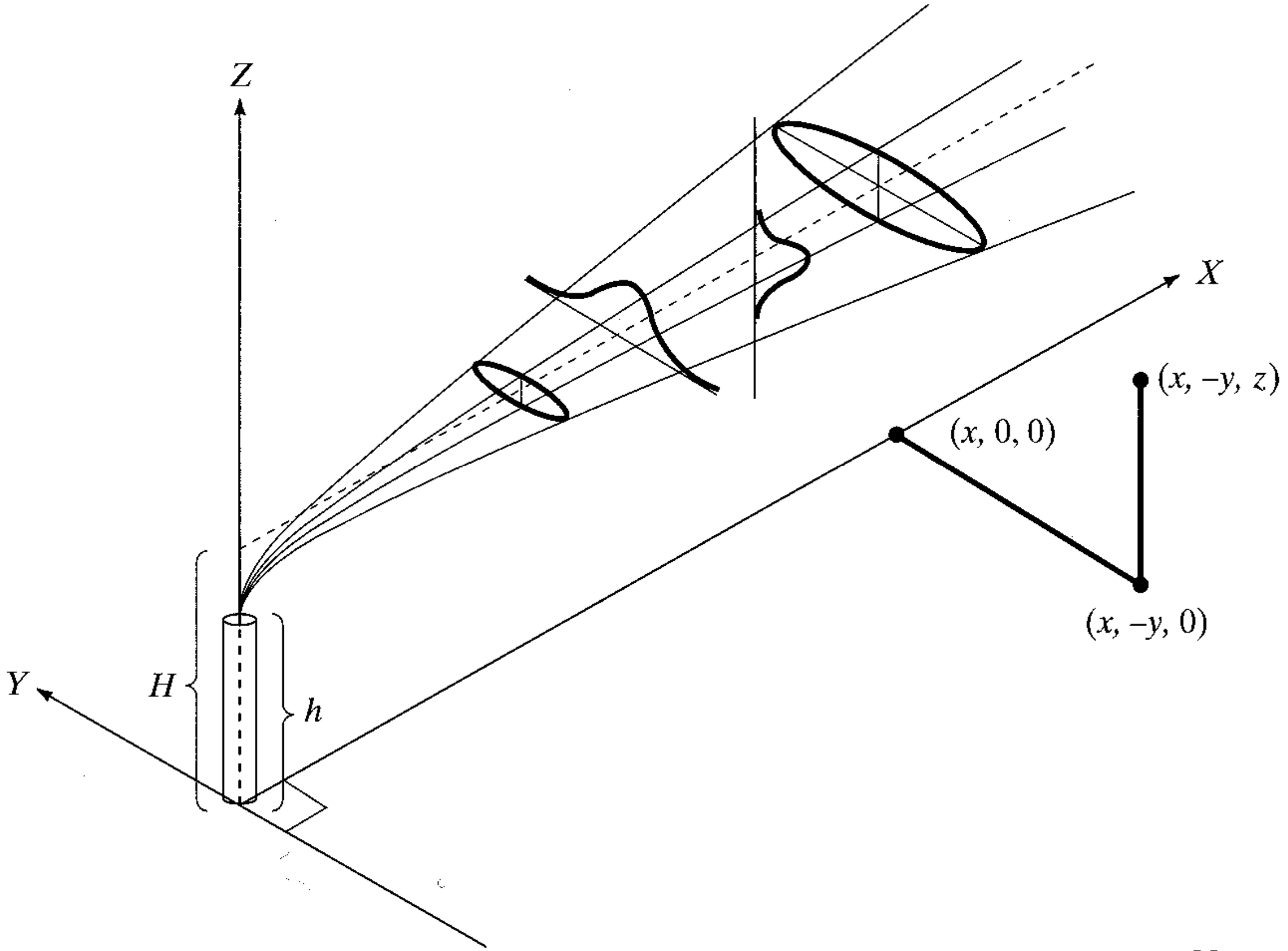
- Inputs to GPM
  - Height of chimney and Source strength
  - Wind rose data
  - Atmospheric stability of the region

Point Source Gaussian Plume Model



Masters & Ela, 2008

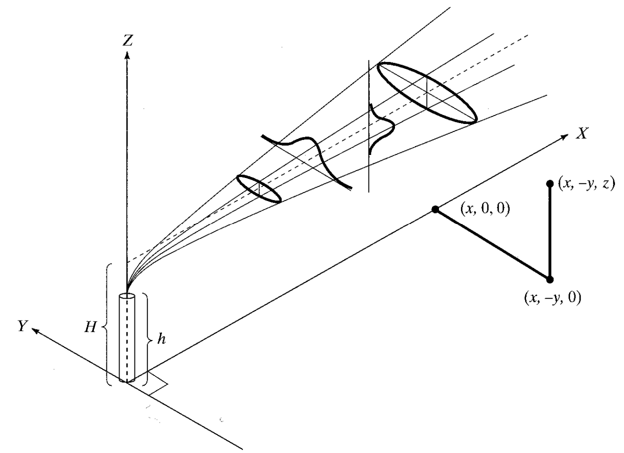
Point Source Gaussian Plume Model



Masters & Ela, 2008

GPM: Model Structure & Assumptions

- pollutants released from a "virtual point source"
- advective transport by wind
- dispersive transport (spreading) follows normal (Gaussian) distribution away from trajectory
- constant emission rate
- wind speed constant with time and elevation
- pollutant is conservative (no reaction)
- terrain is flat and unobstructed
- uniform atmospheric stability



Point Source GPM: Mathematical expression

$$C(x, y, 0) = \left[\frac{Q}{\pi s_y s_z u_H}\right]\left[\exp\left[-\frac{1}{2}\left(\frac{y}{s_y}\right)^2\right]\right]\left[\exp\left[-\frac{1}{2}\left(\frac{H}{s_z}\right)^2\right]\right]$$

Where,

C = downwind concentration at ground level ($\mu g/m^3$)

Q = emission rate of pollutant ($\mu g/s$)

s_y, s_z = plume standard deviations (m)

u = wind speed (m/s)

x, y, z = distances (m)

H = Effective Stack Height (m)

Point Source GPM: Effective Stack Height

$$H = h + \Delta H$$

where, H = Effective stack height (m)

h = height of physical stack (m)

ΔH = plume rise (m)

- Holland's formula

$$\Delta H = \frac{v_s d}{u}\left[1.5 + \left(2.68\times10^{-3}(P)\left(\frac{T_s - T_a}{T_s}\right)d\right)\right]$$

where, v_s = stack velocity (m/s)

d = stack diameter (m)

u = wind speed (m)

P = atmospheric Pressure, millibars

T_s = stack gas temperature (°K)

T_a = air temperature (°K)

Holland's formula, however, does not take into account the meteorology of the atmosphere, and good for certain atmospheric conditions only

Point Source GPM: Stability Categories

TABLE 11–6 Key to Stability Categories

Surface Wind Speed (at 10 m) ($m \cdot s^{-1}$)	Day[a] Incoming Solar Radiation			Night[a]	
	Strong	Moderate	Slight	Thinly Overcast or $\geq \frac{4}{8}$ Low Cloud	$\leq \frac{3}{8}$ 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

