AIR POLLUTION MODELING

Ch 6 de Nevers
Nov., 23, 2015

AP MODELING

- To plan and execute air pollution control programs designed to meet the requirements of these laws, one must predict the ambient air concentrations that will result from any planned set of emissions.
- We may probably need to use some kind of predictions of ambient contaminant concentrations, made possible by air pollutant concentration models.
- Perfect air pollutant concentration model allowing us to predict the concentrations from any set of pollutant emissions, for any specified meteorological conditions, at any location, for any time period, with total confidence ARE FAR from availability.

AP MODELING

- All models are simplifications of reality. The models in this chapter are useful.
- All of the models presented here are simple material balances.
- A material balance is an accounting in which one applies the general balance equation to some species. In our case the species being accounted for is the air pollutant under study.
- We will consider three kinds of models:

A. Source - oriented models:

  - Grid or ***box models (single*** & multiple; with or ***without chemical reactions***)
  - Diffusion or ***dispersion models for single*** or multiple ***point source***s

B. Receptor - oriented models

Classification by Source

- Emissions from **source types** are modeled differently

Point source	Gaussian plume model (e.g. ISC-AERMOD)
Mobile source	Roadway models (e.g. CALINE, CAL3QHC)
Area source	Flexible source models (e.g. CALPUFF)

BOX MODELS

- Conservation of mass principle applied to relatively large scale systems such as an urban airshed:

INPUT - OUTPUT + GENERATION - CONSUMPTION = ACCUMULATION (6.1)

- All such models are applied to one air pollutant at a time.
- Most models can be used for several different pollutants, but they must be applied separately to each. No models presented here apply to “air pollution in general.”
- Steady state rarely of interest, we are usually interested in modeling, explaining, predicting, preventing severe air pollution episodes of a transient nature
- Wind, emission, and ambient monitoring data required for meaningful modelling work

FIXED-BOX MODELS

- Consider a rectangular city as shown in Fig. 6.1.
- Make the following major simplifying assumptions:

1. The city is a rectangle with dimensions W and L and with one side parallel to the wind direction.
2. Atmospheric turbulence produces complete and total mixing of pollutants up to the mixing height H and no mixing above this height.
3. Turbulence is strong enough in the upwind direction that the pollutant concentration is uniform in the whole volume of air over the city. This assumption is quite *contrary to what we observe in nature* but permits a great simplification of the mathematics.
4. The wind blows in the x direction with velocity u. This velocity is constant and is independent of time, location, or elevation above the ground. This is *also contrary to observation*; wind speeds increase with elevation. Here we use the average u between that at the ground and that at H.

Figure 6.1 de Nevers

Simple box model of a rectangular city

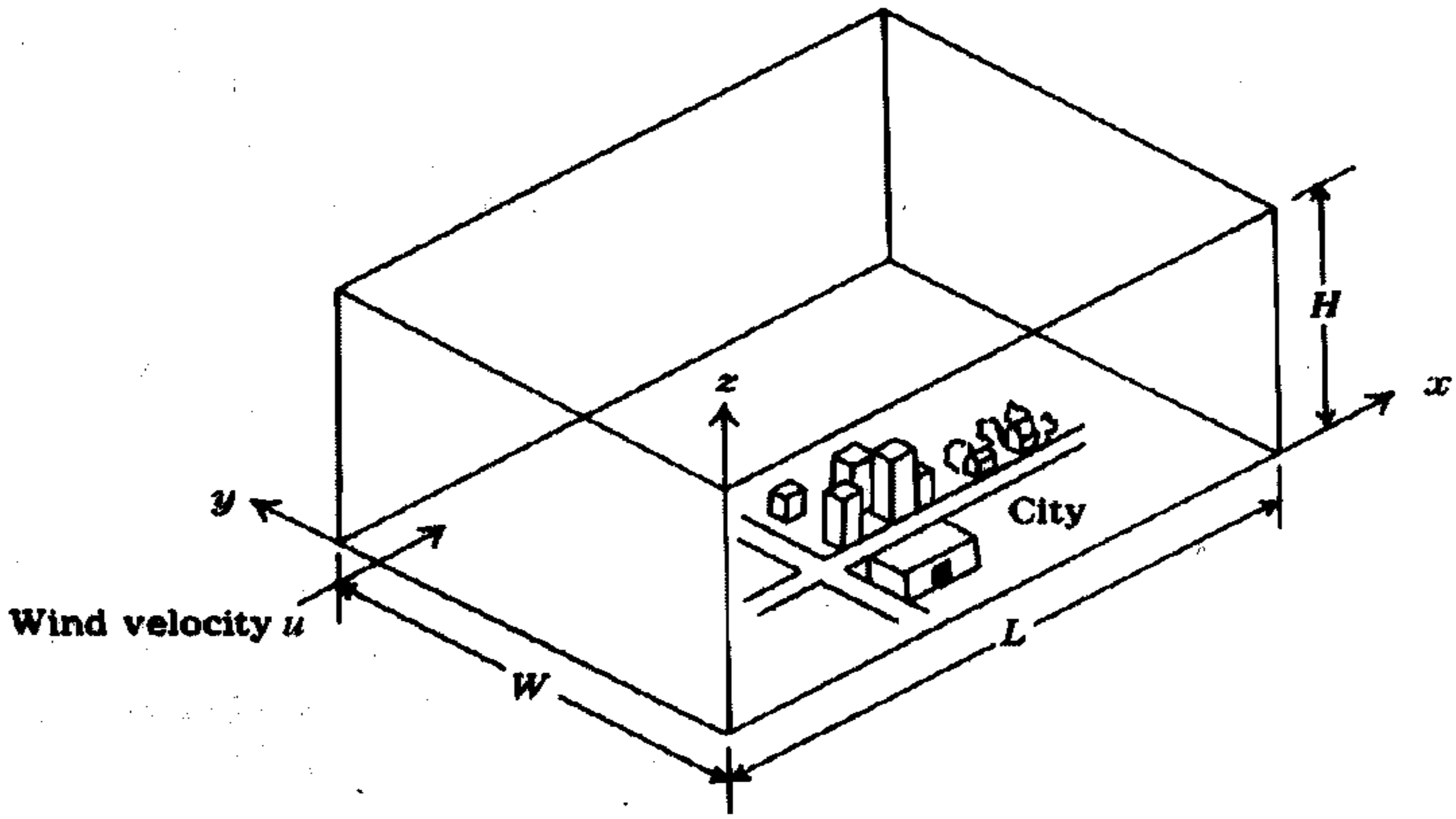


FIGURE 6.1
Rectangular city, showing meaning of symbols used in the fixed-box model.

