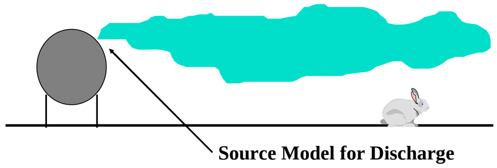
Chemical Process Safety

Chapter 5: Dispersion Models

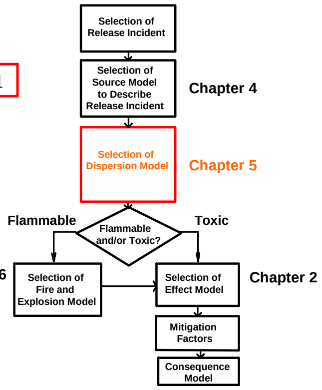


Wind--->

<--Mixing with fresh air-->

Source Model for Discharge
thru hole

Figure 4-1



Selection of Release Incident

Selection of Source Model to Describe Release Incident

Chapter 4

Selection of Dispersion Model

Chapter 5

Flammable

Flammable and/or Toxic?

Toxic

Chapter 6

Selection of Fire and Explosion Model

Selection of Effect Model

Chapter 2

Mitigation Factors

Consequence Model

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.

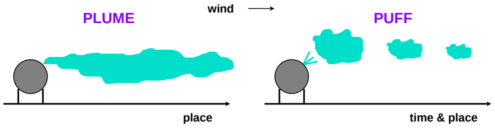
Why? To determine the consequences.

Results: Downwind concentrations (x,y,z)

Area affected

Downwind evacuation distances

Dispersion



Continuous release

Instantaneous release

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

difficult

Atmospheric stability

MAINLY DETERMINED BY VERTICAL TEMPERATURE GRADIENT

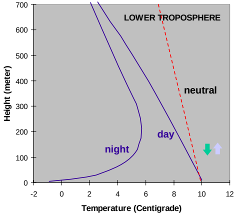
⊕ heat & radiation balance troposphere and surface

⊖ convective air flows

- incident sunlight
- cloud coverage
- wind speed

season
time of day
night

Figure 5-3



Adiabatic temperature gradient humid air: 0.5 °C / 100 m

Atmospheric stability

Unstable: 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.

STABILITY CLASSES A - F

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

Table 5-1

Atmospheric stability

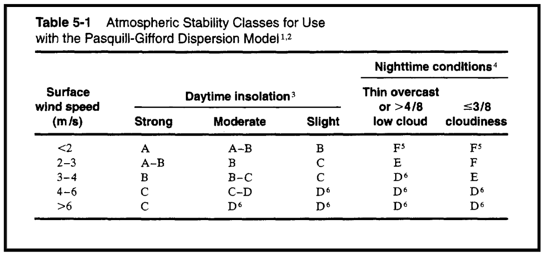


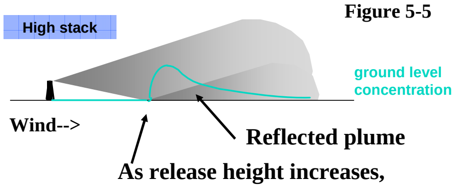
Table 5-1 Atmospheric Stability Classes for Use with the Pasquill-Gifford Dispersion Model[1,2]

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

See qualifying notes below table!

Release Height Effect

Figure 5-5

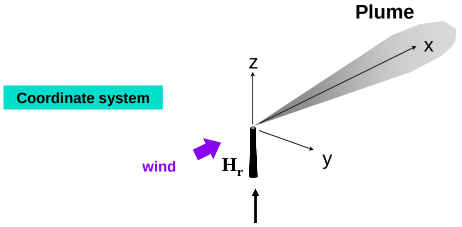


Wind-->

Reflected plume

As release height increases, downwind concentration decreases.

Coordinate systems

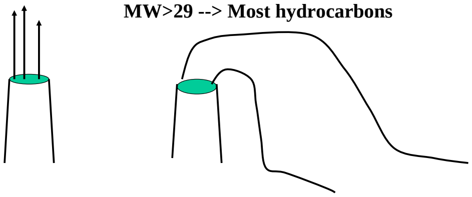


H_r = Release Height

Origin at ground level: (x,y,z) = (0,0,0)

Release Momentum and Buoyancy

MW>29 --> Most hydrocarbons



Jet Release

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

Dispersion Models

Dispersion models are based on a mass balance.

Two approaches:

1. Use eddy diffusivities, *K*, to represent turbulence.

   Advantage: nice tidy theoretical model.

   Disadvantage: *K = K(x,y,z)*, and impossible to measure. See text.

2. Use dispersion coefficients which represent the standard deviations in the concentration profiles.

   Advantage: easy to measure and correlate.