A Extremely Unstable

B Moderately Unstable

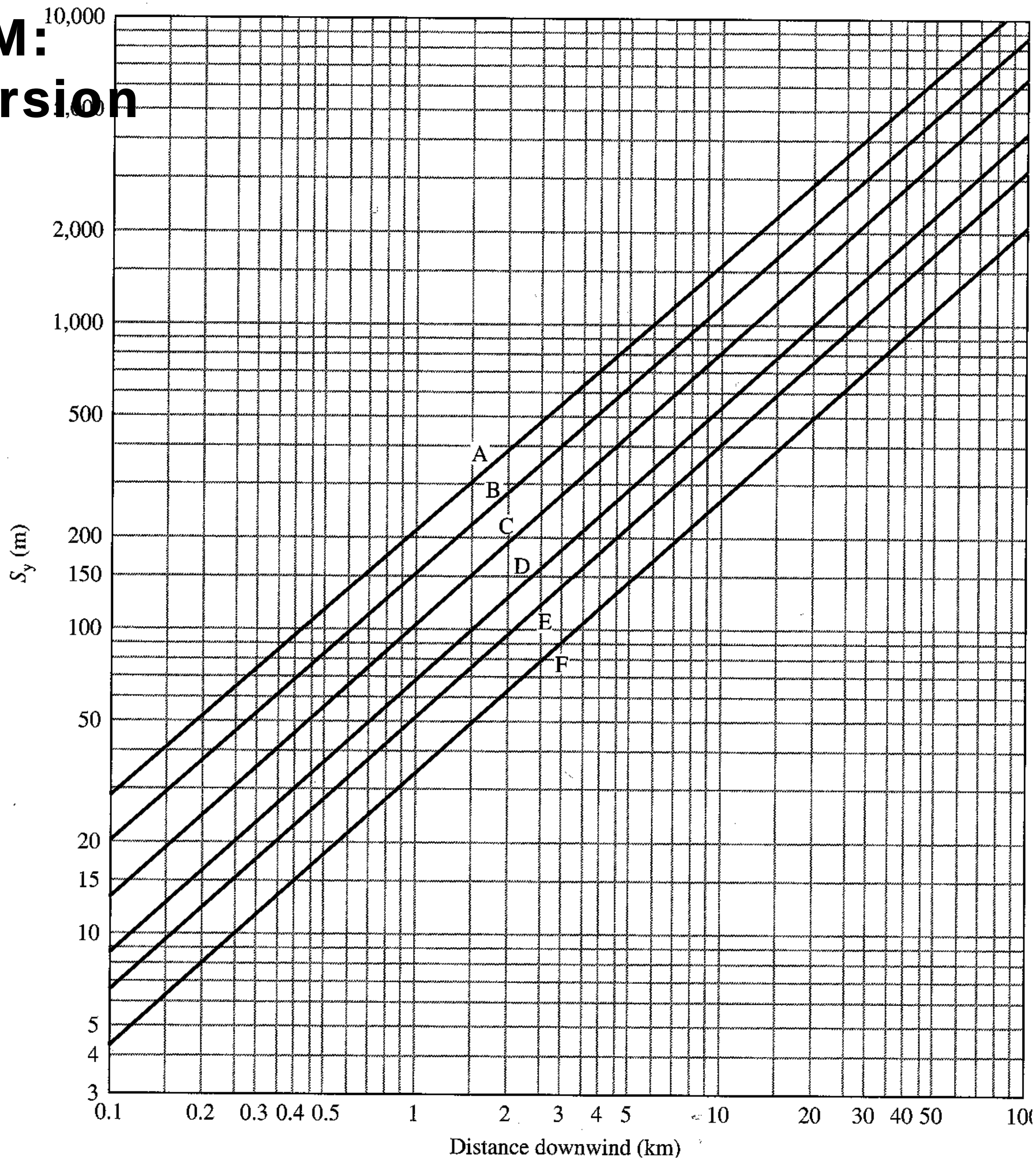
C Slightly Unstable

D Neutral

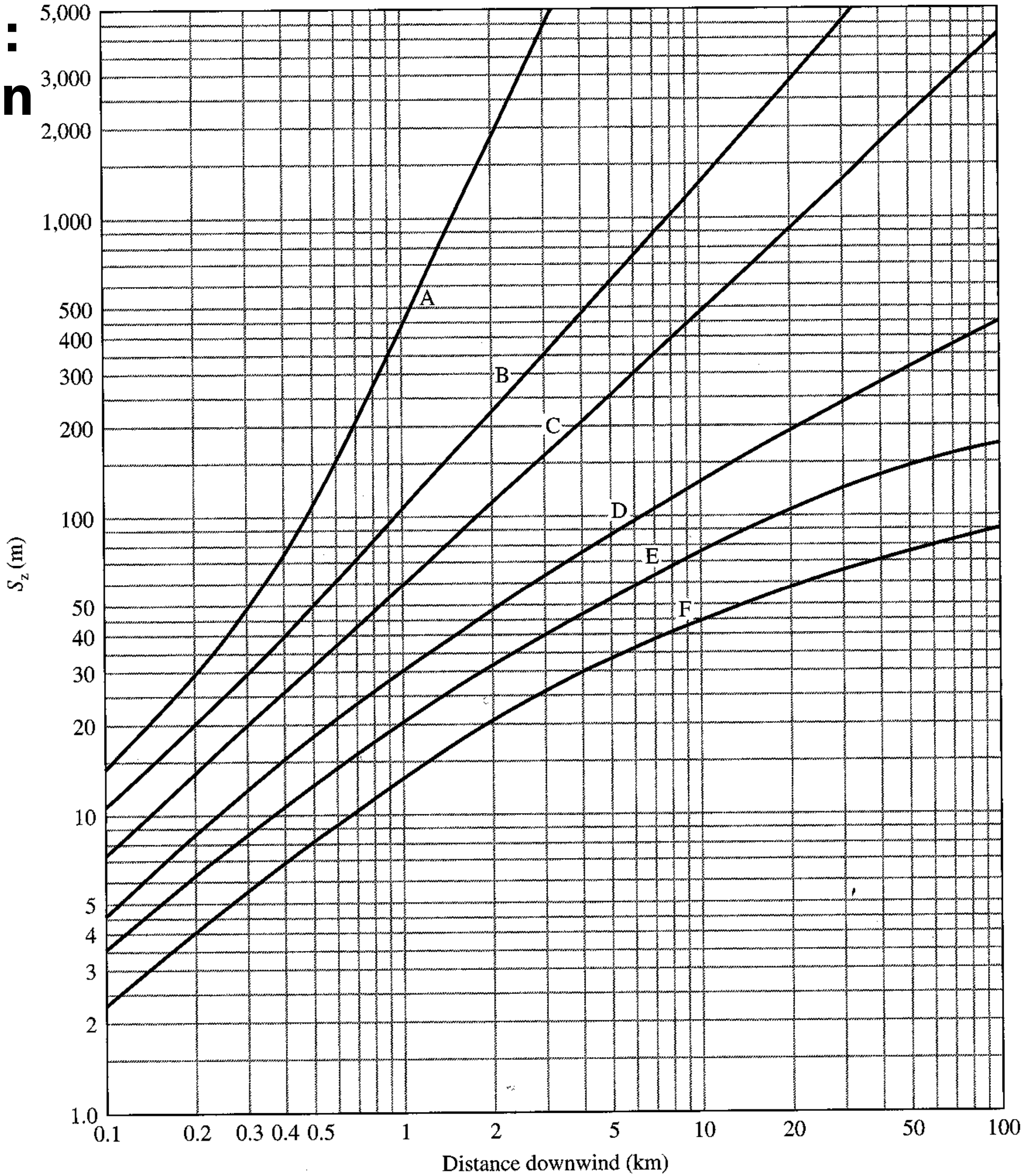
E Slightly Stable

F Moderately Stable

Point Source GPM: Horizontal Dispersion (s_y)



Point Source GPM: Vertical Dispersion (s_z)



Point Source GPM:
Vertical & horizontal Dispersion (sy, s_z)

$$\sigma_y = a\,x^{0.894}$$

$$\sigma_z = cx^d + f$$

TABLE 7.8

Values of the Constants *a*, *c*, *d*, and *f* for Use in (7.47) and (7.48)

		$x \leq 1$ km			$x \geq 1$ km		
Stability	*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

Note: The computed values of σ will be in meters when x is given in kilometers.
Source: Martin, 1976.