FIXED-BOX MODELS

5. The concentration of pollutant in the air entering the city (at x = 0) is constant and is equal to b (b for “background” concentration, a term borrowed from the nuclear field, from which many of the early air pollution meteorologists came). Concentrations in this model and in most of this chapter are usually in units of g/m3 or micrograms/m3.
6. The air pollutant emission rate of the city is Q (typically expressed in g/s). This is normally given as an emission rate per unit area, q, in g/s.m2. We can convert from one to the other by:

$$Q = q. A$$

   where A is the area of the city, which equals W times L in this case. This emission rate is constant and unchanging with time.
7. No pollutant leaves or enters through the top of the box, nor through the sides that are parallel to the wind direction.
8. The pollutant in question is sufficiently long-lived in the atmosphere that the destruction rate in Eq. (6.1) is zero.

FIXED-BOX MODELS

- Now evaluate all of the terms in Eq. (6.1). Choose as our system the volume WLH.
- All assumptions indicate that flows and emission rates are independent of time.
- For any steady-state situation , the accumulation rate is zero.
- We may treat the emission rate Q either as a generation rate or as a flow into the box through its lower face; either gives exactly the same result.
- Thus, material balance equation becomes:

0= (flow rate in) + (generation rate) = (flow rates out)

(I)The flow rate of pollutant into the upwind side of the city:

Flow rate in = u W H b

FIXED-BOX MODELS

- The first three symbols constitute the volume of air that crosses the upstream boundary of the system per unit time; the student may verify that u WH has dimensions of volume/time. Multiplying it by a concentration (mass/volume), we obtain a mass flow rate (mass/time).

  (II) The generation rate is that of pollutant emitted by the city into the lower face of the system:

  $$\text{Generation rate} = Q = q\, W\, L$$

- According to the preceding assumptions, the concentration in the entire city is constant and is equal to c.
- The only way pollutant leaves the system is by flow out through the downwind face.

  (III) The flow rate out is given by the equation

  $$\text{Flow rate out} = u\, W\, H\, c$$

SIMPLE BOX MODEL OF A CITY

$$c = b + \frac{qL}{uH} \quad ,\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(6.7)$$

b = pollutant concentration in entering air, g/m3

q = pollutant mass emission rate

per unit area in the city (area source), g/s/m2

L = length of box in direction of wind, m

H = mixing height, m

u = wind speed, m/s

c = pollutant concentration in air leaving box, g/m3

Example 6.1. A city has the following description: $W = 5$ km, $L = 15$ km, $u = 3$ m/s, $H = 1000$ m. The upwind, or background, concentration of carbon monoxide is $b = 5\ \mu g/m^3$. The emission rate per unit area is $q = 4 \times 10^{-6}\ g/s \cdot m^2$. What is the concentration c of carbon monoxide over the city?

By direct substitution into Eq. (6.7), we find

$$c = \frac{5\ \mu g}{m^3} + \left(4 \times 10^{-6} \frac{g}{s \cdot m^2}\right)\left[\frac{15{,}000\ m}{(3\ m/s)(1000\ m)}\right]$$

$$= 5 + 20 = 25\ \frac{\mu g}{m^3}$$

■

Notes on BOX MODEL - Equation (6.7)

- Note that W does not enter the calculation or influence the result. This is reasonable for the model chosen; doubling the width of the city while holding q constant would not change c. **(DOWNWIND)**
- Eq. (6.7) is a great simplification of reality. However, it correctly indicates that
  - the upwind concentration for a long-lived pollutant is additive to the concentration produced by the city and that
  - the latter increases with increases in q and L and decreases with increases in u and H.
- The worst assumptions are:
  - that the concentrations at the upwind and downwind edges of the city are the same.
  - that the emissions are uniformly distributed over the area of the city (i.e., q is constant over the whole city).

$$c = b + \frac{qL}{uH}$$

Notes on BOX MODEL Equation (6.7)

- The simple fixed-box model of Eq. (6.7), as well as most of the other models, predicts concentrations for **only one specific** meteorological condition.
- To find the **annual average** concentration of some pollutant, we would have to use the frequency distribution of *various values* of wind direction, u, and H, compute the concentration from Eq. (6.7) *for each value,* and then multiply by the frequency and sum to find the annual average; that is,

$$\begin{pmatrix}\text{Annual}\\ \text{average}\\ \text{concentration}\end{pmatrix} = \sum_{\text{over all meteorologies}} \begin{pmatrix}\text{concentration}\\ \text{for that}\\ \text{meteorology}\end{pmatrix} \begin{pmatrix}\text{frequency of}\\ \text{occurrence of that}\\ \text{meteorology}\end{pmatrix} \tag{6.8}$$

Example 6.2. For the city in Example 6.1, the meteorological conditions described ($u = 3$ m/s, $H = 1000$ m) occur 40 percent of the time. For the remaining 60 percent, the wind blows at right angles to the direction shown in Fig. 6.1 at velocity 6 m/s and the same mixing height. What is the annual average concentration of carbon monoxide in this city?

First we find the concentration for the other meteorological condition using Eq. (6.7). Observe that the wind direction shift has interchanged the values of W and L (see Fig. 6.1). Thus,

$$c = 5\ \frac{\mu\text{g}}{\text{m}^3} + \left(4 \times 10^{-6}\ \frac{\text{g}}{\text{s} \cdot \text{m}^2}\right)\left[\frac{5000\ \text{m}}{(6\ \text{m/s})(1000\ \text{m})}\right] = 8.33\ \frac{\mu\text{g}}{\text{m}^3}$$

Using this value plus the one from Example 6.1 in Eq. (6.8), we find

$$\begin{pmatrix}\text{Annual} \\ \text{average} \\ \text{concentration}\end{pmatrix} = 25\ \frac{\mu\text{g}}{\text{m}^3} \times 0.4 + 8.33\ \frac{\mu\text{g}}{\text{m}^3} \times 0.6 = 15\ \frac{\mu\text{g}}{\text{m}^3} \quad \blacksquare$$

$$c = b + \frac{qL}{uH}$$

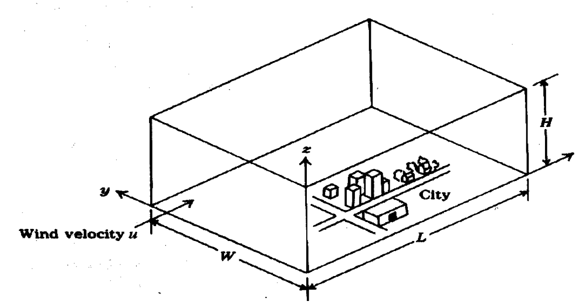


FIGURE 6.1
Rectangular city, showing meaning of symbols used in the fixed-box model.