Gaussian form of plume equation Equation 5-49

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

Top View of plume

--> Wind

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

$Q_m =$ Release rate (mass/time)

$\sigma_y, \sigma_z =$ Dispersion coefficients = f(stability class, downwind distance)

$u =$ Wind speed (length/time)

$y, z =$ Coordinates (length)

$H_r =$ Release height (length)

Atmospheric stability

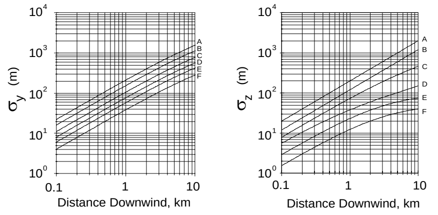
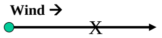


Fig. 5-10

Dispersion coefficients for plume model for rural releases. See Figure 5-11 for urban releases, and Table 5-2 for plume equations. Figure 5-12 and Table 5-3 are for puff model.

Simplified Cases - Plume

Ground Centerline Concentration:



$$< C > (x,0,0) = \frac{Q_m}{\pi \sigma_y \sigma_z u} \exp\left[-\frac{1}{2}\left(\frac{H_r}{\sigma_z} \right)^2 \right] \qquad \textbf{(5-51)}$$

Ground, centerline, release height H_r = 0

$$< C > (x,0,0) = \frac{Q_m}{\pi \sigma_y \sigma_z u} \qquad \textbf{(5-48)}$$

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

Maximum Concentrations - Plume

Always occurs at release point.

For releases above ground, max. concentration on ground occurs downwind.

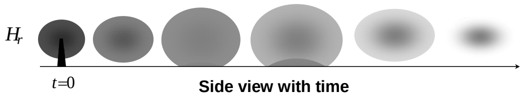
$$(\sigma_z)_{x,\max} = \frac{H_r}{\sqrt{2}} \qquad < C >_{\max} = \frac{2Q_m}{e\pi u H_r^2}\left(\frac{\sigma_z}{\sigma_y} \right)$$

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.**

Puff

Equation 5-54

$$< C > (x,y,z,t) = \frac{Q_m^*}{\sqrt{2}\pi^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left[\frac{1}{2}\left(\frac{y}{\sigma_y} \right)^2 \right] \times \left\{ \exp\left[-\frac{1}{2}\left(\frac{z-H_r}{\sigma_z} \right)^2 \right] + \exp\left[-\frac{1}{2}\left(\frac{z+H_r}{\sigma_z} \right)^2 \right] \right\}$$



***u, t* not explicit in equation**

***x* is implicit thru dispersion coefficients**

Coordinate system moves with puff center at *x=ut*

Assume $\sigma_x = \sigma_y$

Simplified Cases - Puff

Concentration on ground below puff center

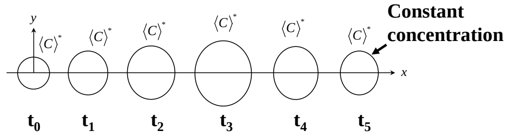
$$< C > (0,0,0) = \frac{Q_m^*}{\sqrt{2}\pi^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left[-\frac{1}{2}\left(\frac{H_r}{\sigma_z} \right)^2 \right] \qquad \textbf{(5-56)}$$

Same as above, with H_r = 0. Puff center on ground.

$$< C > (0,0,0) = \frac{Q_m^*}{\sqrt{2}\pi^{3/2}\sigma_x\sigma_y\sigma_z} \qquad \textbf{(5-41)}$$

Puff center always at release height.

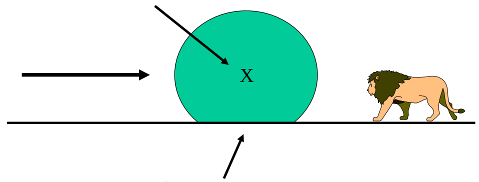
Location of Puff



---> Wind = constant at *u*

Center of puff located at: *x = u t*

Maximum Concentration - Puff



Always at puff center

On ground, max. concentration always occurs directly below puff center.

Example:

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/m^3 (Equation 2-7)

Substitute into Equation 5-52:

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

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

$Q_m = 2.7 \text{ kg/s}$ **Not very much!**

Example:

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 $\sigma_x = \sigma_y$

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

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

Example:

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!

Example:

What size release will result in 10 ppm at fenceline?

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

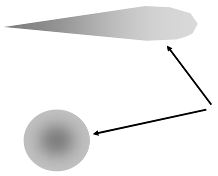
Not very much! Better to contain chemicals than to mitigate after a release!

Isopleths

What: Lines of constant concentration

Plume:

Puff:



10 ppm boundary

Determining Isopleths: Plume and Puff

Divide equation for centerline concentration by equation for ground level concentration. Solve for y, which is crosswind direction.

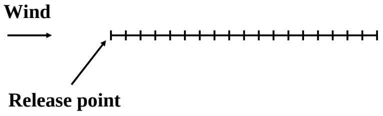
$$y = \sigma_y\sqrt{2\ln\left(\frac{< C > (x,0,0,t)}{< C > (x,y,0,t)}\right)} \qquad \textbf{(5-45)}$$

Downwind, ground centerline conc.

Isopleth conc.

Procedure to Determine Isopleths - 1

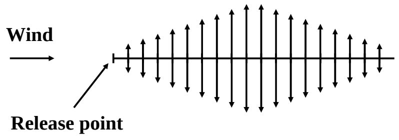
1. Determine concentrations along centerline at fixed points downwind.