Masters & Ela, 2008

Point Source GPM: Wind Speed Correction

- Unless the wind speed at the virtual stack height is known, it must be estimated from the ground wind speed

$$u_2 = u_1 \left(\frac{z_2}{z_1} \right)^p$$

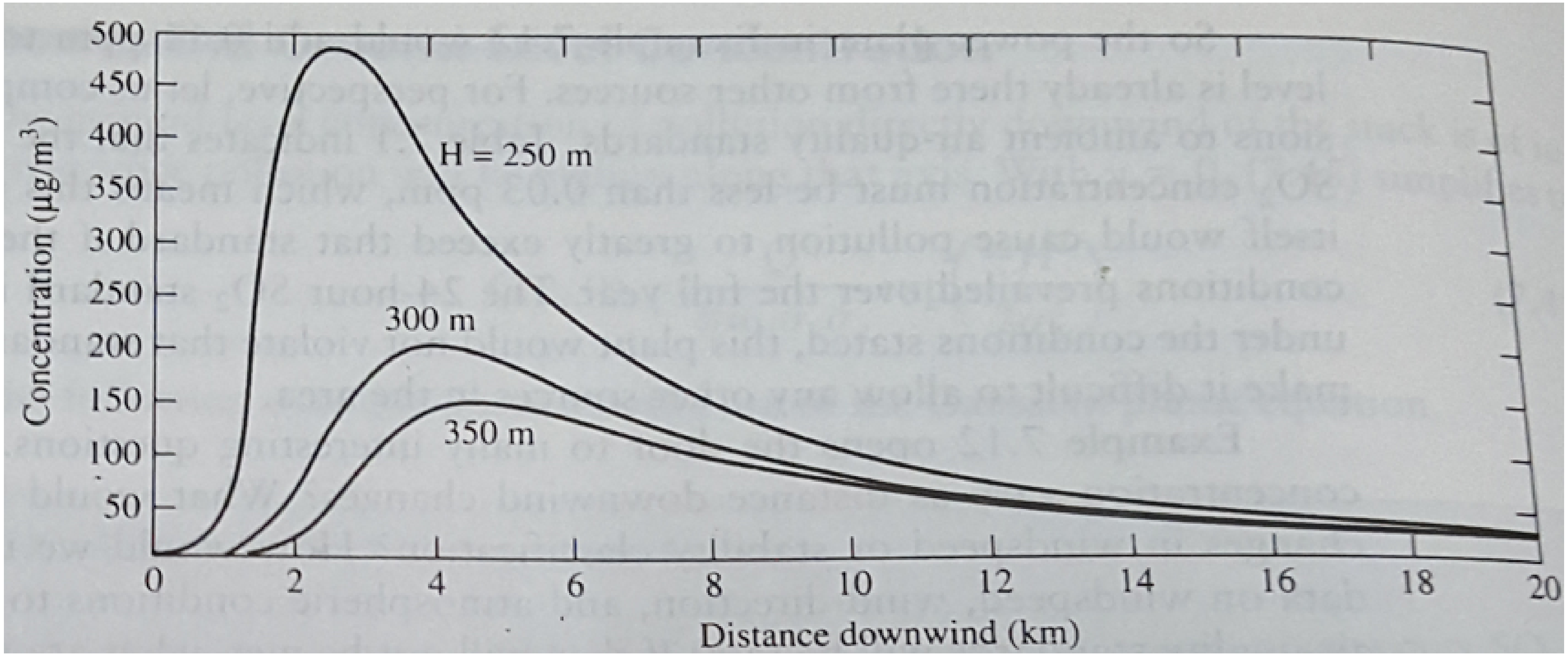
where u_x = wind speed at elevation z_x

p = empirical constant

TABLE 11–8 Exponent p Values for Rural and Urban Regimes

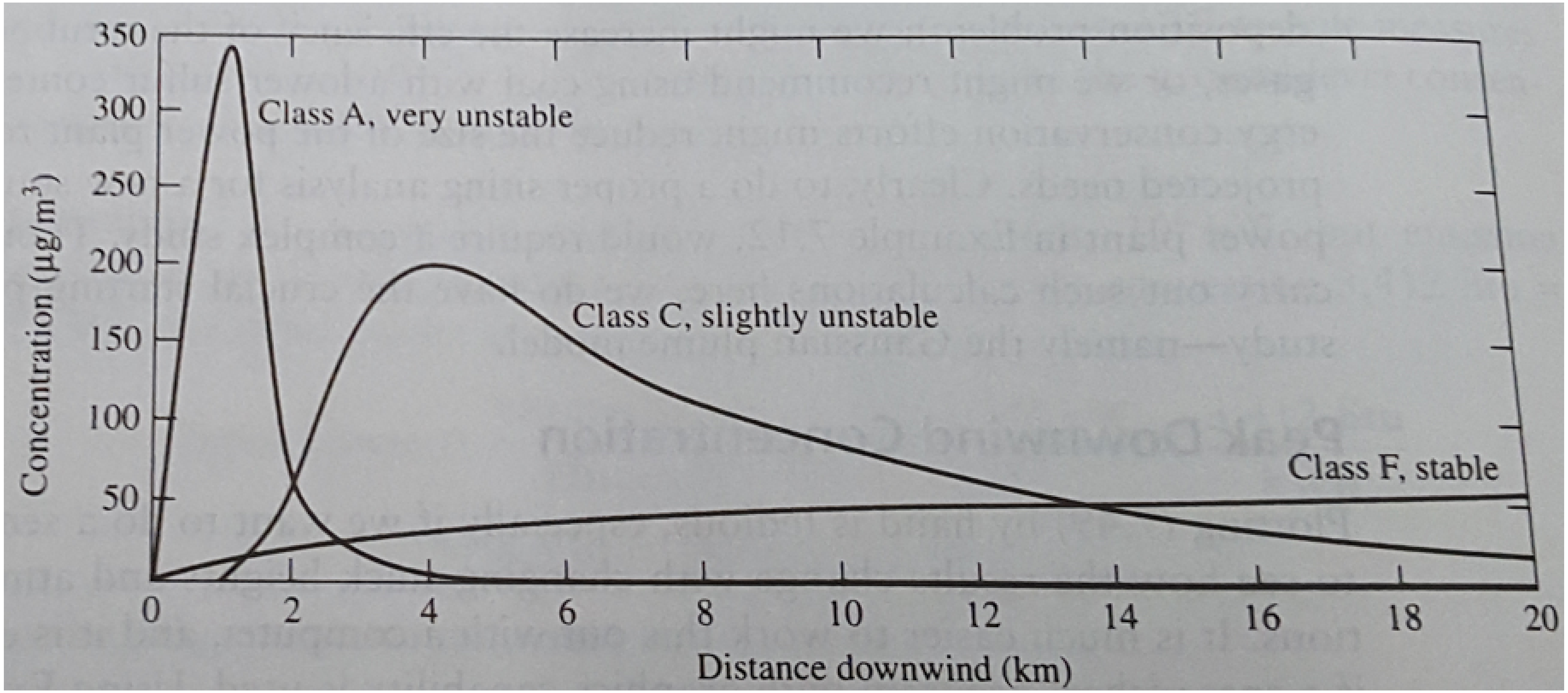
Stability Class	Rural	Urban	Stability Class	Rural	Urban
A	0.07	0.15	D	0.15	0.25
B	0.07	0.15	E	0.35	0.30
C	0.10	0.20	F	0.55	0.30

Point Source GPM:
Effect of effective stack height



Masters & Ela, 2008

Point Source GPM:
Effect of atmospheric stability classification



Masters & Ela, 2008

Point Source GPM

Example !

A stack in an urban area is emitting 80 g/s of NO. It has an effective stack height of 100m. The wind speed is 4 m/s at 10 m. It is a clear summer day with the sun nearly overhead. Estimate the ground level concentration at:

a. 2 km downwind on the centerline, and

b. 2 km downwind, 0.1 km off the centerline.

Point Source GPM: Example !

1. Determine stability class

   Assume wind speed is 4 m/s at ground surface.
   Description suggests strong solar radiation.

   hence *stability class* is **B**

clear summer day with the sun nearly overhead; wind speed 4 m/s at 10 m.

TABLE 11–6 Key to Stability Categories

Surface Wind Speed (at 10 m) ($m \cdot s^{-1}$)	Day[a] Incoming Solar Radiation: Strong	Moderate	Slight	Night[a]: Thinly Overcast or $\geq \frac{4}{8}$ Low Cloud	$\leq \frac{3}{8}$ 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

Point Source GPM: Example !

