Process Safety Engineering:

Toxic Release and Dispersion Models

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Practical and Potential Releases

During an accident process equipment can release toxic materials very quickly

- Explosive rupture of a process vessel due to excess pressure
- Rupture of a pipeline with material under high pressure
- Rupture of tank with material above boiling point
- Rupture of a train or truck following an accident.

- ✓ **Identify the Design basis**

  What process situations can lead to a release, and which are the worst situations

- ✓ **Source Model**

  What are the process conditions and hence what will be the state of the release and rate of release

- ✓ **Dispersion Model**

  Using prevailing conditions (or worst case) determine how far the materials could spread

Dispersion Models

What?

- Describe how vapors are transported downwind of a release. Valid between 100 m to 10 km.

- Below 100 m use ventilation equations Chapt. 3.
- Above 10 km: almost unpredictable.

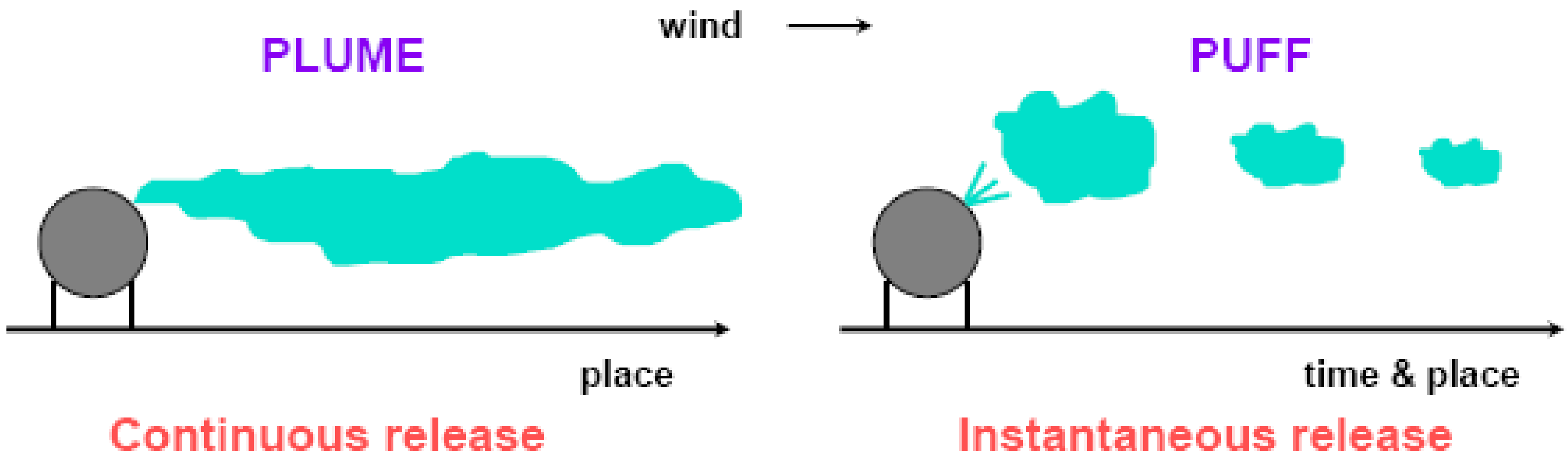
Why?

To determine the consequences.

Results:

- ✓ Downwind concentrations (x, y, z)
- ✓ Area affected
- ✓ Downwind evacuation distances

Dispersion

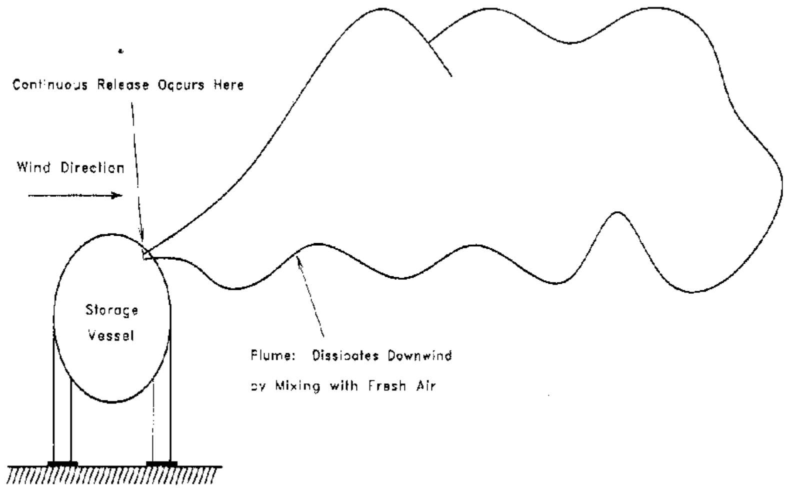


DOWNWIND DILUTION BY MIXING WITH FRESH AIR

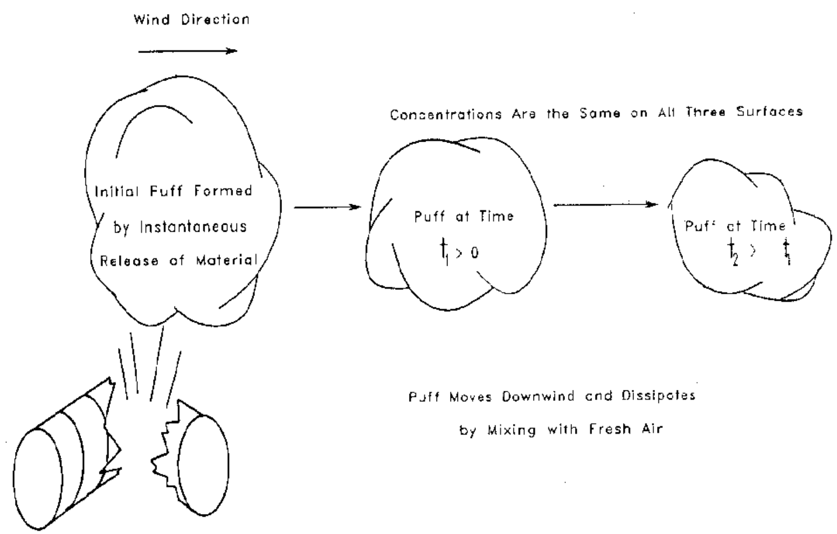
ATMOSPHERIC DISPERSION

- Wind speed
- Atmospheric stability: vertical temp. profile
- Roughness ground: buildings, structures, trees, water
- Height of release above ground level
- Momentum and buoyancy: effective height

- Plume models were originally developed for dispersion from a smoke stack.
- In an emergency if there is a leak in a large tank then a plume can develop.