AP Plumes

Gaussian plume

- Pollutants have a longer time to diffuse laterally ***before*** the high concentration region of the plume touches ground

- So, the maximum concentration at ground level is not found at the source but at some distance from the stack

- The magnitude of the *maximum concentration* and *where it is expected* to occur are two of the most important questions involved in the effectiveness of an exhaust stack.

DIFFUSION MODELS: GAUSSIAN PLUME

FIGURE 6.3 DE NEVERS

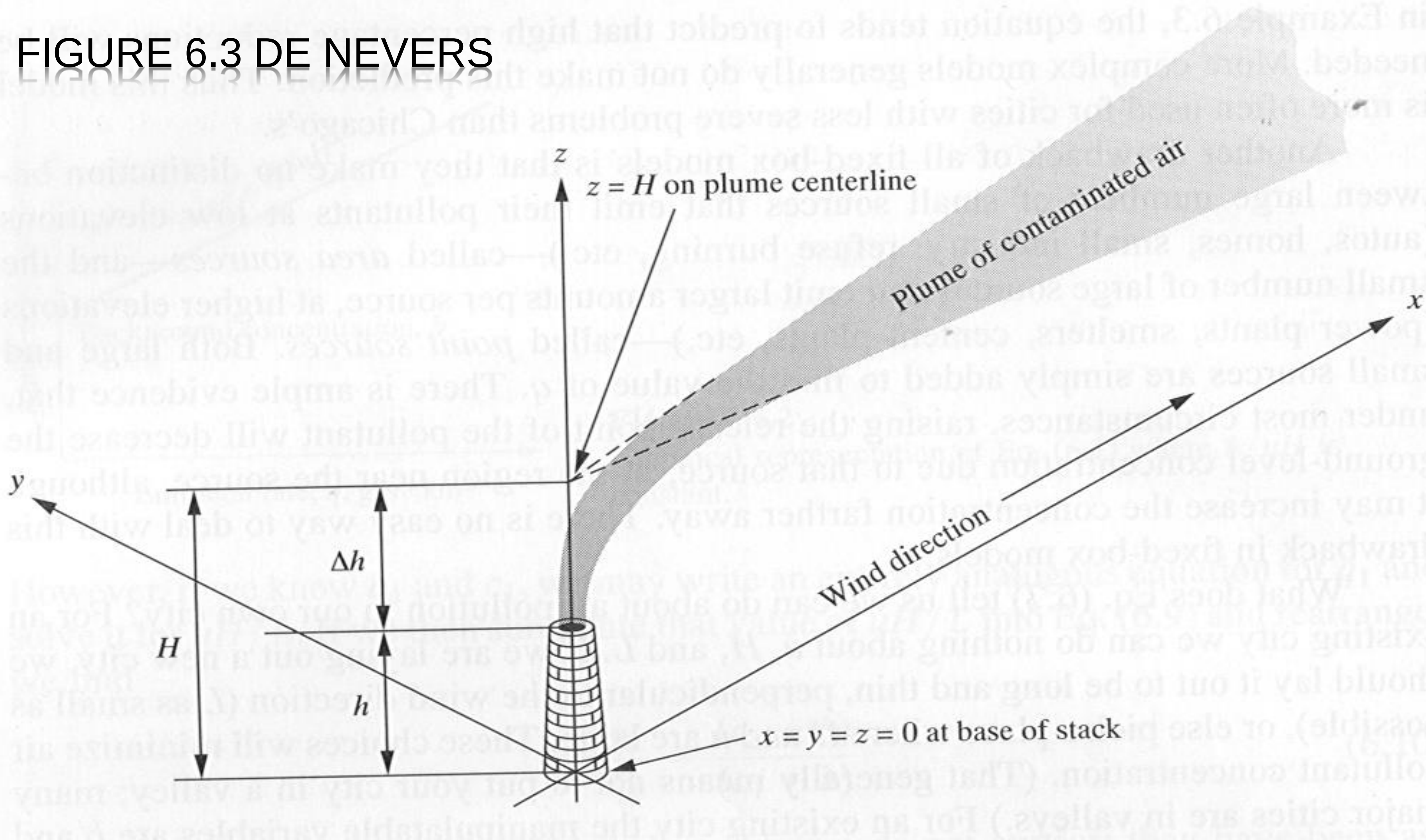


FIGURE 6.3
Coordinate system and nomenclature for the Gaussian plume idea.

ATMOSPHERIC DISPERSION

- Factors Affecting Dispersion of Air Pollutants

- The factors that affect the transport, dilution, and dispersion of air pollutants can generally be categorized in terms of:

  1. the emission point characteristics,
  2. the nature of the pollutant material,
  3. meteorological conditions, and
  4. effects of terrain and anthropogenic structures.

- We will integrate the <u>first and third factors</u> to describe the qualitative aspects of calculating pollutant concentrations and follow this with a quantitative model.