2. Estimate the wind speed at the effective stack height

   Note: effective stack height given – no need to calculate using Holland's formula

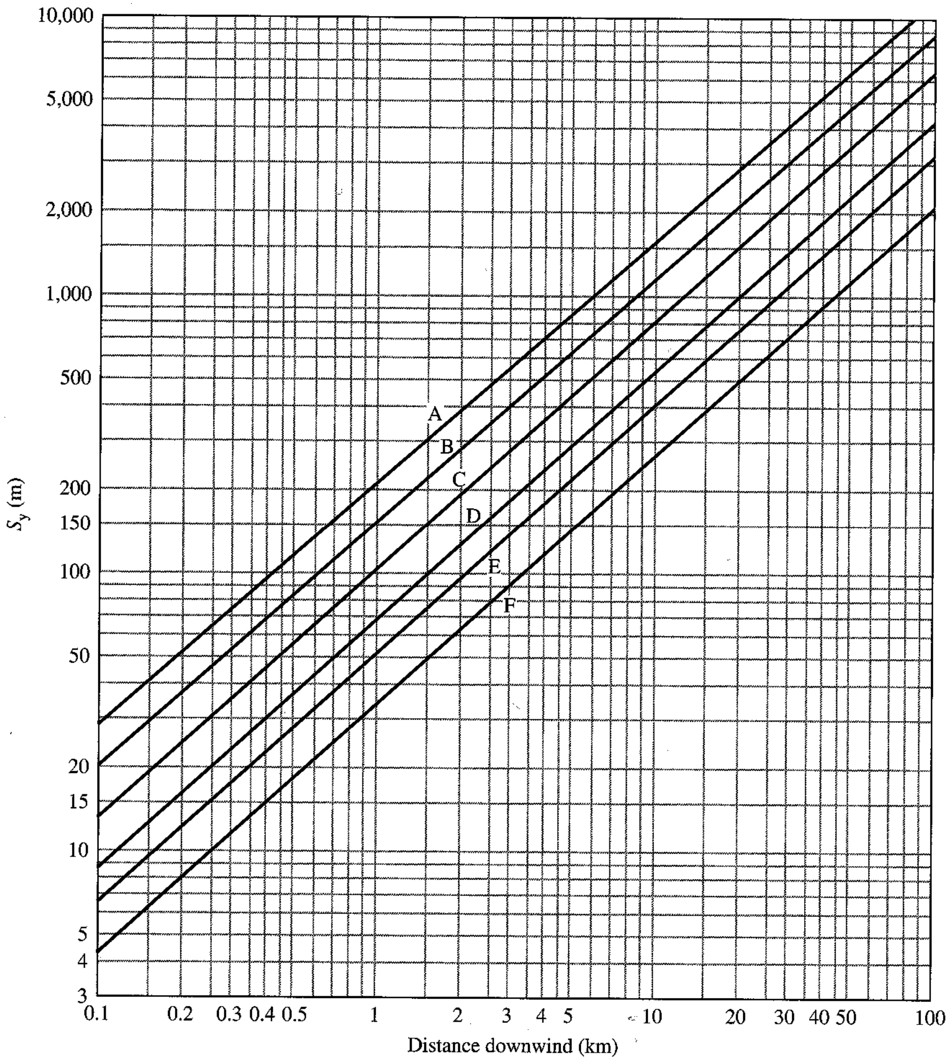
TABLE 11–8 Exponent p Values for Rural and Urban Regimes

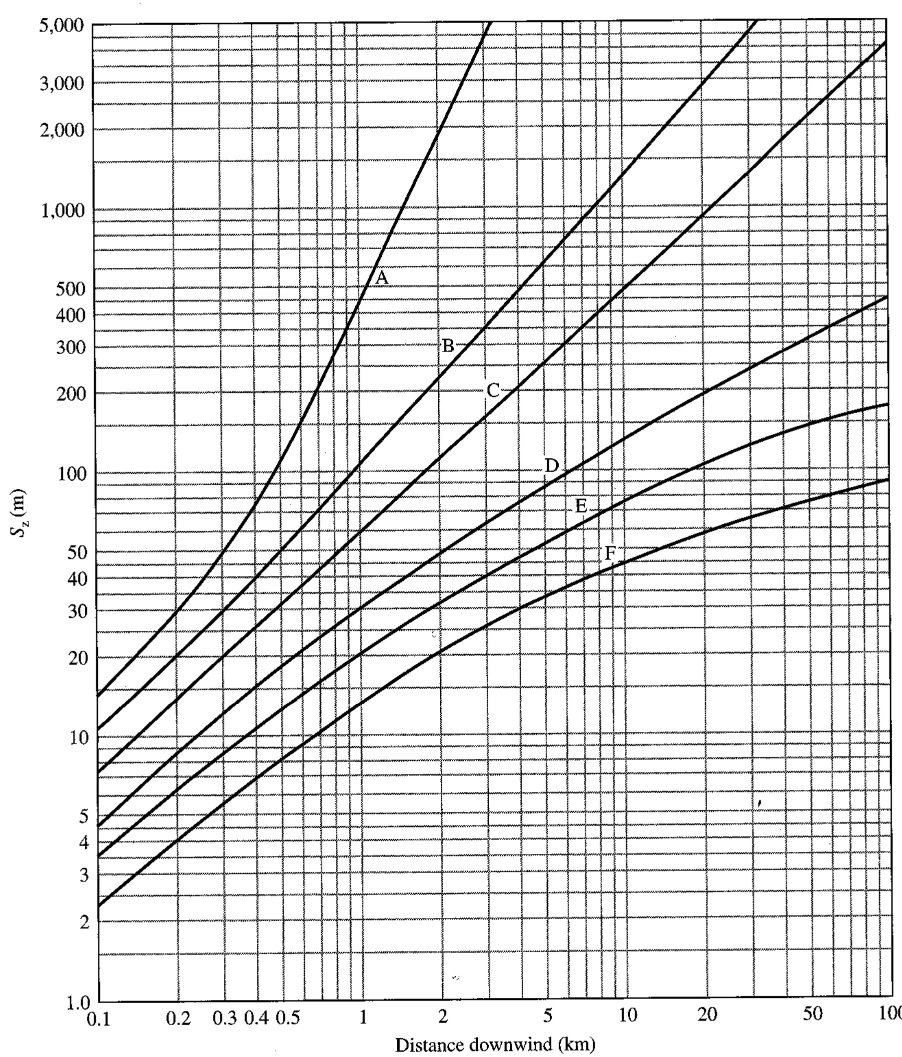
Stability Class	Rural	Urban	Stability Class	Rural	Urban
A	0.07	0.15	D	0.15	0.25
B	0.07	0.15	E	0.35	0.30
C	0.10	0.20	F	0.55	0.30

$$u_2 = u_1\left(\frac{z_2}{z_1}\right)^p = 4\left(\frac{100}{10}\right)^{0.15} = 5.65\,\text{m/s}$$

Point Source GPM: Example !