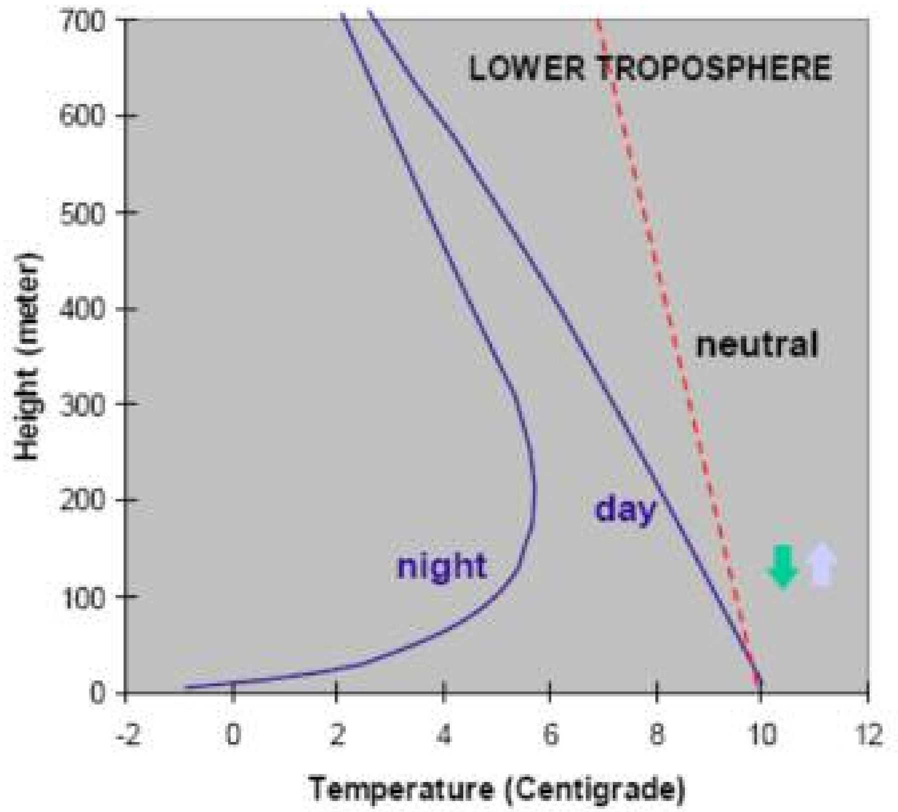
- Puff models are used when you have essentially an instantaneous release and the cloud is swept downwind.
- No significant plume develops



Atmospheric stability

MAINLY DETERMINED BY VERTICAL TEMPERATURE GRADIENT

- **Unstable** atmospheric conditions: Sun heats ground faster than heat can be removed so that air temperature near the ground is higher than the air temperature at higher elevations.
- **Neutral**: The air above the ground warms and the wind speed increases, reducing the effect of solar input.
- **Stable**: The sun cannot heat the ground as fast as the ground cools - temperature at ground is lower.



Atmospheric stability

STABILITY CLASSES A - F

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

Table 5-1

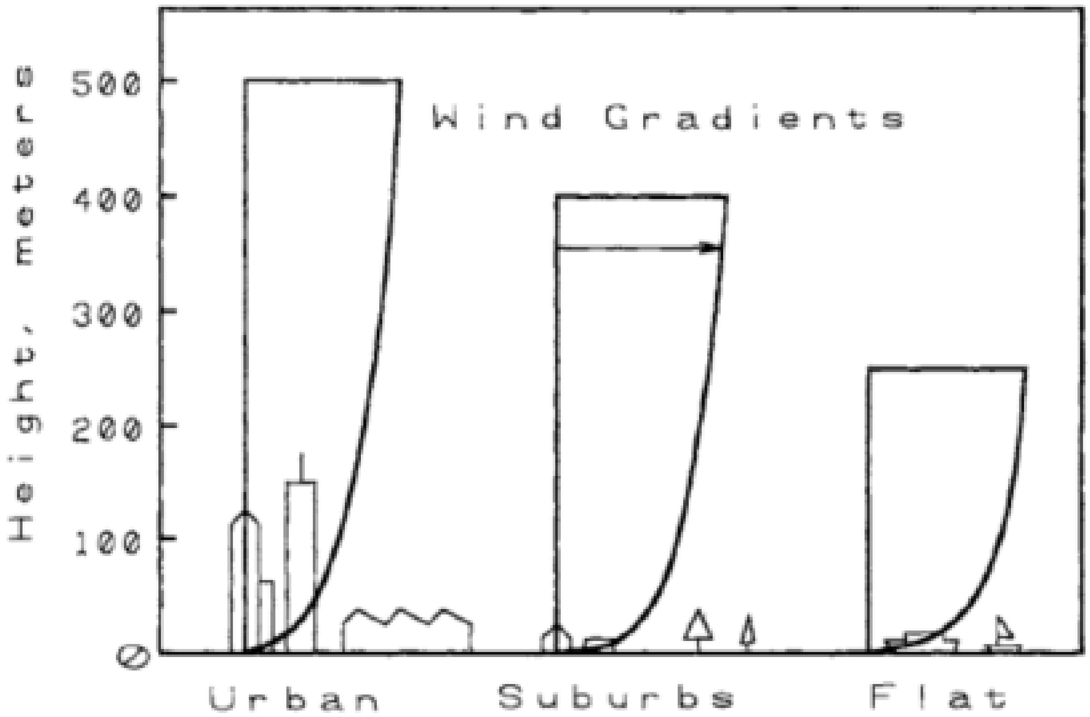
Table 5-1 Atmospheric Stability Classes for Use with the Pasquill-Gifford Dispersion Model[1,2]