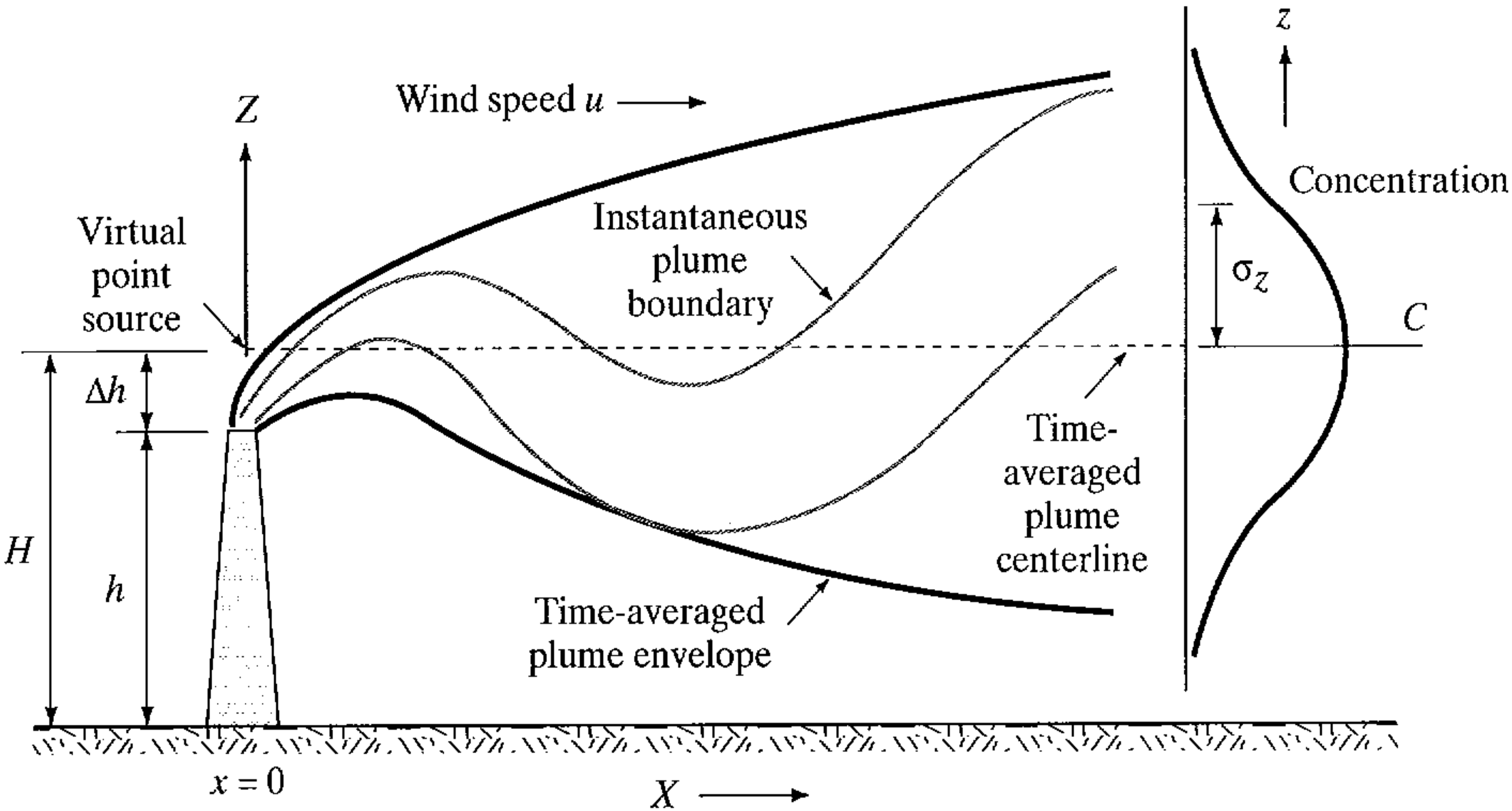
Dispersion Modeling

- General considerations and use of models.
  - A dispersion model is a mathematical description of the meteorological transport and dispersion process that is quantified in terms of source and meteorological parameters during a particular time.
  - The resultant numerical calculations yield estimates of concentrations of the particular pollutant for specific locations and times.

Model Assumptions

- Gaussian dispersion modeling based on a number of assumptions including
  - Horizontal and vertical pollutant concentrations in the plume are normally distributed (double Gaussian distribution)
  - Steady-state conditions (constant source emission strength)
  - Wind speed, direction and diffusion characteristics of the plume are constant
  - Mass transfer due to bulk motion in the x-direction far out-shadows the contribution due to mass diffusion
  - Conservation of mass, i.e. no chemical transformations take place