3. Determine σ_y and σ_z

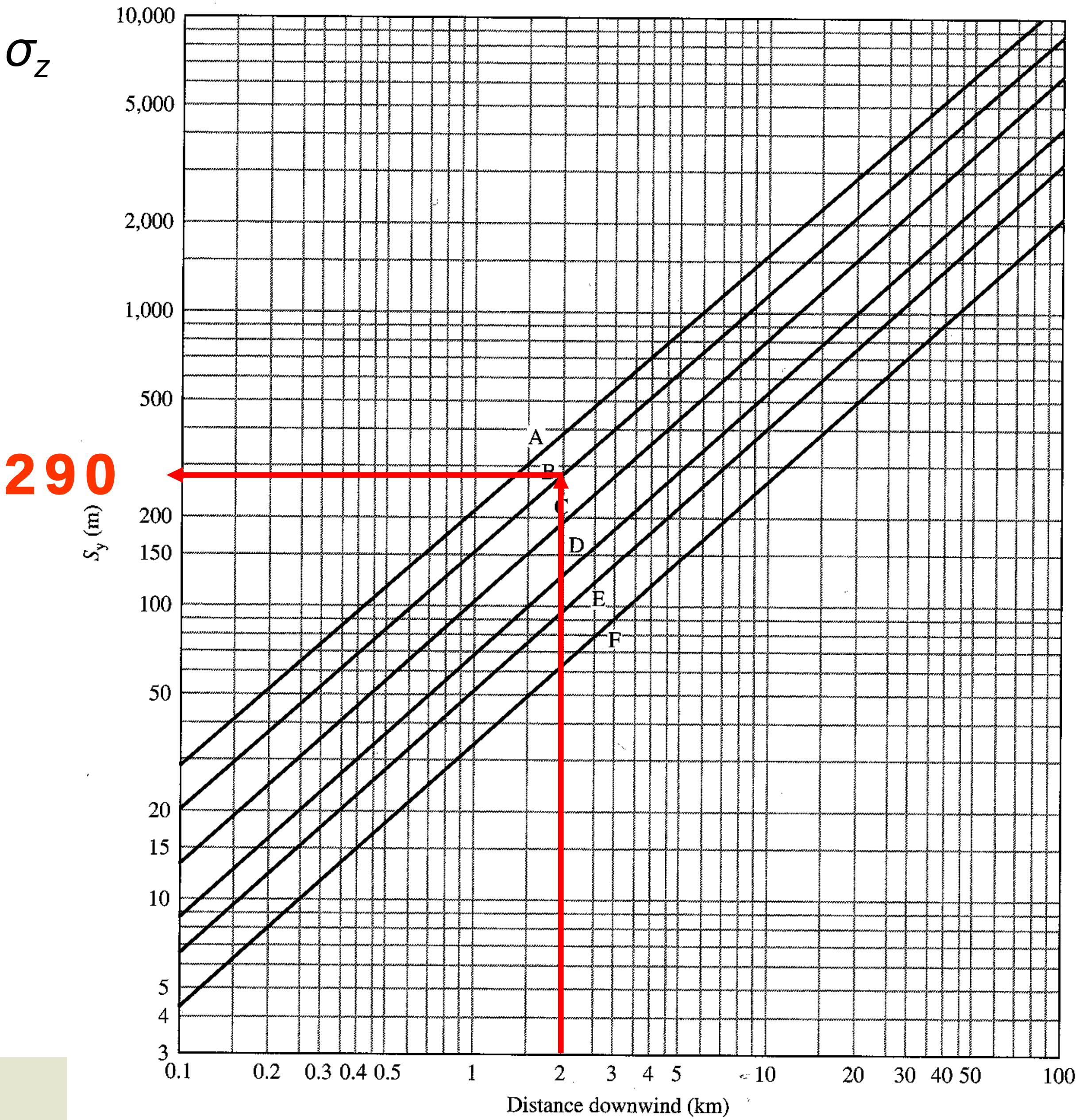




Point Source GPM: Example !

3. Determine σ_y and σ_z

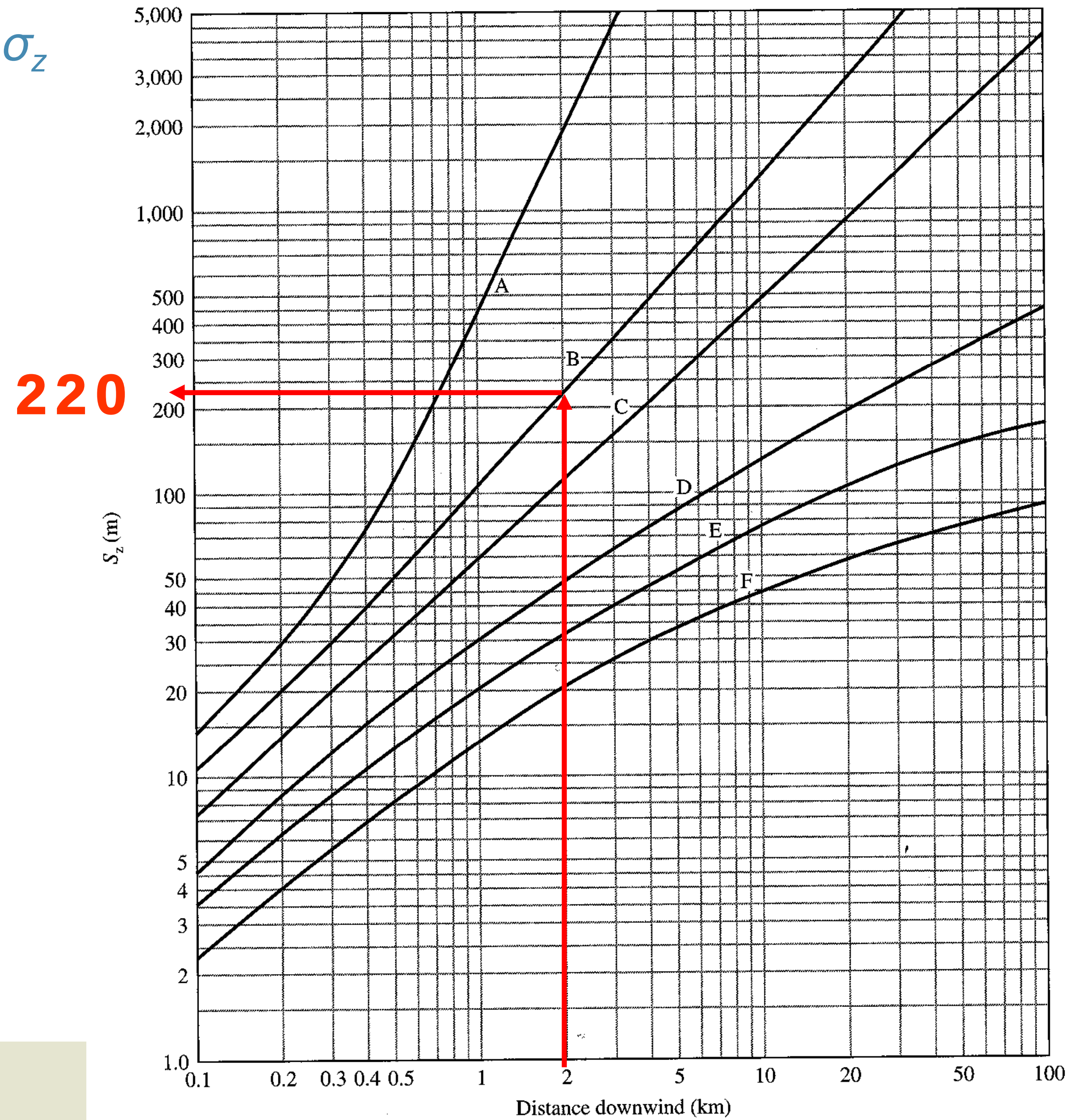
σ_y = 290



Point Source GPM: Example !

3. Determine σ_y and σ_z

σ_z = 220



Point Source GPM: Example !

4. Determine concentration using the Eqn.

   a. x = 2000, y = 0

$$C(2000,0) = \frac{80}{\pi(290)(220)(5.6)} \exp\left[-\frac{1}{2}\left(\frac{0}{290}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{100}{220}\right)^2\right]$$

$$C(2000,0) = 6.37 \times 10^{-5}\ \mathrm{g/m^3} = 63.7\ \mu\mathrm{g/m^3}$$

Point Source GPM: Example !

