# **Dispersion Models**

## **Exposure to Release**

#### **Predict effects of exposure near the surface.**



#### **Stages**

- **1. Source**
- **2. Acceleration, Diffusion**
- **3. Gravity**
- **4. Transition**
- **5. Surface**
- **6. Turbulence**

#### **Predict % affected by the exposure.**

# **Fluids Beyond the Sources**

- **Effluent properties dominate near a leak**
- **Material then migrates and mixes with air**
- **Ambient conditions eventually dominate**
	- $⊩$  **Pressure, temperature, wind velocity, humidity, sun light**
- $\textcolor{red}{\textbf{■}}$  **Transport and mixing with air at a vapor cloud boundary**
- $\frac{1}{2}$  **/sopleth: constant concentration boundary of a vapor cloud**

## Accidental Flow



# **Dispersion Modeling Needed**

**Goals: prevent releases; mitigation Prevent**

**Inherent safety practices: reduction, substitution, attenuation**

**Process design and integrity**

**PSM management; PHA**

**Mitigation measures**

**Emergency response planning**

10/15/2011 5

## **Hazard Levels**

- **Concentration**
- **Air velocity and turbulence**
- **Time period of release;** *C***(***time***) following release**
- **<b>↓Position of cloud relative to ground**

## **Gaussian Dispersion Pattern**



## **Dispersion Parameters**

- **Cloud of effluents expands, mixes with air**
- **Mixing dilutes the effluent:** *C* **decreases**
- **Lower downwind** *C* ⇒ *greater area* **affected**
- $\textcolor{red}{\textbf{↓}}$  **Dominant dispersion mechanism: turbulent dispersion** ⇒ **horizontal and vertical movement**
- **Mixing rate depends on** *u***, atmosphere stability, buoyancy**

#### **Light winds, strong sun** ⇒ **most unstable: rapid diffusion**



#### **Plume & Puff**







## **Plume Model**

- **Steady state concentration from a continuous source, e.g. smokestack**
- **Initially increases in size, additions from source**
- **Steady state: same amount of effluent added to plume as is mixed with air; constant volume**
- **Source stopped: plume size decreases as mixing with air is dominant, plume returns to source origin, finally disappears.**

## **Puff Model**

- **Cloud formed from a fixed amount of effluent, e.g., from a ruptured vessel**
- $\textcolor{red}{\textbf{�}{\textbf{F}}}$  **Release over a short period of time that source is active**
- **Movement from source: dependent on air velocity**
- **Material mixes with air, boundary diminished in size, finally disappears**

$$
\frac{\partial \langle C \rangle}{\partial t} + \langle u_j \rangle \frac{\partial \langle C \rangle}{\partial x_j} = \frac{\partial}{\partial x_j} \left( K_j \frac{\partial \langle C \rangle}{\partial x_j} \right)
$$
  
\nPlumes\n
$$
\frac{Plume}{\text{Of Putf}}
$$
\n1. SS,  $\langle u_j \rangle = 0, K_j = K^*$   $\langle C \rangle (r) = \frac{Q_m}{4\pi K^* r}$   
\n3. NSS,  $\langle u_j \rangle = 0, K_j = K^*$   $\langle C(r, t) \rangle = \frac{Q_m}{4\pi K^* r}$   $\text{erfc} \left( \frac{r}{2\sqrt{K^* t}} \right)$   
\n4. SS,  $\langle u_j \rangle = \langle u_x \rangle = u, K_j = K^*$   $\langle C(r) \rangle = \frac{Q_m}{4\pi K^* r} \exp \left( -\frac{u(r - x)}{2K^*} \right)$   
\n6. SS,  $\langle u_j \rangle = \langle u_x \rangle = u, K_x, K_y, K_z$  Source