2. Use equation (5-45) to find y at each fixed point.

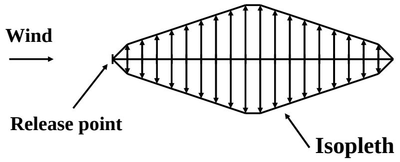
Procedure to Determine Isopleths - 2

3. Plot +y and - y at each fixed point.



Procedure to Determine Isopleths - 3

4. Connect the points.



Worst Case on Ground- Plume and Puff

Want maximum <C> downwind

Plume: Centerline, ground, $H_r = 0$

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

Puff: Center of puff on ground, $H_r = 0$

$$\langle C \rangle (x,0,0) = \frac{Q_m^*}{\sqrt{2}\pi^{3/2} \sigma_x \sigma_y \sigma_z u}$$

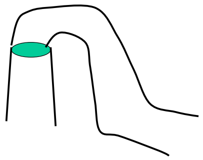
Specify: Q_m and Q_m^* at maximum

σ's are minimum --> F stability

u is minimum within stability class --> 2 m/s

(EPA suggests 1.5 m/s!)

Dense Gas Dispersion



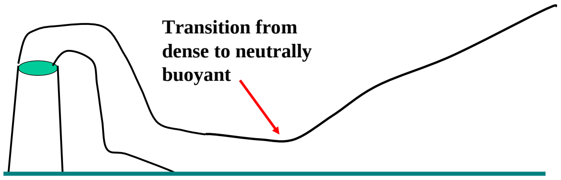
Heavier than air!

Britter-McQuaid Dense Gas Dispersion Model:

Based on dimensionless groups and available experimental data.

See pages 195-199.

Dense Gas Dispersion



Results in shorter distances if only dense gas.
Results in longer distances if dense gas coupled with Gaussian dispersion.

Toxic Effect Criteria

What concentration should we use for emergency releases?

Cannot use PEL or TWA since these are for continuous work exposures – values are too low for short-term exposures.

ERPGs – Emergency Response Planning Guidelines, issued by American Industrial Hygiene Association

EEGLs – Emergency Response Guidance Levels, issued by National Academy of Sciences/National Research Council.

LOC – Level of Concern from EPA

Toxic Endpoints promulgated by EPA as part of RMP

ERPG: Emergency Response Planning Guideline

ERPG-1: max. airborne concentration below which it is believed nearly all individuals can be exposed for up to 1-hr without experiencing effects other than mild transient adverse health effects or perceiving a clearly defined objectionable odor.

ERPG-2: max. airborne conc. below which it is believed nearly all individuals can be exposed up to 1 hr without experiencing or developing irreversible or other serious health effects or symptoms that could impair their ability to take protective action.

ERPG: Emergency Response Planning Guideline

ERPG-3: max. airborne concentration below which it is believed nearly all individuals can be exposed for up to 1-hour without experiencing or developing life-threatening health effects.

Table 5-6	ERPG-1	ERPG-2	ERPG-3
Ammonia	25 ppm	200 ppm	1000 ppm
Chlorine	1 ppm	3 ppm	20 ppm
Monomethylamine	10 ppm	100 ppm	500 ppm
Toluene	50 ppm	300 ppm	1000 ppm

EEGL: Emergency Exposure Guidance Levels

A concentration of a gas, vapor, or aerosol that is judged acceptable and allows exposed individuals to perform specific tasks during emergency conditions lasting from 1 to 24 hours.

Table 5-7	1-hr EEGL	24-hr EEGL
Ammonia	100 ppm	
Chlorine	3 ppm	0.5 ppm
Toluene	200 ppm	100 ppm

IDLH: Immediately Dangerous to Life and Health

A concentration that poses a threat of exposure to airborne contaminants when that exposure is likely to cause death or immediate or delayed permanent adverse health effects or prevent escape from such an environment.

Available from OSHA (osha.gov) or NIOSH Pocket Guide.

Ammonia	50 ppm
Chlorine	10 ppm
Toluene	500 ppm

LOC: Level of Concern

The max. concentration of an extremely hazardous substance in air that will not cause serious irreversible health effects in the general population when exposed to the substance for relatively short duration.

See EPA for values.

Toxic Endpoints

Must be used for dispersion modeling required for the EPA RMP. Values are, in order of preference, ERPG-2 or LOC.

Table 5-8

Ammonia	0.14 mg/L
Chlorine	0.0087 mg/L
Chloroform	0.49 mg/L

Proposed Hierarchy to Estimate Values

Table 5-9: ORDER IS REVERSED IN TABLE!

Primary	Secondary	Benzene
ERPG-3:	**EEGL (30-min)**	**1000 ppm**
	IDLH	**500 ppm**
ERPG-2:	**EEGL (60 min)**	**150 ppm**
	LOC	
	PEL-C	
	TLV-C	
	5 x TLV-TWA	**50 ppm**

Proposed Hierarchy to Estimate Values (con't)

Primary	Secondary	Benzene
ERPG-1:	**PEL-STEL**	**50 ppm**
	TLV-STEL	**5 ppm**
	3 x TLV-TWA	**30 ppm**