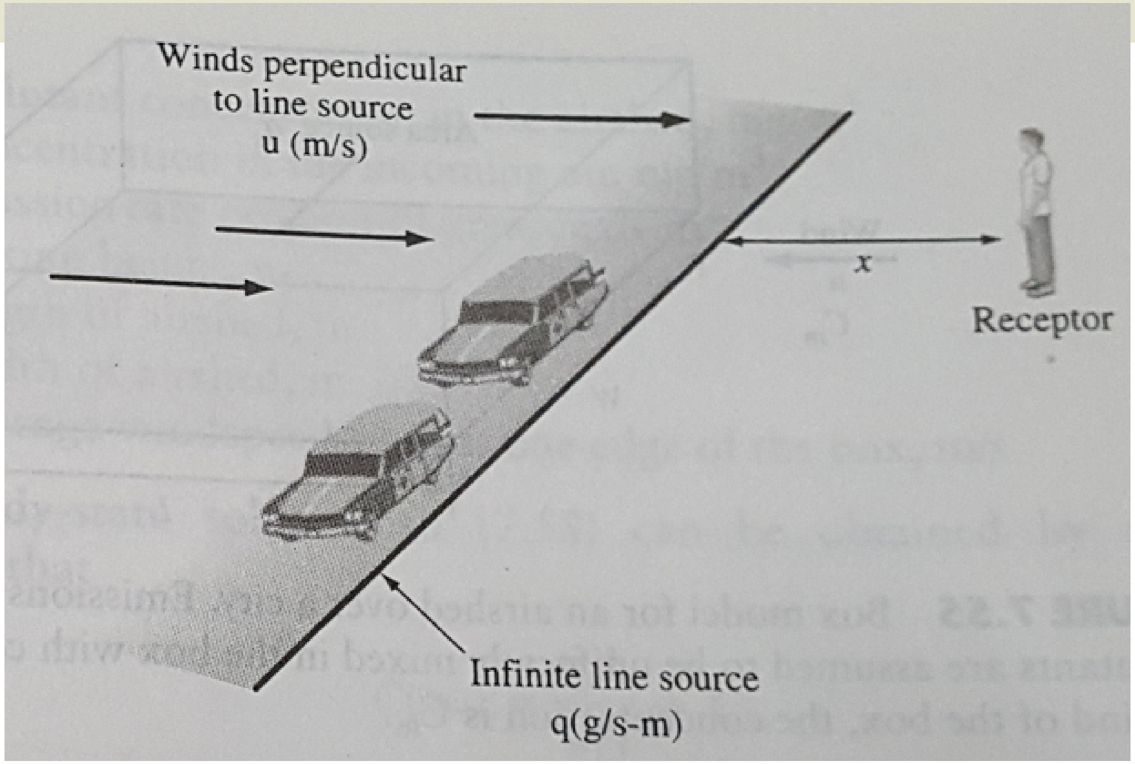
4. Determine concentration using the Eqn.

   b. x = 2000, y = 0.1 km (= 100m)

$$C(2000{,}100) = \frac{80}{\pi(290)(220)(5.6)} \exp\left[-\frac{1}{2}\left(\frac{100}{290}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{100}{220}\right)^2\right]$$

$$C(2000{,}0) = 6.00 \times 10^{-5}\ \mathrm{g/m^3} = 60\ \mu\mathrm{g/m^3}$$

Line Source Dispersion Model



- Useful in certain conditions where source is distributed along a line with continuous emissions

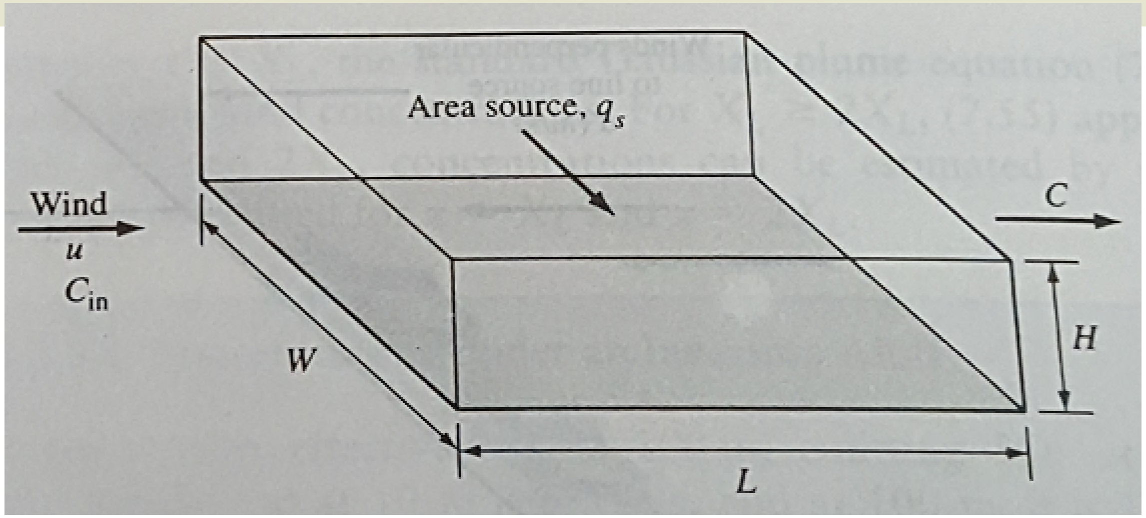
- Hence, ground level conc. of pollutant at a distance perpendicular distance x can be obtained by:

$$C(x) = \frac{2q}{\sqrt{2\pi}\,\sigma_z u}$$

Where

q = emission rate per unit distance along the line (g/m-s)

Area Source Model

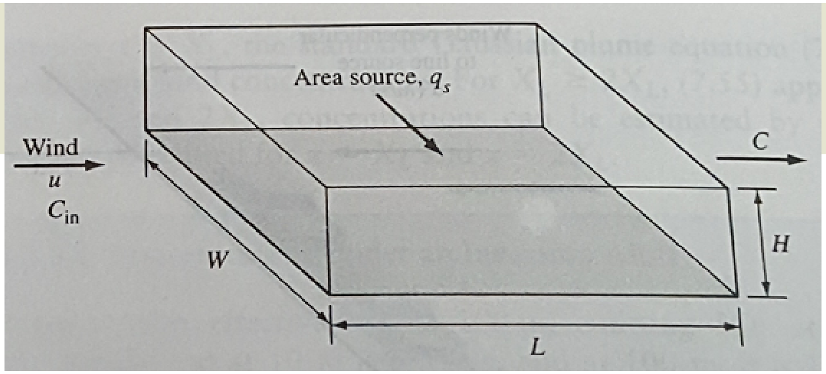


- Useful for distributed sources spread over an area
- e.g. Box model for an airshed over a city
- Pollutants are assumed to be uniformly mixed in the box

- If we assume the pollutant is conservative, then

$$\begin{pmatrix}\text{Rate of change of}\\ \text{pollution in the box}\end{pmatrix} = \begin{pmatrix}\text{Rate of pollution}\\ \text{entering the box}\end{pmatrix} - \begin{pmatrix}\text{Rate of pollution}\\ \text{leaving the box}\end{pmatrix}$$

Area Source Model



- If we assume the pollutant is conservative, then

$$LWH\frac{dC}{dt} = q_s LW + WHuC_{in} - WHuC$$

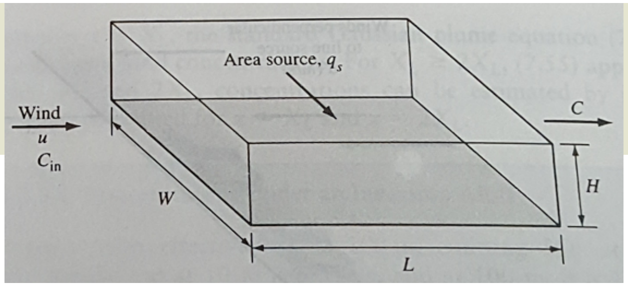
where

C = pollutant concentration in the airshed, mg/m^3
C_{in} = concentration in the incoming air, mg/m^3
q_s = emission rate per unit of area, mg/s-m^2
H = mixing height, m
L = length of airshed, m
W = width of airshed, m
u = average windspeed against one edge of the box, m/s

- Hence the steady state solution of the above equation, by simply setting $dC/dt = 0$, is:

$$C(\infty) = \frac{q_s L}{uH} + C_{in}$$

Area Source Model



$$LWH\frac{dC}{dt} = q_s LW + WHuC_{in} - WHuC$$

- The time-dependent change in the pollutant concentration in the city can be obtained by following:

$$C(t) = \left(\frac{q_s L}{uH} + C_{in}\right)(1 - e^{-ut/L}) + C(0)e^{-ut/L}$$

Where, C(0) is the concentration in the airshed at t=0

- If we assume incoming wind blow relatively no pollution in the box, C(0)=0 then:

$$C(t) = \frac{q_s L}{uH}(1 - e^{-ut/L})$$

Box Model: Example !