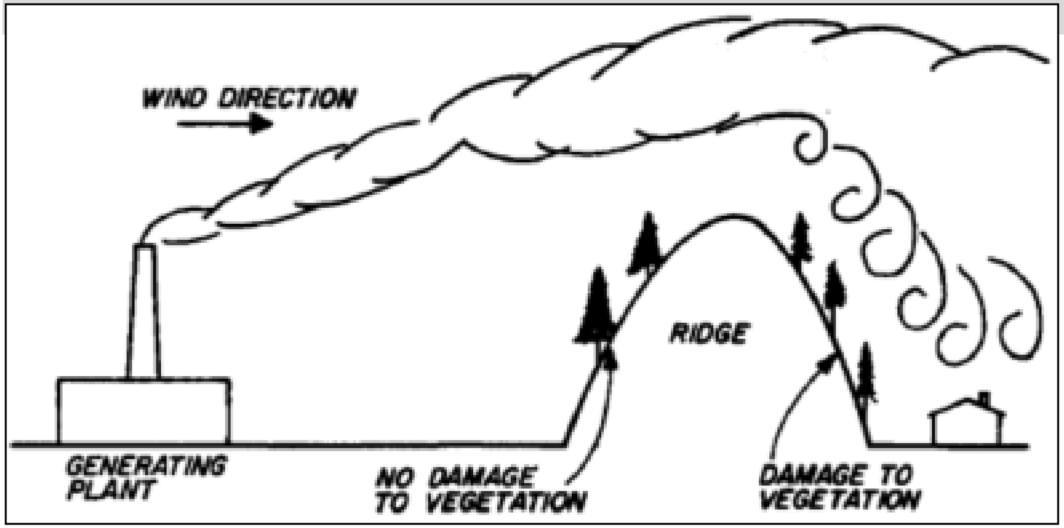
Surface wind speed (m/s)	Daytime insolation[3]			Nighttime conditions[4]	
	Strong	Moderate	Slight	Thin overcast or >4/8 low cloud	≤3/8 cloudiness
<2	A	A–B	B	F[5]	F[5]
2–3	A–B	B	C	E	F
3–4	B	B–C	C	D[6]	E
4–6	C	C–D	D[6]	D[6]	D[6]
>6	C	D[6]	D[6]	D[6]	D[6]

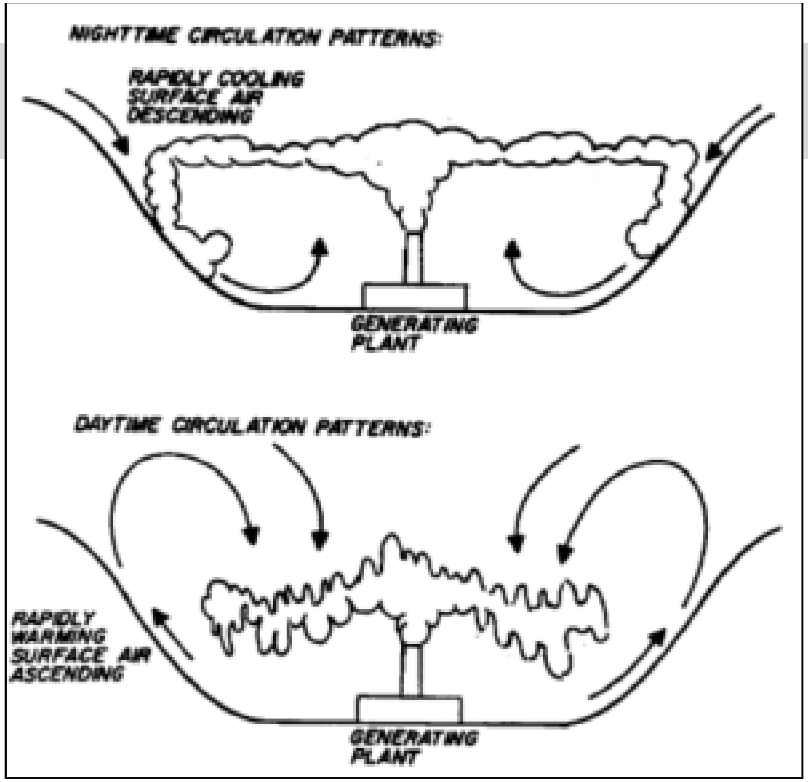
Ground conditions

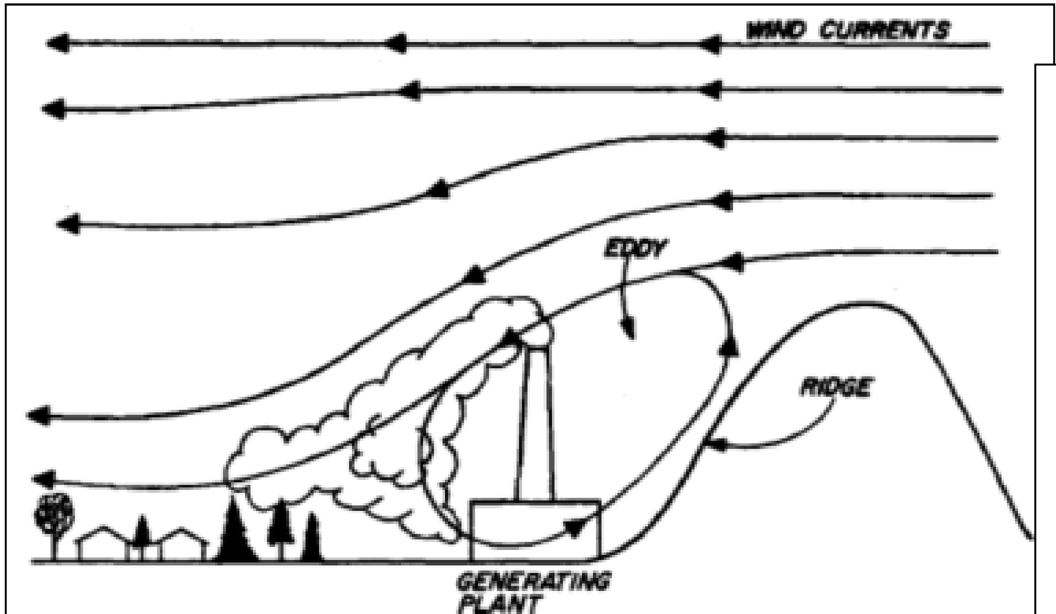
- Ground conditions affect the mechanical mixing at the surface and the wind profile with height.