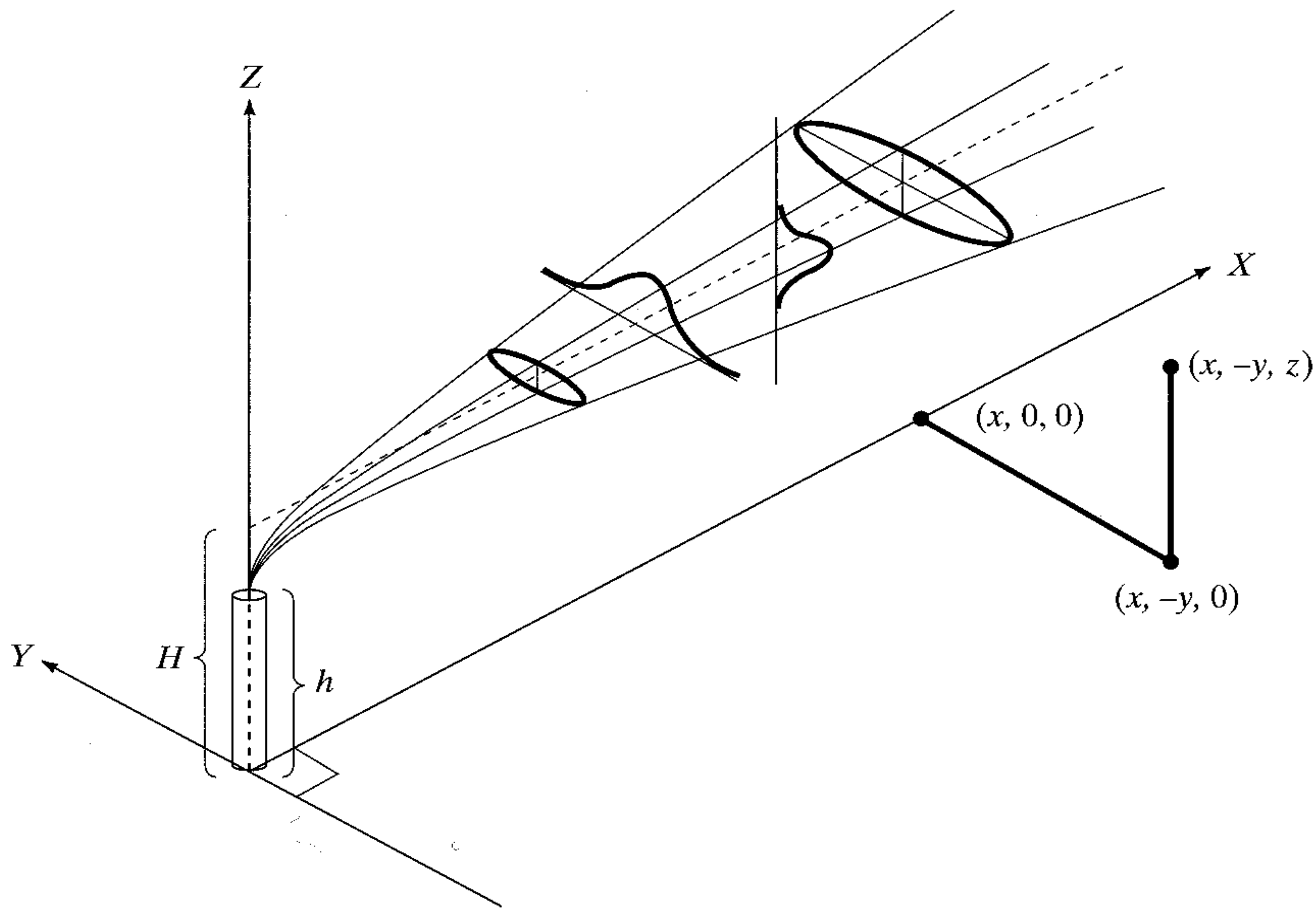
Point Source Gaussian Model



Gaussian Plume Model

- Employs a 3D axis system of downwind, crosswind, and vertical with the origin at the ground
- Assumes
  - the concentrations from a continuously emitting plume are proportional to the emission rate
  - The concentrations are diluted by the wind at the point of emission at a rate inversely proportional to the wind speed
  - The time averaged (~ 1h) pollutant concentrations crosswind and vertically near the source are well described by Gaussian distributions
  - The standard deviations of plume concentration in these two directions are empirically related to the level of turbulence in the atmosphere and increase with distance from the source

Point Source Plume



BASIC GAUSSIAN PLUME EQUATION

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

Equation 6-27

wind speed, u (m/s)

continuous release of Q (g/s) of pollutant at : x = y = 0 (stack location) and

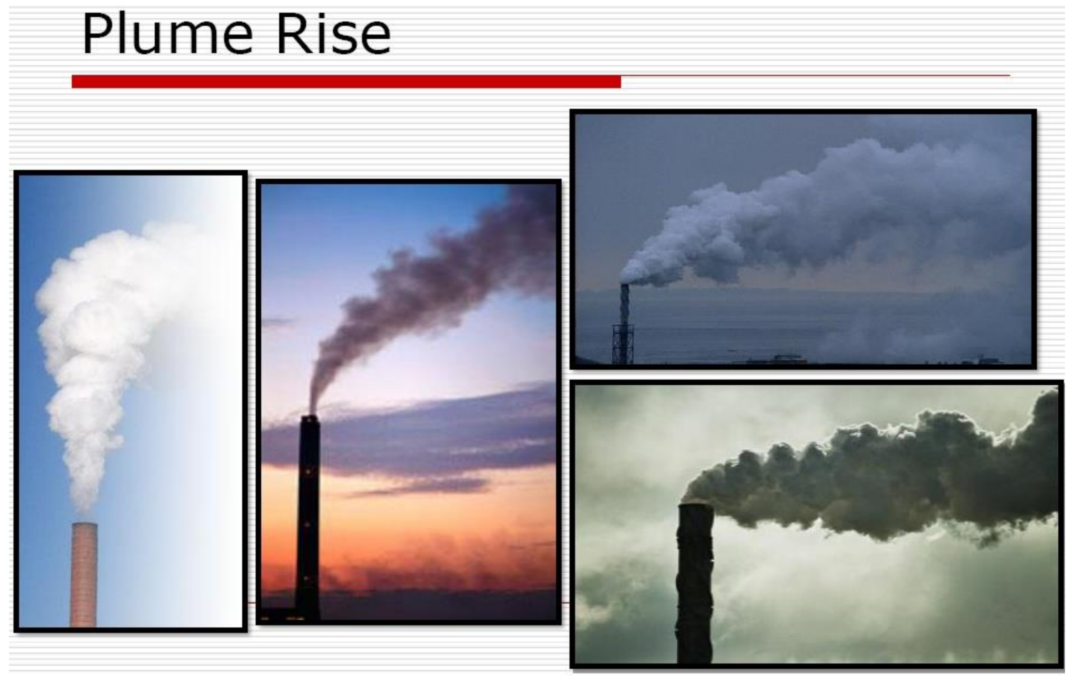
z = H (the effective stack height)

H = h + Δh

h : physical stack height,

Δh : plume rise due to buoyancy

Effective Stack Height



$$H = h + \Delta h$$

where:

H = effective stack height (m)

h = height of physical stack (m)

Δh = plume rise (m)

Effective Stack Height

- **Holland's formula**

$$\Delta h = \frac{v_s}{u}\left[1.5 + \left(2.68 \times 10^{-2}(P)\left(\frac{T_s - T_a}{T_a}\right)d\right)\right]$$

where v_s = stack velocity (m/s)

d = stack diameter (m)

u = wind speed (m)

P = pressure (kPa)

T_s = stack temperature (K)

T_a = air temperature (K)

Holland's Simple Equation

- For large power plants, the heat emission rate (Q_H) is usually reported instead of stack temperature

$$\Delta h = 1.5 \frac{v_s d_s}{u} + 9.6 \frac{Q_H}{u}$$

v_s = stack exit velocity (m/s)
d_s = stack diameter (m)
u = wind velocity (m/s)
Q_H = heat emission rate (MW)

BASIC GAUSSIAN PLUME EQUATION

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

Equation 6-27

- ✓ u (m/s): wind speed
- ✓ Q (g/s): continuous release of of pollutant at :
  x = y = 0 (stack location)
- ✓ z = H: effective stack height)

H = h + Δh

h : physical stack height,

Δh : plume rise due to buoyancy

DISPERSION COEFFICIENTS

$$\sigma_y = \sqrt{\frac{2K_y x}{u}} \qquad \sigma_z = \sqrt{\frac{2K_z x}{u}}$$

K_y and K_z = dispersion coefficients (approx. proportional to wind speed)

K_y/u and K_z/u approximately constant

σ_y and σ_z (standard deviations); they vary with $x^{(1/2)}$

Field observations show more complex variation

(Figures 6.7 and 6.8 de Nevers)

Wind speed and solar flux combine to give stability classes

A - F (Table 6.1 de Nevers)