9. 
$$
S_{10^{15/20}j_1}^{S} \geq u_x \geq u, K_x, K_y, K_{\text{net-1-NC}}^{S} \geq 0
$$

$$
\frac{\partial \langle C \rangle}{\partial t} + \langle u_j \rangle \frac{\partial \langle C \rangle}{\partial x_j} = \frac{\partial}{\partial x_j} \left( K_j \frac{\partial \langle C \rangle}{\partial x_j} \right)
$$
  
\nPlumes\n
$$
\frac{P_{lume}}{\text{Of Putf}}
$$
\n
$$
\text{Out Putf}
$$
\n
$$
\langle C(r,t) \rangle = \frac{Q_m}{8(\pi K^* t)^{3/2}} \exp\left(-\frac{r^2}{4K^* t}\right)
$$
\n
$$
2. \langle u_j \rangle = 0, K_j = K^*
$$
\n
$$
5. \langle u_j \rangle = 0, K_x, K_y, K_z
$$

7. 
$$
\langle u_j \rangle = \langle u_x \rangle = u, K_x, K_y, K_z
$$

$$
8. \langle u_j \rangle = 0, K_x, K_y, K_z
$$
Source

## **Neutrally Buoyant Dispersion**

**No reactions; small effect of molecular diffusion**

- **Mixing mechanism: air turbulence**
- **Turbulence** ⇒**fluctuations in** *C, u*

$$
\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_j} (u_j C) = 0
$$
\n*u<sub>j</sub>*, air velocity  
\n*u<sub>j</sub>* =  $\langle u_j \rangle + u_j$   $\rightarrow$  *C* =  $\langle C \rangle + C$ 

 $u'_{j}$ , $C'$  , fluctuation components

# **Eddy Diffusivity,** *K<sup>j</sup>*

**Represent** *C* **fluctuation due to turbulence**

$$
\langle u'_j \rangle = 0; \ \langle C'_j \rangle = 0
$$

$$
\langle u_j C' \rangle = -K_j \frac{\partial \langle C \rangle}{\partial x_j}
$$

#### **Governing equation:**

$$
\frac{\partial \langle C \rangle}{\partial t} + \langle u_j \rangle \frac{\partial \langle C \rangle}{\partial x_j} = \frac{\partial}{\partial x_j} \left( K_j \frac{\partial \langle C \rangle}{\partial x_j} \right)
$$

10/15/2011 METU-NCC 16

### **1. Steady State, Point Release, No Wind**

 $\downarrow Q_m$  constant; C independant of *t*, wind,  $u \sim 0$  $\uparrow$  **Constant**  $K_i = K^*$  **in all directions** 



**Polar coordinates, integrate over** *r* **:**

$$
\langle C \rangle(r) = \frac{Q_m}{4\pi K^* r}
$$

$$
Q_m
$$
, source term

$$
r = \sqrt{x^2 + y^2 + z^2}
$$

### **2. Puff Release, No Wind**

 $\downarrow$  Wind velocity,  $u \sim 0$  $\uparrow$  **Constant**  $K_i = K^*$  in all directions

$$
\frac{1}{K^*} \frac{\partial \langle C \rangle}{\partial t} = \frac{\partial^2 \langle C \rangle}{\partial x^2} + \frac{\partial^2 \langle C \rangle}{\partial y^2} + \frac{\partial^2 \langle C \rangle}{\partial z^2}
$$

**Instantaneous concentration:**



#### **3. Non SS Point Release, No Wind**

 $\downarrow Q_m$  constant; wind,  $u \sim 0$  $\angle$  **Constant**  $K_i = K^*$  **in all directions** 

$$
\frac{1}{K^*} \frac{\partial \langle C \rangle}{\partial t} = \frac{\partial^2 \langle C \rangle}{\partial x^2} + \frac{\partial^2 \langle C \rangle}{\partial y^2} + \frac{\partial^2 \langle C \rangle}{\partial z^2}
$$

**Integrate instantaneous concentration:**

$$
\langle C(r,t) \rangle = \frac{Q_m}{4\pi K^* r} erf \left( \frac{r}{2\sqrt{K^* t}} \right)
$$