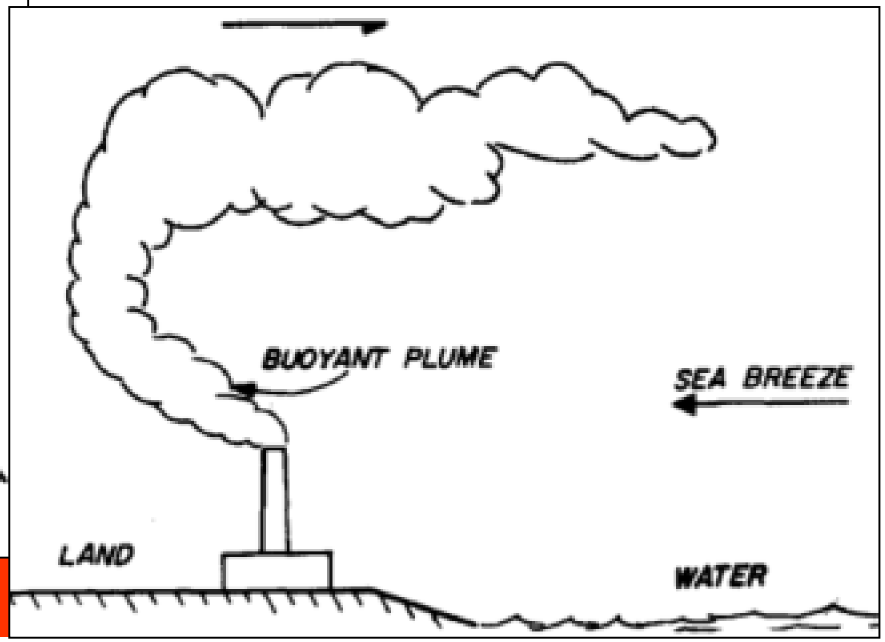
- Trees and buildings increase mixing, whereas lakes and open areas decrease it




WIND DIRECTION
RIDGE
GENERATING PLANT
NO DAMAGE TO VEGETATION
DAMAGE TO VEGETATION

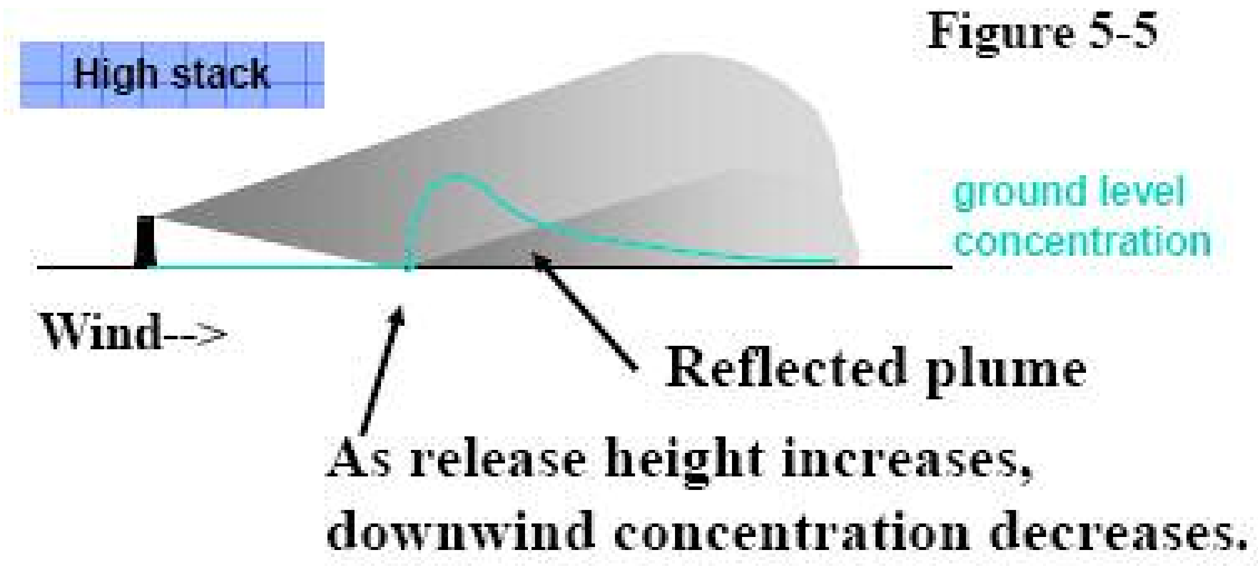

NIGHTTIME CIRCULATION PATTERNS:
RAPIDLY COOLING SURFACE AIR DESCENDING
GENERATING PLANT
DAYTIME CIRCULATION PATTERNS:
RAPIDLY WARMING SURFACE AIR ASCENDING
GENERATING PLANT


WIND CURRENTS
EDDY
RIDGE
GENERATING PLANT


BUOYANT PLUME
SEA BREEZE
LAND
WATER

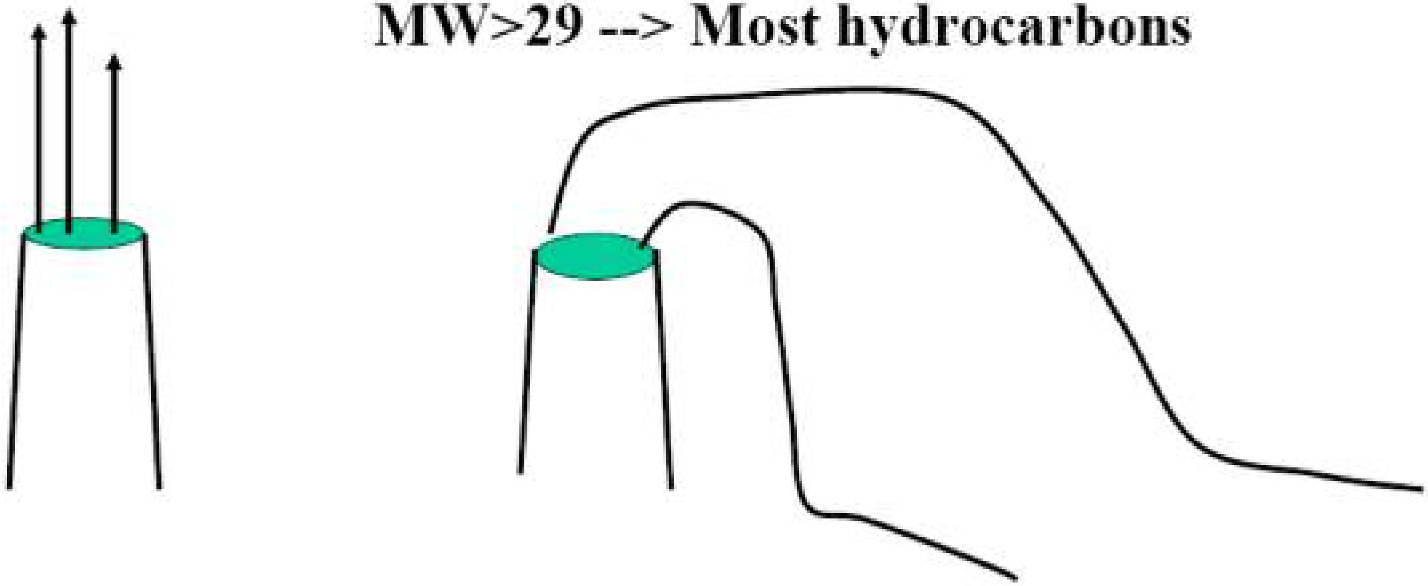
Release Height Effect

- The release height significantly affects ground-level concentrations.
- As the release height increases, ground-level concentrations are reduced because the plume must disperse a greater distance vertically.