In a square city of 15 km a side, there are 2,00,000 cars on the road, each driven 30 km between 4-6pm, and each emitting 3 g/km of CO. It's a clear winter evening with radiation inversion restricting mixing height to 20 m. The wind is bringing clean air at a steady rate of 1.0 m/s, along an edge of the city. Using box model estimate CO at 6 pm if there was no CO in air at 4 pm, and only source of CO is cars. Assume CO is conservative and uniform mixing in the box.

First, calculate the CO emissions, q_s (in units of mass/area-time):

$$q_s = \frac{200000 cars \times 30\, km / car \times 3\, g / km}{(15 \times 10^3 m)^2 \times 3600 s / hr \times 2 hr}$$

$$= 1.1 \times 10^{-5} \; g / s - m^2$$

Box Model: Example !

In a square city of 15 km a side, there are 20,000 cars on the road, each driven 30 km between 4-6pm, and each emitting 3 g/km of CO. It's a clear winter evening with radiation inversion restricting mixing height to 20 m. The wind is bringing <u>clean air</u> at a steady rate of 1.0 m/s, along an edge of the city. Using box model estimate CO at 6 pm if there was <u>no CO in air at 4 pm</u>, and only source of CO is cars. Assume CO is conservative and uniform mixing in the box.

$$C(t) = \left(\frac{q_s L}{uH} + C_{\text{in}}\right)(1 - e^{-ut/L}) + C(0)e^{-ut/L}$$

Hence,

$$C(t) = \frac{q_s L}{uH}(1 - e^{-ut/L})$$

$$C(2hr) = \frac{1.1\times10^{-5}\, g/s-m^2 \times 15\times10^3\, m}{(15\times10^3\, m)^2 \times 3600 s/hr \times 2hr}\left[1 - \exp\left(\frac{-1.0 m/s \times 7200 s}{15\times10^3\, m}\right)\right]$$

$$= 3.2\times10^{-3}\ \ g/m^3$$

Indoor Box Model

- Similar to urban airshed, a box model can be used for indoor environments

- e.g. a basic mass balance for pollution in the building/ room, assuming well-mixed conditions:

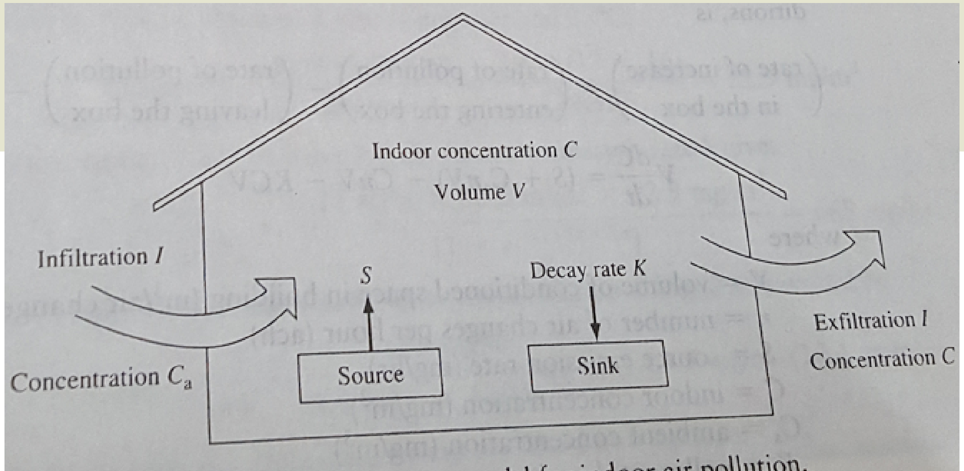


FIGURE 7.65 Box model for indoor air pollution.

$$\begin{pmatrix}\text{rate of increase}\\ \text{in the box}\end{pmatrix} = \begin{pmatrix}\text{rate of pollution}\\ \text{entering the box}\end{pmatrix} - \begin{pmatrix}\text{rate of pollution}\\ \text{leaving the box}\end{pmatrix} - \begin{pmatrix}\text{rate of decay}\\ \text{in the box}\end{pmatrix}$$

$$V\frac{dC}{dt} = (S + C_a nV) - CnV - KCV$$

where

V = volume of conditioned space in building (m^3/air change)
n = number of air changes per hour (ach)
S = source emission rate (mg/hr)
C = indoor concentration (mg/m^3)
C_a = ambient concentration (mg/m^3)
K = pollutant decay rate or reactivity (1/hr)

Indoor Box Model

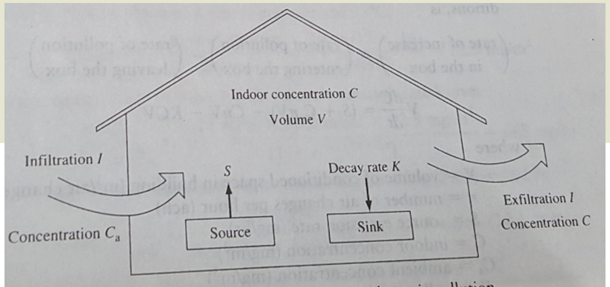


FIGURE 7.65 Box model for indoor air pollution.

- Steady-state indoor pollutant conc., by setting $dC/dt = 0$, will be:

$$C(\infty) = \frac{(S/V) + C_a n}{n + K}$$

- Time-dependant variation of indoor pollutant conc. can be obtained by:

$$C(t) = \left[\frac{(S/V) + C_a n}{n + K}\right]\left[1 - e^{-(n+K)t}\right] + C(0)e^{-(n+K)t}$$

- For pollutants such as CO and NO_2, which can be treated as conservative (K=0), also, if ambient conc. is negligible (C_a=0), and before a source is operated indoors (C(0)=0), then:

$$C(t) = \left(\frac{S}{nV}\right)(1 - e^{-nt})$$

Indoor Box Model: Example !

An outdoor airflow of 0.047 m^3/s enters a 3 m high room having a 100 m^2 of new wall-to-wall carpet. If one square meter carpet gives off formaldehyde (HCHO) at a rate of 0.1 $\mu g/s$, assuming outdoor air is formaldehyde free and formaldehyde is conservative:

1. What is the outdoor air change rate for the room?
2. What is the formaldehyde conc. under steady state?
3. If the carpet is removed very quickly from the room, how long would it take for the formaldehyde to reach 5% of its initial conc.?

1. Air change rate, n = Q/V

$$n = \frac{0.047 m^3/s}{(3m \times 100 m^2)} \times 3600 s/hr$$

$$= 0.56/hr$$ = *0.56 ACH*

Indoor Box Model: Example !

An outdoor airflow of 0.047 m^3/s enters a 3 m high room having a 100 m^2 of new wall-to-wall carpet. If one square meter carpet gives off formaldehyde (HCHO) at a rate of 0.1 μg/s, assuming outdoor air is formaldehyde free and formaldehyde is conservative:

2. What is the formaldehyde conc. under steady state?

2. Formaldehyde conc. under steady state,

$$C(t) = \left[\frac{(S/V) + C_a n}{n + K}\right]\left[1 - e^{-(n+K)t}\right] + C(0)e^{-(n+K)t}$$

$$C(\infty) = \frac{S/V}{n} = \frac{S}{Q}$$

$$= \frac{0.1\mu g/(s.m^2)\times 100m^2}{0.0476m^3/s} = 213\mu g/m^3$$

Indoor Box Model: Example !

An outdoor airflow of 0.047 m^3/s enters a 3 m high room having a 100 m^2 of new wall-to-wall carpet. If one square meter carpet gives off formaldehyde (HCHO) at a rate of 0.1 μg/s, assuming outdoor air is formaldehyde free and formaldehyde is conservative:

3. If the carpet is removed very quickly from the room, how long would it take for the formaldehyde to reach 5% of its initial conc.?