#### **Error function & its Integration**



### **4. SS Point Source with Wind**

*Q<sup>m</sup>* **constant;** *C* **independent of** *t* **Wind in** *x* **direction,** *u<sup>x</sup>* **constant**  $\uparrow$  **Constant**  $K_i = K^*$  in all directions



10/15/2011 METU-NCC

21

## **5. Puff with No Wind, K<sup>j</sup> Varies**

*Q\*<sup>m</sup>* **constant; Puff release**  $\neq$  No wind(<u<sub>**j**</sub>> =0)  $\bf{K}$ <sup>*★*</sup> *K<sup>\*</sup>*, but constant in all directions

$$
\frac{\partial \langle C \rangle}{\partial t} = K_x \frac{\partial^2 \langle C \rangle}{\partial x^2} + K_y \frac{\partial^2 \langle C \rangle}{\partial y^2} + K_z \frac{\partial^2 \langle C \rangle}{\partial z^2}
$$

$$
\langle C \rangle (x, y, z, t) = \frac{Q_m^*}{8(\pi t)^{3/2} \sqrt{K_x K_y K_z}} \exp \left[ -\frac{1}{4t} \left( \frac{x^2}{K_x} + \frac{y^2}{K_y} + \frac{z^2}{K_z} \right) \right]
$$

#### **6. SS Point Source with Wind, K<sup>j</sup> Varies**

*Q<sup>m</sup>* **constant;** *C* **independent of** *t* **Wind in** *x* **direction,** *u<sup>x</sup>* **constant**  $\bf{K}$ <sup>*★*</sup> *K<sup>\*</sup>*, but constant in all directions



#### **7. Puff with Wind**

#### *Q\*<sup>m</sup>* **constant; Puff release**

- **Wind in x direction only(** $\langle u_j \rangle = \langle u_x \rangle = u = constant$ )
- $\bullet$  *K*<sup>*j*</sup> ≠ *K<sup>\*</sup>*, but constant in all directions

$$
\frac{\partial \langle C \rangle}{\partial t} = K_x \frac{\partial^2 \langle C \rangle}{\partial (x - ut)^2} + K_y \frac{\partial^2 \langle C \rangle}{\partial y^2} + K_z \frac{\partial^2 \langle C \rangle}{\partial z^2}
$$

$$
\langle C \rangle (x, y, z, t) = \frac{Q_m^*}{8(\pi t)^{3/2} \sqrt{K_x K_y K_z}} \exp\left[ -\frac{1}{4t} \left( \frac{(x - ut)^2}{K_x} + \frac{y^2}{K_y} + \frac{z^2}{K_z} \right) \right]
$$

#### **8. Puff with No Wind, Source on Ground**

*Q\*<sup>m</sup>* **constant; Puff release**  $\neq$  No wind(<u<sub>**j**</sub>> =0)  $\mathbf{K}_i \neq \mathbf{K}^*$ , but constant in all directions

$$
\frac{\partial \langle C \rangle}{\partial t} = K_x \frac{\partial^2 \langle C \rangle}{\partial x^2} + K_y \frac{\partial^2 \langle C \rangle}{\partial y^2} + K_z \frac{\partial^2 \langle C \rangle}{\partial z^2}
$$

$$
\langle C \rangle(x,y,z,t) = \frac{Q_m^*}{\left(4\pi\right)^{3/2} \sqrt{K_x K_y K_z}} \exp\left[-\frac{1}{4t} \left(\frac{x^2}{K_x} + \frac{y^2}{K_y} + \frac{z^2}{K_z}\right)\right]
$$

#### **Impervious boundary** 10/15/2011 **METU-NCC** 25

#### **9. SS Point Source with Source on Ground**

*Q<sup>m</sup>* **constant;** *C* **independent of** *t* **Wind in** *x* **direction,** *u<sup>x</sup>* **constant**  $\bf{K}$ <sup>*★*</sup> *K<sup>\*</sup>*, but constant in all directions