Release Momentum and Buoyancy

MW>29 --> Most hydrocarbons

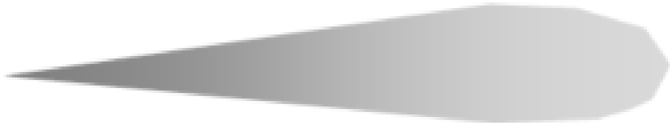


Jet Release

Heavier than air. Gas becomes neutral downwind as it mixes with air.

Gaussian form of plume equation

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



Top View of plume

--> Wind

$\langle C \rangle (x,y,z) =$ Ave. conc. (20-30 min ave)

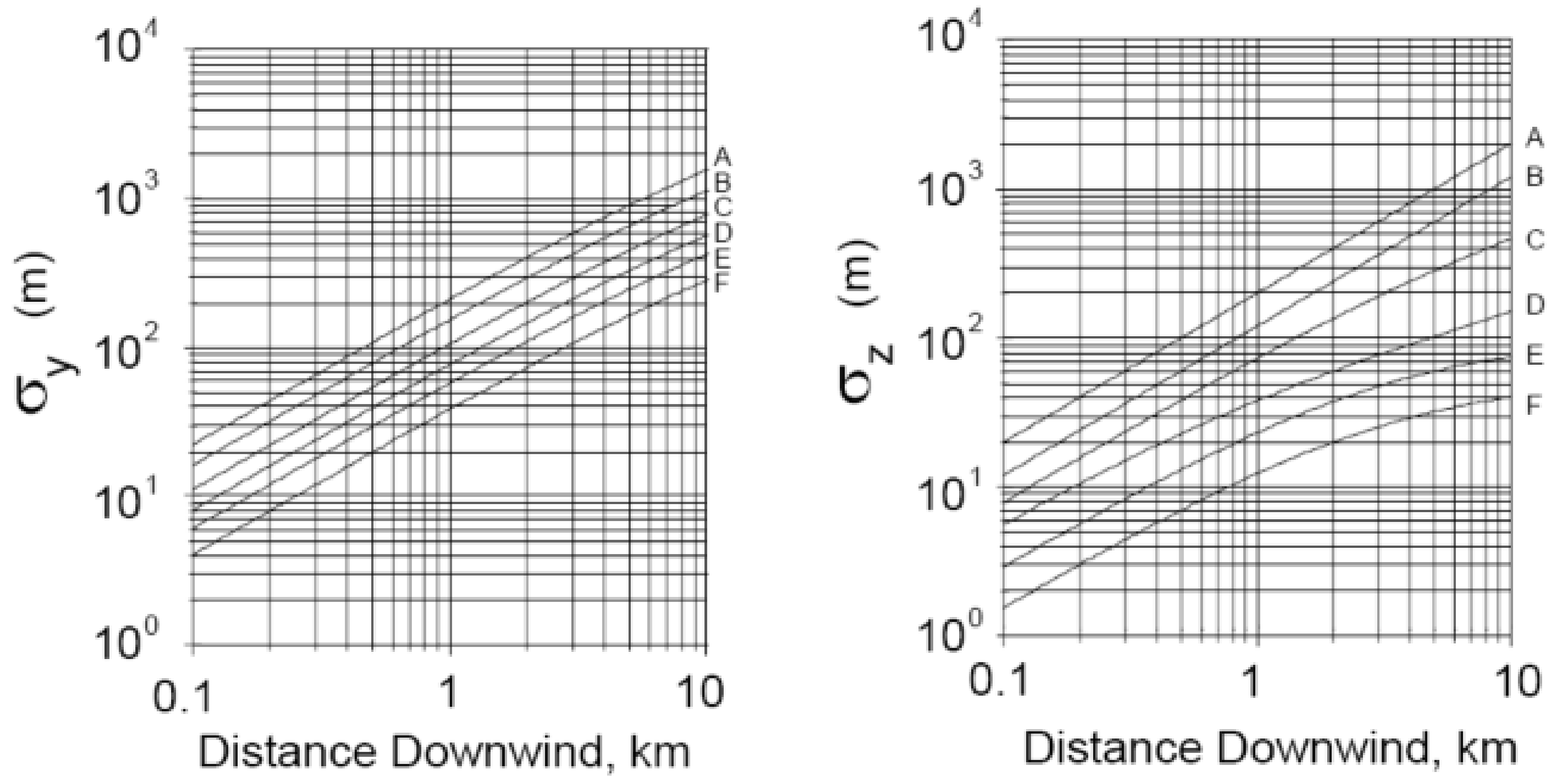
Q_m = Release rate (mass/time)

σ_y, σ_z = Dispersion coefficients = f(stability class, downwind distance)