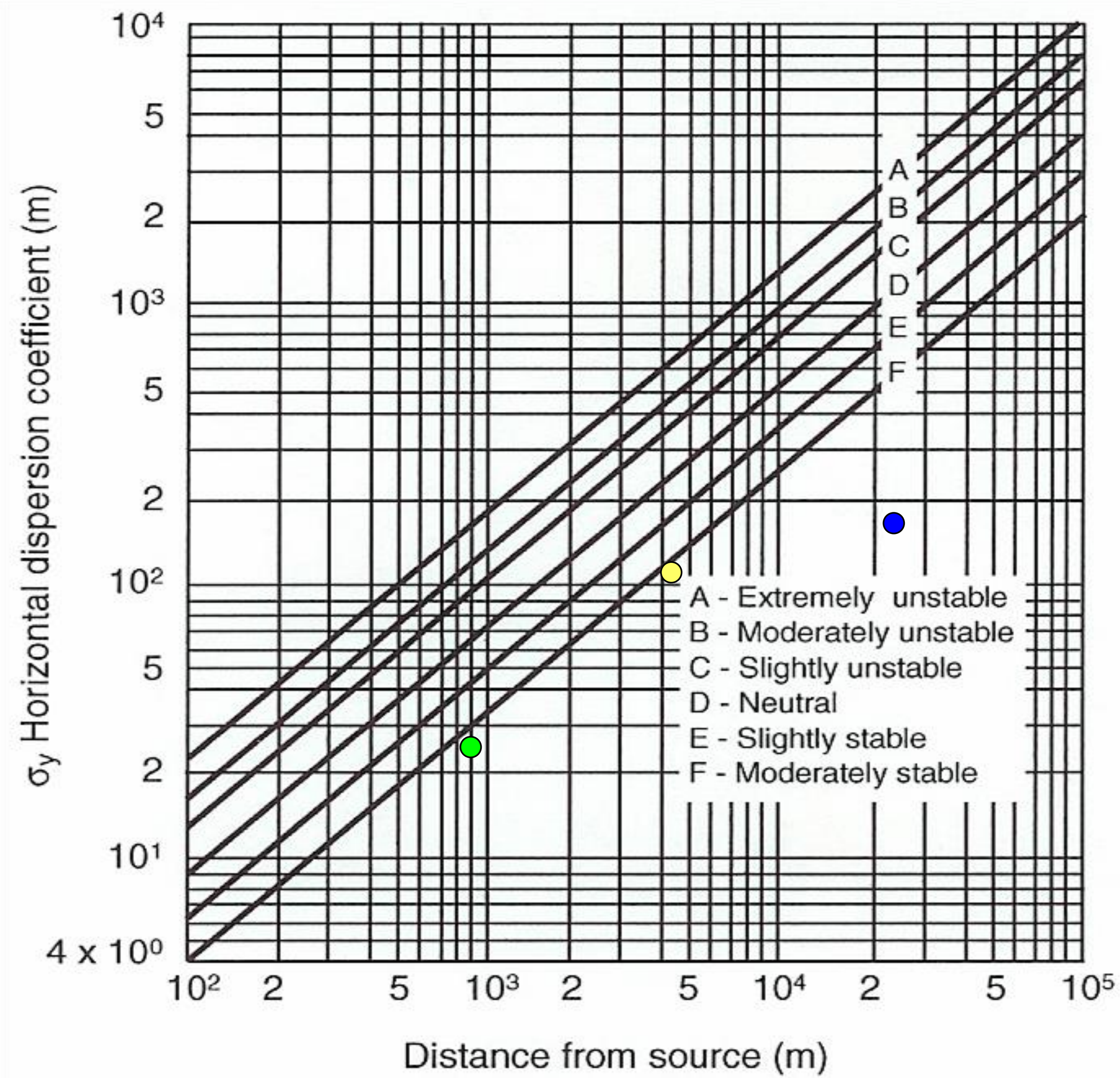
Stability Classes

TABLE 6.1
Key to stability categories

Surface wind speed (at 10 m), m/s	Day			Night	
	Incoming solar radiation				
	Strong	Moderate	Slight	Thinly overcast or $\geq \frac{4}{8}$ cloud	Clear or $\leq \frac{3}{8}$ cloud
0–2	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

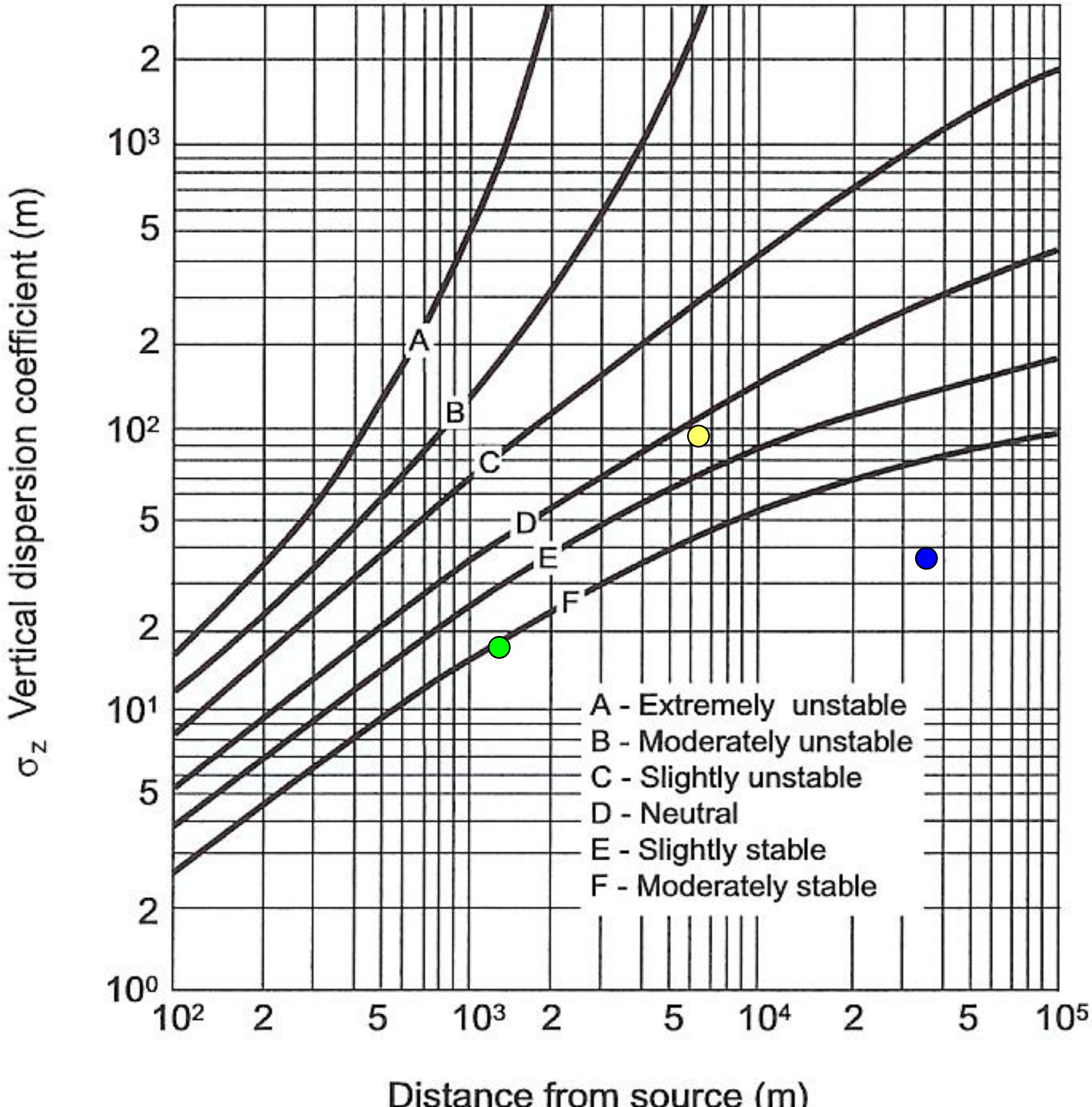
Source: Ref. 6.