10/15/2011 METU-NCC 26

#### **10. SS Point Source with Source at Height H<sup>r</sup> above the Ground**

- *Q<sup>m</sup>* **constant;** *C* **independent of** *t*
- **Wind in** *x* **direction,** *u<sup>x</sup>* **constant**
- $\mathbf{K}_i \neq \mathbf{K}^*$ , but constant in all directions



## **Consequence Analysis (Ex)**



#### **Risk contour**

## **Consequence Analysis (Ex)**



10/15/2011 METU-NCC 29



## **Pasquill-Gifford Model**

*K<sup>j</sup>* **values difficult to measure**



**Define:** *dispersion coefficient ~* **st dev for** *C*   $\sigma_i$  $\frac{2}{i}$  = 1 2 *C* 2 (*ut*) 2*n i* **=** *x, y, z; n,* **parameter**

 $\sigma_{_j}$  $\sigma$  : functions of downwind distance, *x*, and **atmospheric conditions in stability classes,** *A - F***, based on sunlight and wind speed. Tab 5-1, p. 187**

 $\sigma_j$  values for rural or urban plumes, or puffs from Figs **5-10 - 5-12 or Tabs 5-1 - 5-3, pp., 187-189**

#### Nighttime conditions<sup>4</sup> **Surface** Thin overcast Daytime insolation<sup>3</sup> wind speed or  $>4/8$  $\leq 3/8$  $(m/s)$ Strong Moderate Slight low cloud cloudiness  $< 2$  $A-B$  $F<sup>5</sup>$ A B.  $F5$  $2 - 3$  $A-B$ B C F.  $\mathbf F$  $3 - 4$ В  $B-C$ €  $D<sup>6</sup>$ Е  $C-D$  $4 - 6$  $\mathcal{C}$  $D<sub>6</sub>$ D 6. D<sup>6</sup>  $\mathcal{C}$  $>6$ D<sup>6</sup>  $\mathbf{D}^6$ D<sup>6</sup> D°

#### Table 5-1 Atmospheric Stability Classes for Use with the Pasquill-Gifford Dispersion Model<sup>1,2</sup>

- **A: Extremely unstable B: Moderately unstable C: Slightly unstable**
- **D: Neutrally stable**
- **E: Slightly stable**
- **C: Moderately stable**

Table 5-2 Recommended Equations for Pasquill-Gifford Dispersion Coefficients for Plume Dispersion<sup>1,2</sup> (the downwind distance x has units of meters)



Table 5-3 Recommended Equations for Pasquill-Gifford Dispersion Coefficients for Puff Dispersion<sup>1,2</sup> (the downwind distance  $x$  has units of meters)





Figure 5-10 Dispersion coefficients for Pasquill-Gifford plume model for rural releases.



Dispersion coefficients for Pasquill-Gifford plume model for urban releases. Figure 5-11



Figure 5-12 Dispersion coefficients for Pasquill-Gifford puff model.

## **Atmospheric Stability Classes**



*Day Temperature*

**Stability classes classify level of turbulance:**  14<sub>5/2</sub> least stable; F, most stable (Tab. 5-1, p. 187)<sup>38</sup>

### **11. Puff, Ground Source,** *u* **Constant**

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

#### **Ground concentration:** *z* **= 0**

**Ground concentration along**  $x: y = z = 0$ 

#### **Center of moving puff,** *x* **=** *ut***:**

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

## **Total Dose**

$$
D_{tid}(x, y, z) = \int_0^\infty \langle C \rangle(x, y, z, t) dt
$$

### **Puff, ground source, constant** *u***:**

**Ground level:** 
$$
D_{tid}(x, y, 0) = \frac{Q_m^*}{\pi \sigma_y \sigma_z u} \exp\left(-\frac{1}{2} \frac{y^2}{\sigma_y^2}\right)
$$