3. Time for HCHO to reach its 5% value,

$$C(t) = \left[\frac{(S/V) + C_a n}{n + K}\right]\left[1 - e^{-(n+K)t}\right] + C(0)e^{-(n+K)t}$$

$$C(t) = C(0)e^{-nt}$$ or $$C(t)/C(0) = e^{-nt}$$

=> $$0.05 = e^{-0.56t}$$

Therefore, *t = 5.3 hr*

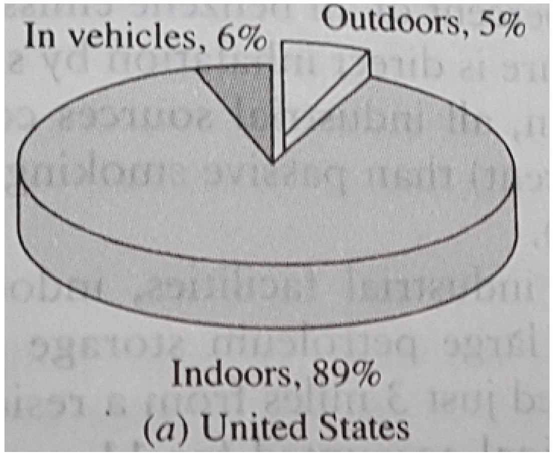
Need for Indoor Models:
… so to estimate Indoor Exposures

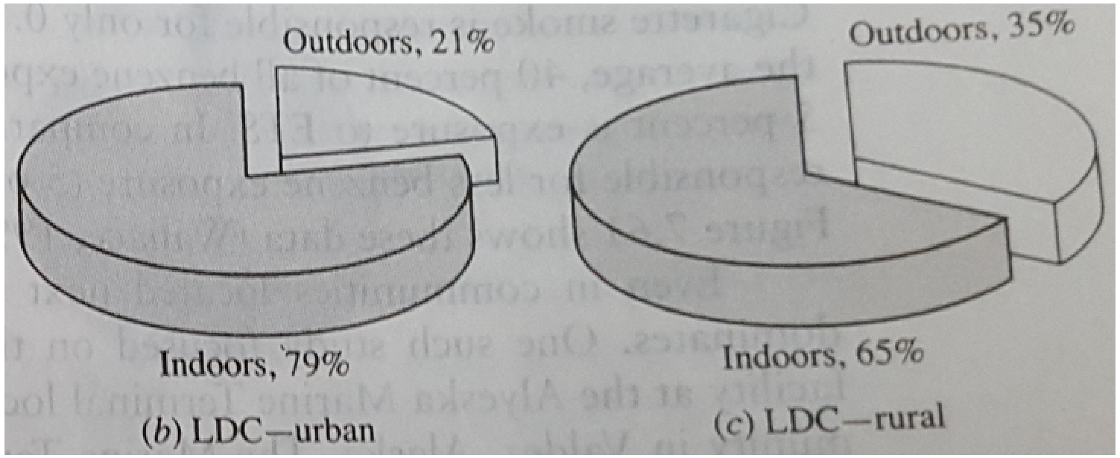
- Outdoor models needed so to manage air quality in ambient environments where no measurements are available

- But as far as human health effects are concerned, what matters is not the pollutants' conc., but what humans get exposed to!

Exposure = concentration x duration of time in contact

- Contact duration depends on where people spend their time





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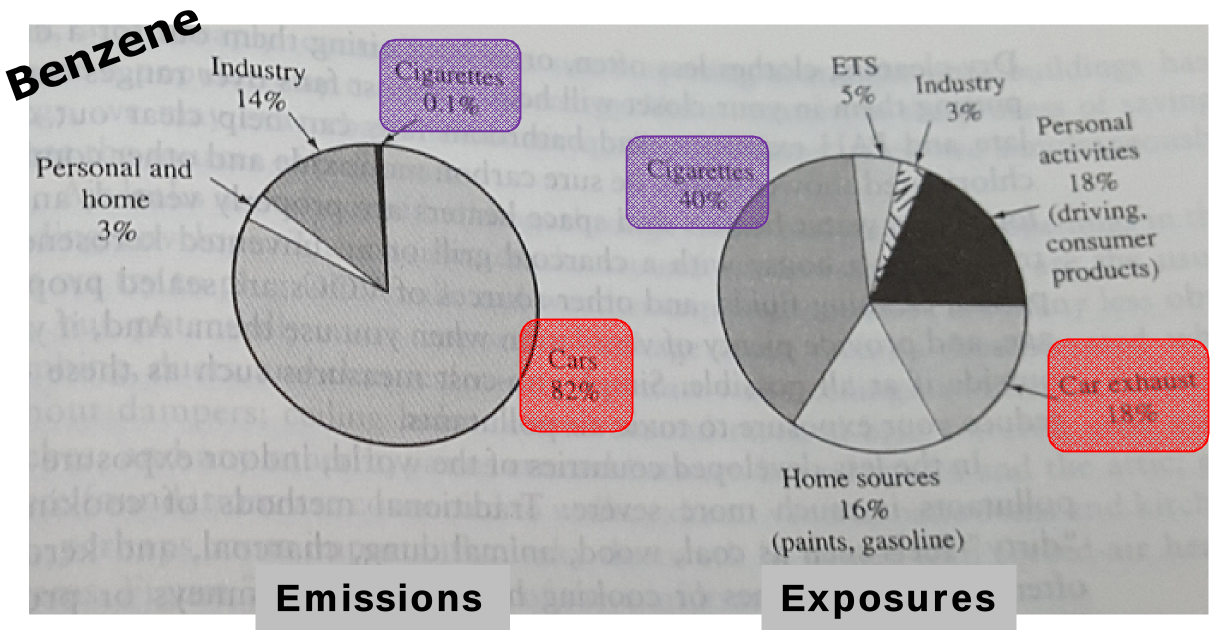
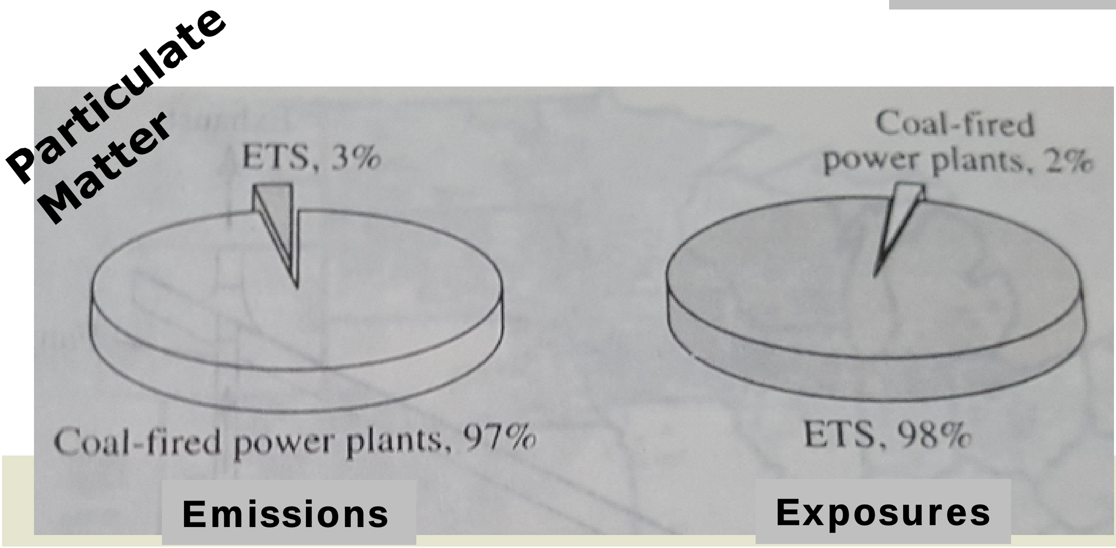
Air Pollution Exposures

- Some of the largest emissions may have lowest exposures and vice-versa





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