Note: The neutral class D should be assumed for overcast conditions during day or night.



Dispersion Coefficients: Horizontal

FIGURE 6.7 DE NEVERS



Dispersion Coefficients: Vertical

FIGURE 6.8 DE NEVERS

Determining Sky Conditions

Description	Fraction	Meaning
Clear	0	No clouds
Few	0 to 2/8	Few clouds visible
Scattered	3/8 to 4/8	Partly cloudy
Broken	5/8 to 7/8	Mostly cloudy
Overcast	8/8	Sky is covered by clouds
Sky obscured	--	Hidden by fog, smoke, …

Height of Cloud Bases

	Tropics	Middle Lat.	Polar
High	20,000 to 60,000 ft	16,000 to 43,000 ft	10,000 to 26,000 ft
Middle	6,500 to 26,000 ft	6,500 to 23,000 ft	6,500 to 13,000 ft
Low	surface to 6,500 ft	surface to 6,500 ft	surface to 6,500 ft

Note how cloud heights lower at higher latitude.

Atmospheric stability

- Two governing factors:
  - Temperature gradient (lapse rate)
  - Turbulence due to wind

- Dry adiabatic lapse rate : 10 ºC / km
- Saturated adiabatic lapse rate : 6 ºC /km
- “Standard” profile : 6.6 ºC / km

Special Cases: ground level

1) We are most interested in ground level, z=0, concentrations (where humans and other life forms reside); c at ground level:

$$c(x,y,0,H)=\frac{Q}{\pi\sigma_y\sigma_z\bar{u}}\left\{\exp\left(\frac{-y^2}{2\sigma_y^2}\right)\right\}\left\{\exp\left(\frac{-H^2}{2\sigma_z^2}\right)\right\}$$

2) On the center line, z=y=0, where concentrations are at their maximum; directly downwind (along the plume line, parallel to the wind direction); c at ground level:

$$c(x,0,0,H)=\frac{Q}{\pi\sigma_y\sigma_z\bar{u}}\left\{\exp\left(\frac{-H^2}{2\sigma_z^2}\right)\right\}$$

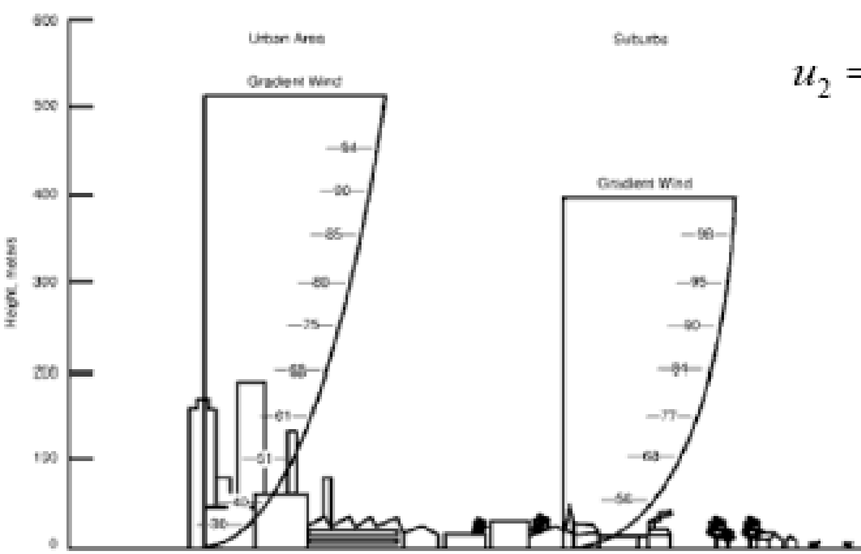
Special Cases: ground level

3) Assuming effective stack height, H =0 (correct for surface burning), the model is simplified as follows:

$$c(x,0,0,0) = \frac{Q}{\pi \sigma_y \sigma_z \bar{u}}$$

Wind Speed as a Function of Height

- The wind speed (u_2) at stack height (z_2) can be estimated using surface wind measurement(u1 @ z1):



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

Dependence of p as a function of stability and surface roughness

Stability	urban	rural
A	0.15	0.07
B	0.15	0.07
C	0.2	0.1
D	0.25	0.15
E	0.3	0.35
F	0.3	0.35

Wind speed example

- Calculation wind speed at 477m if the wind speed at 10m above surface is 2 m/s. Assume neutral condition in urban area.

$$U_{477} = U_{10} * (477/10)^{0.25}$$

$$= 2 * 2.62 = 5.3 \text{ m/s}$$

Summarize – Gaussian Dispersion Problem

- Determine stability class
- Calculate plume rise
- Calculate wind speed
- Calculate $\sigma_y \sigma_z$
- Calculate pollutant concentration

Example: Gaussian Model

A stack in an *urban area* is emitting 80 g/s of NO.

It has an effective stack height, H of 100 m.

The wind speed is 4 m/s at 10 m (~ Ground Level).

It is a clear summer day with the sun nearly overhead.

Estimate the ground level concentration of NO at:

a) 2 km downwind on the centerline and

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

Solution of Example

1. Determine stability class:

   Assume wind speed is 4 km at ground surface.
   Description suggests strong solar radiation.