**Along** 
$$
\mathbf{x}: D_{tid}(x,0,0) = \frac{Q_m^*}{\pi \sigma_y \sigma_z u}
$$

### **12. Plume, Ground Source,** *u* **Constant**

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

**Ground**  $C(x,y,0)$  **:**  $z = 0$ 

Ground,  $C(x,0,0)$  along  $x: y = z = 0$ 

**Isopleth concentration,** *C***\* :** 

$$
y = \pm \sigma_y \sqrt{2 \ln \left( \frac{\langle C(x,0,0,t) \rangle}{\langle C(x,y,0,t) \rangle} \right)} = \pm \sigma_y \sqrt{2 \ln \left( \frac{\langle C(x,0,0,t) \rangle}{\langle C^* \rangle} \right)}
$$

## **13. Plume, Source at H<sup>r</sup> ,** *u* **Constant**



## **Model Implementation**

- **Plume** *Cmax***: release position**
- **Puff** *Cmax***: center of cloud**
- **↓ If atmosphere conditions not known, assume worst case for highest** *C***.**
- **If wind speed not known, assume 2 m/s**
- **Consider P-G model assumptions: neutral buoyancy, turbulent mixing, time concentrations (10 min), 0.1 - 10 km distances**

### **Britter-McQuaid Dense Gas Model**

- **Ground level releases; rural, flat terrain**
- **Atmospheric stability effects not included**
- **Mixing from drop by gravity of effluent into air**
- **Main parameters: initial buoyancy,** *g<sup>o</sup>* **, initial volume flux,** *q<sup>o</sup>* **, or total initial volume,***V<sup>o</sup>* **, wind speed at 10 m elevation,** *u*

$$
g_o = g(\rho_o - \rho_a)/\rho_a
$$

#### $\boldsymbol{\rho}_a$  = density of ambient air

10/15/2011 METU-NCC 44

## **Applicability of B-M Model**



**If model criteria satisfied, use Figs 5-13, 5-14 or Tabs**  10/15/2011 **5-4, 5-5 to est. C or downwind distance, x** 45

## **Implementation of B-M Model**

*C<sup>o</sup>* **= 1 for pure material initially released** *Cm/ C<sup>o</sup>* **: ratio of material conc in air to pure**

$$
q_o = q_L \frac{\rho_L}{\rho_V} \quad \textbf{q}_L \text{ : liquid volumetric discharge rate}
$$

 $V_o = q_o R_d$ : initial volume, Puff

**Adjust conc for density at** *Ta* **:**



*Ce* **: effective conc**

- *C\** **: unadjusted conc**
- *To* **: T at release, K**
- *Ta* **: T ambient, K**





**Table 5-4** Equations Used to Approximate the Curves in the Britter-McQuaid Correlations Provided in Figure 5-13 for Plumes



Table 5-4 Equations Used to Approximate the Curves in the Britter-McQuaid Correlations Provided in Figure 5-13 for Plumes

Concentration ratio $(C_n/C_o)$	Valid range for $\alpha = \log\left(\frac{g_o^2 q_o}{\sigma} \right)^{1/5}$	$\beta = log$	
0.01	$\alpha \leq -0.70$	2.25	
	$-0.70 < \alpha \leq -0.29$	$0.49\alpha + 2.59$	
	$-0.29 < \alpha \le -0.20$	2.45	
	$-0.20 < \alpha \leq 1$	$-0.52\alpha + 2.35$	
0.005	$\alpha \leq -0.67$	2.40	
	$-0.67 < \alpha \leq -0.28$	$0.59\alpha + 2.80$	
	$-0.28 < \alpha \leq -0.15$	2.63	
	$-0.15 < \alpha \leq 1$	$-0.49\alpha + 2.56$	
0.002	$\alpha \leq -0.69$	2.6	
0.002	$-0.69 < \alpha \le -0.25$	$0.39\alpha + 2.87$	
0.002	$-0.25 < \alpha \le -0.13$	2.77	
0.002	$-0.13 < \alpha \leq 1$	$-0.50\alpha + 2.71$	