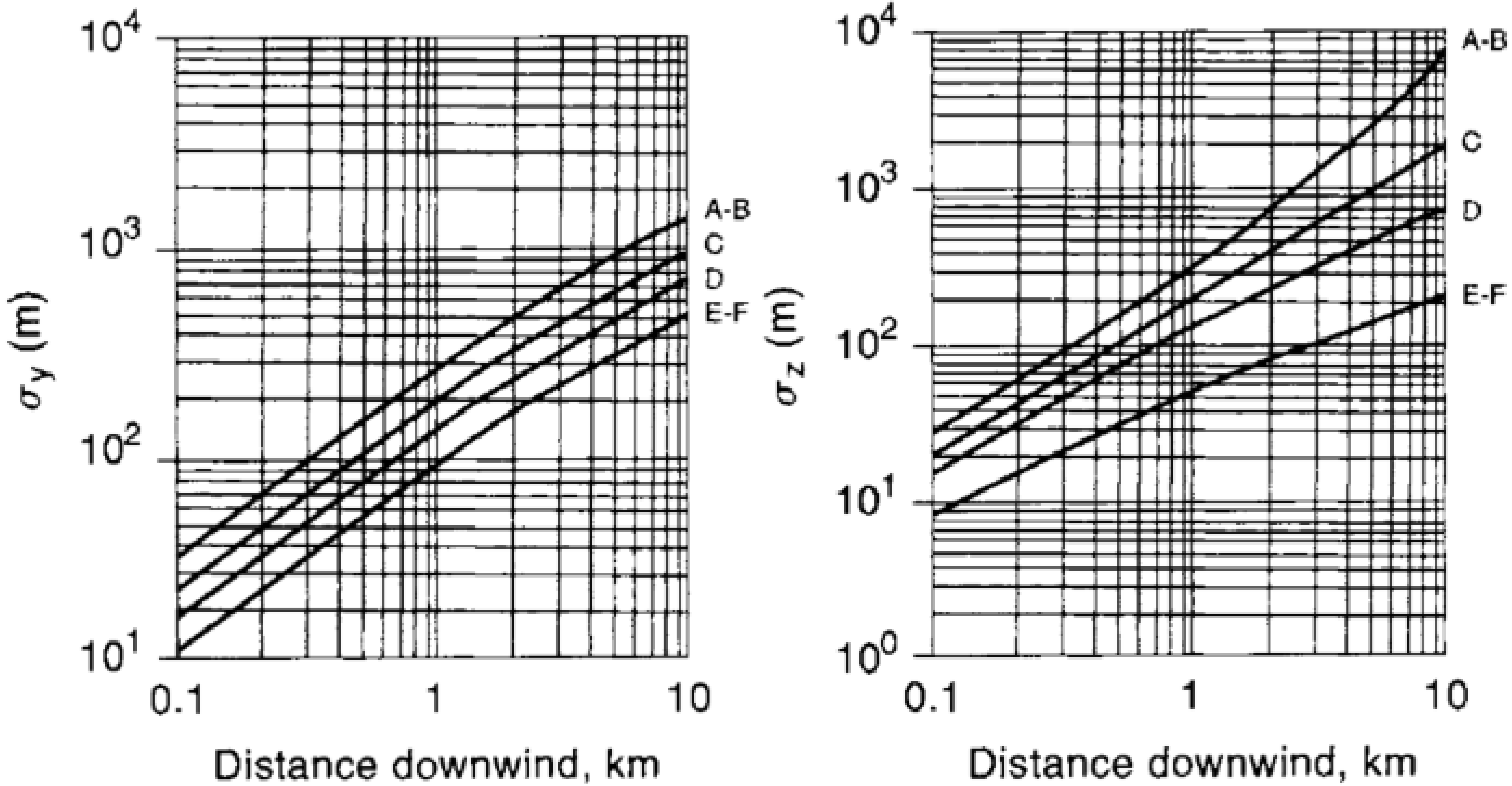
u = Wind speed (length/time)

y, z = Coordinates (length)

H_r = Release height (length)



Dispersion coefficients for plume model for rural releases.



Dispersion coefficients for plume model for urban releases.

Table 5-2 Recommended Equations for Pasquill-Gifford Dispersion Coefficients for Plume Dispersion[1,2] (the downwind distance *x* has units of meters)

Pasquill-Gifford stability class	σ_y (m)	σ_z (m)
Rural conditions		
A	$0.22x(1 + 0.0001x)^{-1/2}$	$0.20x$
B	$0.16x(1 + 0.0001x)^{-1/2}$	$0.12x$
C	$0.11x(1 + 0.0001x)^{-1/2}$	$0.08x(1 + 0.0002x)^{-1/2}$
D	$0.08x(1 + 0.0001x)^{-1/2}$	$0.06x(1 + 0.0015x)^{-1/2}$
E	$0.06x(1 + 0.0001x)^{-1/2}$	$0.03x(1 + 0.0003x)^{1}$
F	$0.04x(1 + 0.0001x)^{-1/2}$	$0.016x(1 + 0.0003x)^{-1}$
Urban conditions		
A–B	$0.32x(1 + 0.0004x)^{-1/2}$	$0.24x(1 + 0.0001x)^{+1/2}$
D	$0.22x(1 + 0.0004x)^{-1/2}$	$0.20x$
D	$0.16x(1 + 0.0004x)^{-1/2}$	$0.14x(1 + 0.0003x)^{-1/2}$
E–F	$0.11x(1 + 0.0004x)^{-1/2}$	$0.08x(1 + 0.0015x)^{-1/2}$

A–F are defined in Table 5-1.

Table 5-1 Atmospheric Stability Classes for Use with the Pasquill-Gifford Dispersion Model[1,2]

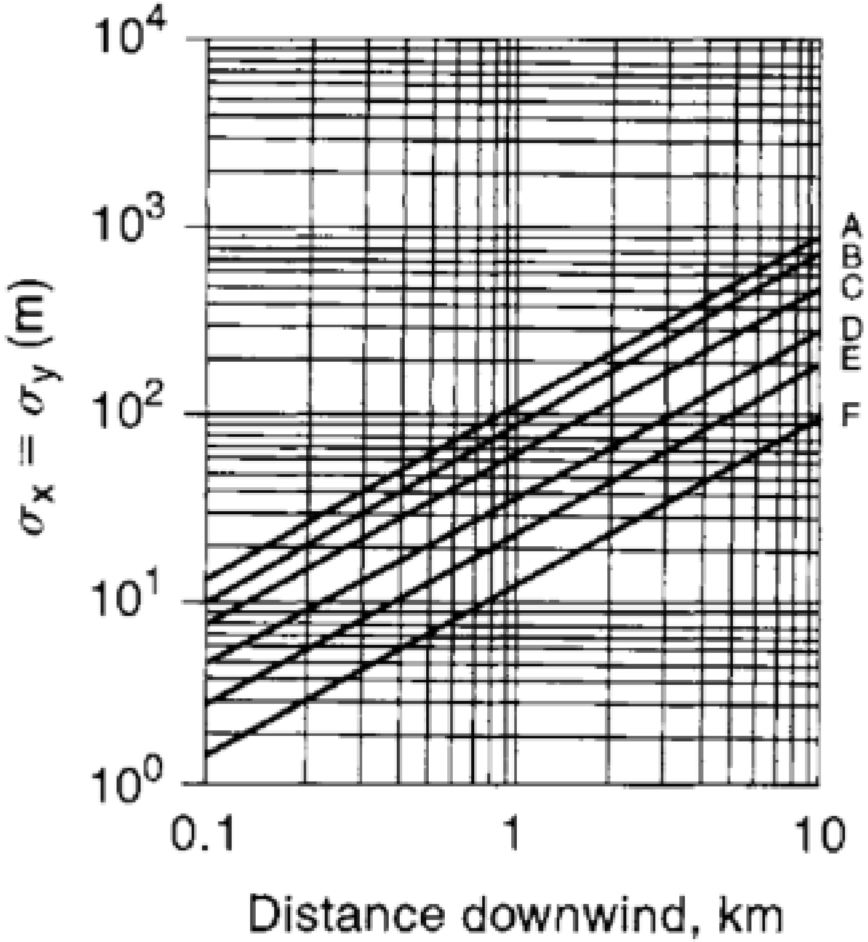
Surface wind speed (m/s)	Daytime insolation[3]			Nighttime conditions[4]	
	Strong	Moderate	Slight	Thin overcast or >4/8 low cloud	≤3/8 cloudiness
<2	A	A–B	B	F[5]	F[5]
2–3	A–B	B	C	E	F
3–4	B	B–C	C	D[6]	E
4–6	C	C–D	D[6]	D[6]	D[6]
>6	C	D[6]	D[6]	D[6]	D[6]