   Stability class: B

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

2. Estimate the wind speed at the effective stack height (u_2)

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

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

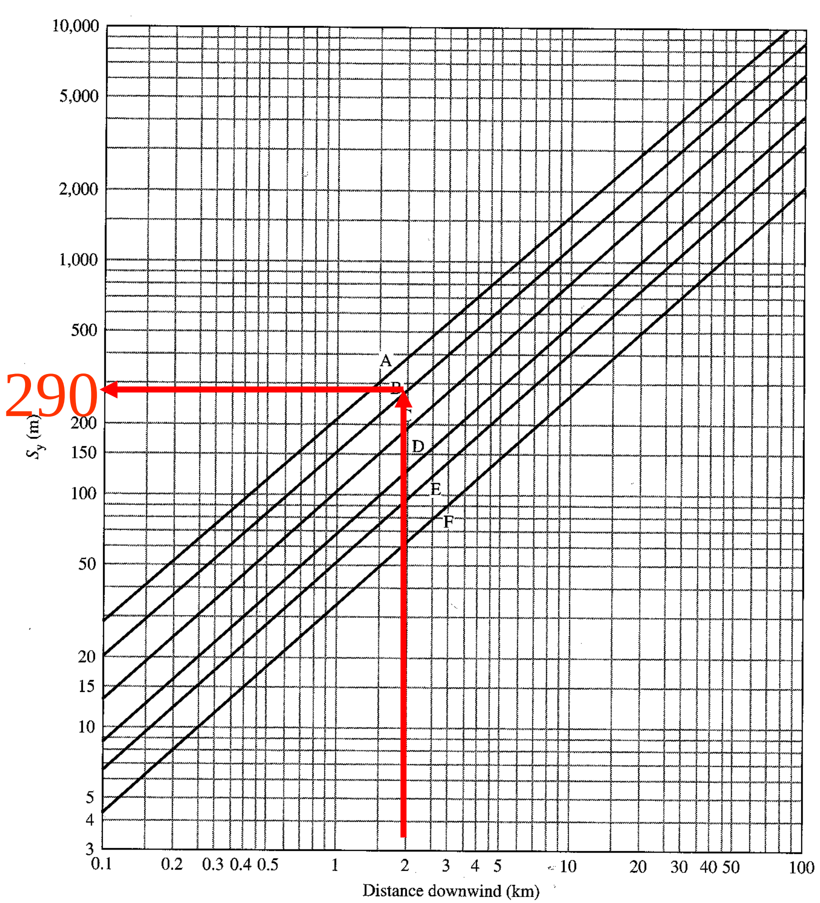
Stability Class	Rural	Urban	Stability Class	Rural	Urban
A	0.07	0.15	D	0.15	0.25
B	0.07	0.15	E	0.35	0.30
C	0.10	0.20	F	0.55	0.30

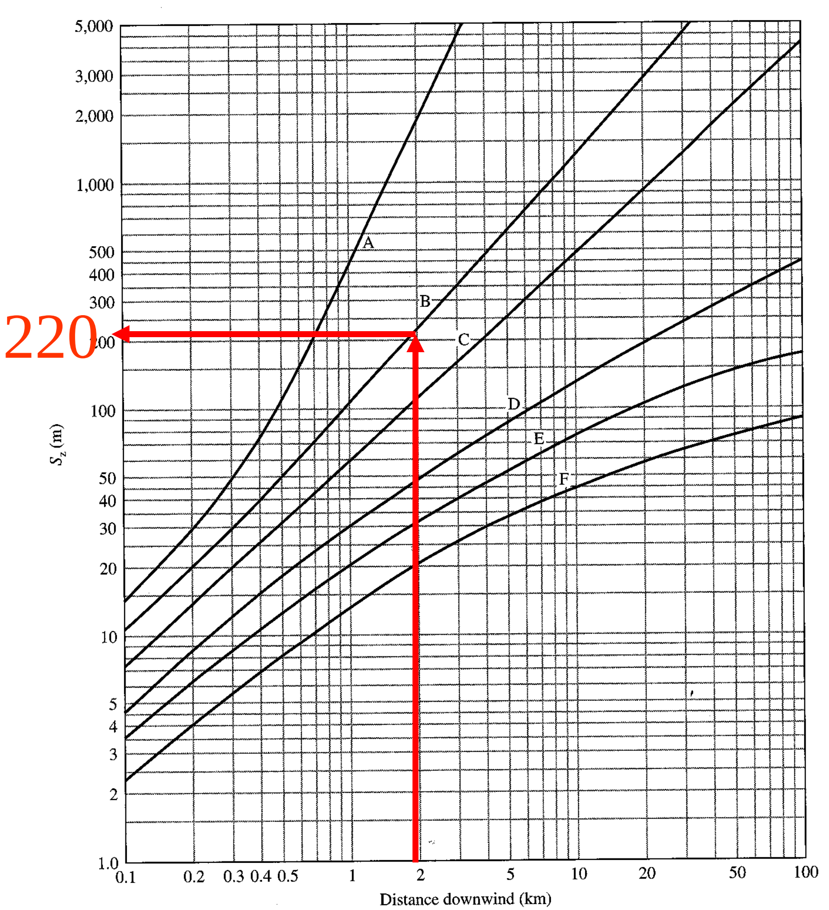
$$u_2 = u_1 \left(\frac{z_2}{z_1} \right)^p = 4 \left(\frac{100}{10} \right)^{0.15} = 5.65 \, \text{m/s}$$

3. Determine σ_y and σ_z

$\sigma_y = 290$

$\sigma_z = 220$





4. Determine concentration using the Eq.

$$c(x, y, 0, H) = \frac{Q_p}{\pi \sigma_y \sigma_z \bar{u}} \left\{ \exp\left(\frac{-y^2}{2\sigma_y^2} \right) \right\} \left\{ \exp\left(\frac{-H^2}{2\sigma_z^2} \right) \right\}$$

x = 2000 m, y = 0, z = 0 (@ centerline)

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

$$C(2000,0,0) = 6.43 \times 10^{-5}\ \text{g/m}^3 = 64.3\ \mu\text{g/m}^3$$

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

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

$$C(2000,0,0) = 6.06 \times 10^{-5}\ \text{g/m}^3 = 60.6\ \mu\text{g/m}^3$$

Maximum Ground Level Concentration

Under moderately stable to near neutral conditions,

$$\sigma_y = k_1 \sigma_z$$

The ground level concentration **at the center line** is

$$C(x,0,0) = \frac{Q}{\pi k_1 \sigma_z^2 u} \exp\left[-\frac{H^2}{2\sigma_z^2}\right]$$

The maximum occurs at $dC / d\sigma_z = 0 \quad \Rightarrow \sigma_z = \frac{H}{\sqrt{2}}$

See GRAPH next

Once σ_z is determined, x can be known and subsequently C.

$$C(x,0,0) = \frac{Q}{\pi \sigma_y \sigma_z u} \exp[-1] = 0.1171 \frac{Q}{\sigma_y \sigma_z u}$$