Concentration ratio $(C_{m}/C_{o})$	Valid range for $g_\mathrm{o} V_\mathrm{o}^{\dagger/3}$ \ $^{1/2}$ $\alpha = \log$	$\frac{x}{1^{1/3}}$ $\beta = \log$
0.1	$\alpha \leq -0.44$ $-0.44 < \alpha \leq 0.43$ $0.43 < \alpha \leq 1$	0.70 $0.26\alpha + 0.81$ 0.93
0.05	$\alpha \leq -0.56$ $-0.56 < \alpha \le 0.31$ $0.31 < \alpha \leq 1.0$	0.85 $0.26\alpha + 1.0$ $-0.12\alpha + 1.12$
0.02	$\alpha \leq -0.66$ $-0.66 < \alpha \le 0.32$ $0.32 < \alpha \leq 1$	0.95 $0.36\alpha + 1.19$ $-0.26\alpha + 1.38$
0.01	$\alpha \leq -0.71$ $-0.71 < \alpha \leq 0.37$ $0.37 < \alpha \leq 1$	1.15 $0.34\alpha + 1.39$ $-0.38\alpha + 1.66$
0.005	$\alpha \leq -0.52$ $-0.52 < \alpha \leq 0.24$ $0.24 < \alpha \leq 1$	1.48 $0.26\alpha + 1.62$ $0.30\alpha + 1.75$
0.002	$\alpha \leq 0.27$ $0.27 < \alpha \leq 1$	1.83 $-0.32\alpha + 1.92$
0.001	$\alpha \leq -0.10$ $-0.10 < \alpha \leq 1$	2.075 $-0.27\alpha + 2.05$

Table 5-5 Equations Used to Approximate the Curves in the Britter-McQuaid Correlations Provided in Figure 5-14 for Puffs

## **Toxic Effect Criteria**

- **Normal work hours criteria: TLV-TWA (ACGIH), PEL (OSHA)**
- **Probit correlations for wide ranges of concentrations and exposure times**
- **Criteria for short term exposures at higher than TLV-TWA values: available from many sources**
- **IDLH (NIOSH), 30 min exposures: SCBA required for higher levels**

## **ERPG Toxic Effect Criteria**

- **← American Industrial Hygiene Association (AIHA): Emergency response planning guidelines (ERPG) for exposures up to 1 hour**
- **ERPG-1: mild transient effects**
- **ERPG-2: reversible health effects**
- **ERPG-3: without life-threatening effects**
- **Tab 5-6, pp. 201, 202**
- **Alternative guidelines in lieu of ERPG data: Tab 5-9, p 206**
- **EPA Toxic Endpoints based on ERPG-2**

#### Table 5-6 (continued)





#### Table 5-9 Recommended Hierarchy of Alternative Concentration Guidelines<sup>1</sup>

## **EEGL Toxic Effect Criteria**

- **National Research Council (NRC):**   $\overline{\mathbf{0}}$ **Emergency exposure guidance levels (EEGL)**
- **Acceptable exposure levels for emergency condition tasks up to 1 or up to 24 hours**
- **Includes reversible effects that do not impair work performance**
- **Tab 5-7, p 204**

Table 5-7 Emergency Exposure Guidance Levels (EEGLs) from the National Research Council (NRC) (all values are in ppm unless otherwise noted)



## **Release Mitigation**

- **Part of consequence modeling, Fig 4-1, p 110. Mitigation methods, Tab 5-10, p 214**
- **Mitigation measures depend on likelihood of a release**
- **Preventive: Inherent safety, process and mechanical integrity, training, maintenance, sensors, software**
- **Protective, reduce effect of incidents: curtains, foams, emergency response program**



#### Table 5-10 Release Mitigation Approaches<sup>1</sup>



#### Release Mitigation Approaches<sup>1</sup> Table 5-10

<sup>1</sup>Richard W. Prugh and Robert W. Johnson, Guidelines for Vapor Release Mitigation (New York: American Institute of Chemical Engineers, 1988).