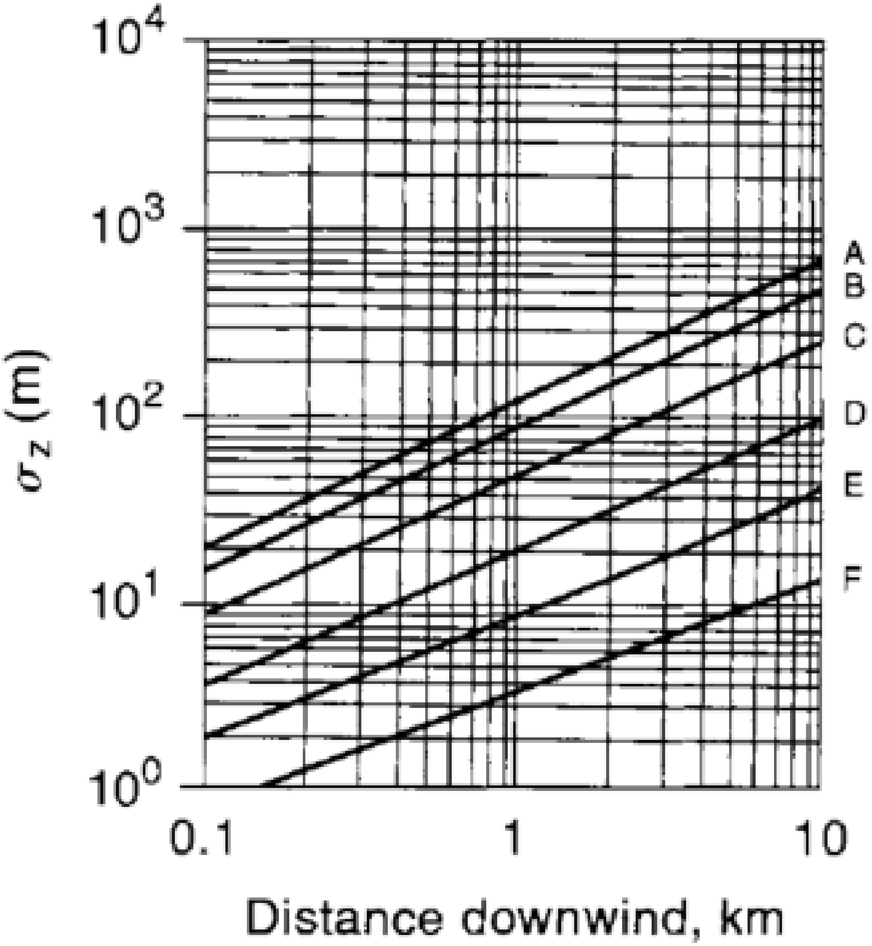
Stability classes:

- A, extremely unstable
- B, moderately unstable
- C, slightly stable
- D, neutrally stable
- E, slightly stable
- F, moderately stable

[3]Strong insolation corresponds to a sunny midday in midsummer in England. Slight insolation to similar conditions in midwinter.

[4]Night refers to the period 1 hour before sunset and 1 hour after dawn.





Dispersion coefficients for Pasquill-Gifford puff model.

Table 5-3 Recommended Equations for Pasquill-Gifford Dispersion Coefficients for Puff Dispersion[1,2] (the downwind distance x has units of meters)

Pasquill-Gifford stability class	σ_y (m) or σ_x (m)	σ_z (m)
A	$0.18x^{0.92}$	$0.60x^{0.75}$
B	$0.14x^{0.92}$	$0.53x^{0.73}$
C	$0.10x^{0.92}$	$0.34x^{0.71}$
D	$0.06x^{0.92}$	$0.15x^{0.70}$
E	$0.04x^{0.92}$	$0.10x^{0.65}$
F	$0.02x^{0.89}$	$0.05x^{0.61}$

A–F are defined in Table 5-1.

[1] R. F. Griffiths, "Errors in the Use of the Briggs Parameterization for Atmospheric Dispersion Coefficients," *Atmospheric Environment* (1994), 28(17): 2861–2865.

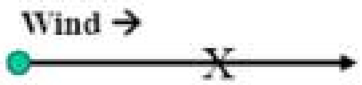
[2] G. A. Briggs, *Diffusion Estimation for Small Emissions*, Report ATDL-106 (Washington, DC: Air Resources, Atmospheric Turbulence, and Diffusion Laboratory, Environmental Research Laboratories, 1974).

Simplified Cases - Plume

The ground-level concentration is found by setting $z = 0$:

$$\langle C\rangle(x, y, 0) = \frac{Q_m}{\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2 - \frac{1}{2}\left(\frac{H_r}{\sigma_z}\right)^2\right].$$

Ground Centerline Concentration:

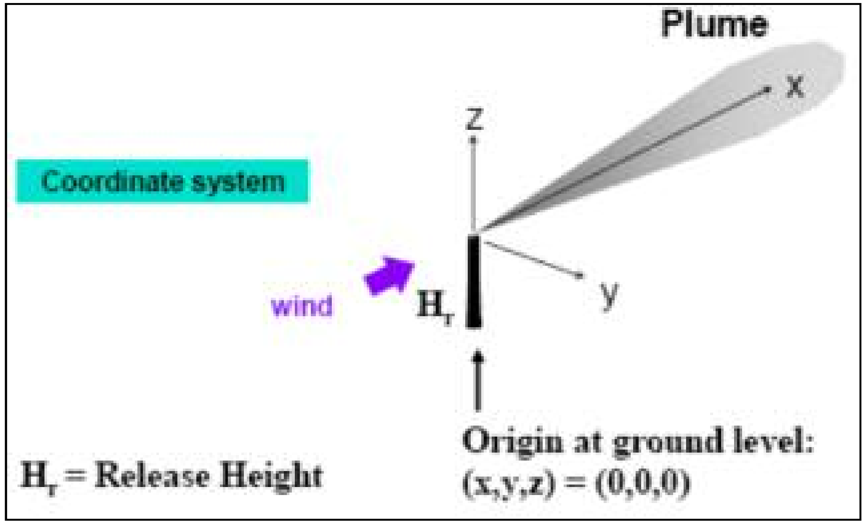


$$< C > (x,0,0) = \frac{Q_m}{\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{H_r}{\sigma_z}\right)^2\right]$$

Ground, centerline, release height $H_r = 0$

$$< C > (x,0,0) = \frac{Q_m}{\pi\sigma_y\sigma_z u}$$

***X* is implicit in the dispersion coefficients!**



Maximum Concentrations - Plume

- Always occurs at release point.
- The distance downwind at which the maximum ground-level concentration occurs: $(\sigma_z)_{x,\max} = \frac{H_r}{\sqrt{2}}$
- For releases above ground, max. concentration on ground occurs downwind: $\langle C \rangle_{\max} = \frac{2Q_m}{e\pi u H_r^2}\left(\frac{\sigma_z}{\sigma_y}\right)$

$$(\sigma_z)_{x,\max} = \frac{H_r}{\sqrt{2}} \qquad \langle C \rangle_{\max} = \frac{2Q_m}{e\pi u H_r^2}\left(\frac{\sigma_z}{\sigma_y}\right)$$

1. Use left equation to determine σ_z

2. Use Figures 5-10 or 5-11 to get x.

3. Determine σ_y **from Figures 5-10 or 5-11.**

4. Calculate <C> from right equation.

Example 1:

10 kg/s of H_2S is released 100 m off of ground. Estimate the concentration 1 km downwind on ground? It is a clear, sunny day, 1 PM, wind speed = 3.5 m/s. Assume rural conditions.

Plume, due to continuous nature of release!

From Table 5-1, Stability Class B.

From Figure 5-10, $\sigma_y = 130 \text{ m}$

From Figure 5-10, $\sigma_z = 120 \text{ m}$

Use Equation 5-51 for a plume.

Example: Apply Equation 5-51

Applies to ground concentration directly downwind of release:

$$\langle C \rangle (x,0,0) = \frac{Q_m}{\pi \sigma_y \sigma_z u} \times \exp\left[-\frac{1}{2}\left(\frac{H_r}{\sigma_z} \right)^2 \right]$$

$$\langle C \rangle (x,0,0) = \frac{10.0 \text{ kg/s}}{(3.14)(130 \text{ m})(120 \text{ m})(3.5 \text{ m/s})} \times \exp\left[-\frac{1}{2}\left(\frac{100 \text{ m}}{120 \text{ m}} \right)^2 \right]$$

$$\langle C \rangle (x,0,0) = 41.2 \times 10^{-6} \text{ kg/m}^3 = 41.2 \text{ mg/m}^3$$

Use Equation 2-7 to get 29.7 ppm. TLV-TWA is 10 ppm.

Example: Where is max. concentration?

Use Equation 5-53:

$$(\sigma_z)_{x,\max} = \frac{H_r}{\sqrt{2}} = \frac{100 \text{ m}}{1.414} = 70.7 \text{ m}$$

Use equation in Table 5-3 to determine downwind distance:

$$\sigma_Z = 0.12x$$

$$70.7 \text{ m} = 0.12x$$

$$x = 590 \text{ m}$$

At this location, from Figure 5-10:

$$\sigma_y = 92 \text{ m}$$

Use Equation 5-52 to calculate max. concentration:

$$< C >_{max} = \frac{2Q_m}{e\pi u H_r^2}\left(\frac{\sigma_z}{\sigma_y}\right) = \frac{(2)(100\ \text{kg/s})}{(2.718)(3.14)(3.5\ \text{m/s})(100\ \text{m})^2}\left(\frac{70.7\ \text{m}}{92\ \text{m}}\right)$$

$$< C >_{max} = 5.14 \times 10^{-4}\ \text{kg/m}^3 = 514\ \text{mg/m}^3 = 370\ \text{ppm}$$

Example: What is max. discharge to result in 10 ppm?

Maximum will occur at same location: $(\sigma_z)_{x,\max} = \frac{H_r}{\sqrt{2}}$

10 ppm = 13.9 mg/m³ (Equation 2-7)

Substitute into Equation 5-52:

$$<C>_{\max} = \frac{2Q_m}{e\pi u H_r^2}\left(\frac{\sigma_z}{\sigma_y}\right)$$

$$13.9 \times 10^{-6} \text{kg/m}^3 = \frac{2Q_m}{(2.71)(3.14)(3.5 \text{ m/s})(100 \text{ m})^2}\left(\frac{70.71 \text{ m}}{92 \text{ m}}\right)$$

$Q_m = 2.7$ kg/s **Not very much!**

Example 2:

10 kg of H_2S is released instantly on the ground. What is concentration at fenceline 100 m away? Same conditions as before.

From Table 5-1, stability class is B.

At x = 0.1 km, from Figure 5-12: $\sigma_y = 10 \text{ m}$ $\sigma_z = 16 \text{ m}$

Use Equation 5-41 for a ground release, centerline conc.:

$$< C > (0,0,0) = \frac{Q_m^*}{\sqrt{2}\pi^{3/2}\sigma_x\sigma_y\sigma_z}$$

Assume $\sigma_x = \sigma_y$

$Q_m^* = 10 \text{ kg} = 10 \times 10^6 \text{ mg}$

$<C> = 79.4 \text{ mg/m}^3 = 571 \text{ ppm}$

How long does it take for puff to reach fenceline?

$$x = ut$$

$$t = \frac{x}{u} = \frac{100\ \text{m}}{3.5\ \text{m/s}} = 28.6\ \text{s after release.}$$

Very little time for an emergency response!

What size release will result in 10 ppm at fenceline?

Same procedure as for plume. Answer is 0.175 kg = 175 gm.

Not very much! Better to contain chemicals than to mitigate after a release!

! Exercises & HW

Examples

5.1 5.2

HW:

5.4 5.9 5.12