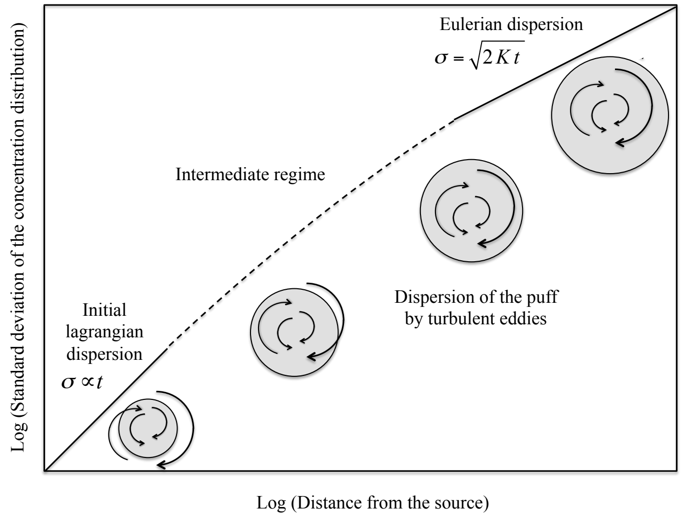
Atmospheric Dispersion

- General considerations on atmospheric dispersion
- Lagrangian representation of turbulence
- Eulerian representation of turbulence
- Lagrangian models of atmospheric dispersion
- Eulerian models of atmospheric dispersion
- Street-canyon models



Atmospheric Dispersion

Dispersion is due to atmospheric turbulence because molecular diffusion is too slow at the time scales relevant to air pollution

Molecular diffusion coefficient: ~10^{-5} m^2/s

Turbulent diffusion coefficient: ~1 m^2/s (stable) to ~100 m^2/s (unstable)

Lagrangian and Eulerian Representations

The lagrangian representation of atmospheric dispersion follows the motion of the pollutants (particles or molecules) with respect to the mean motion of the air parcel (e.g., the stack plume).

The eulerian representation followsthe motion of the pollutants with respect to a fixed reference system (for example a surface monitoring station).

Lagrangian Representation

One assumes that the dispersion process is stochastic (random) and that the atmospheric conditions are uniform and stationary: this leads to a gaussian distribution of the pollutant around the plume centerline.

The concentration integrated over a crosswind plane multiplied by the wind speed must be equal to the emission rate: mass conservation of the emitted pollutant.

If a gaussian distribution is assumed, then the volume of the puff that is within one standard deviation (σ) from the puff center corresponds to 68 % of the initial mass emitted, within 2 σ, 95 %, and within 3 σ, 99.7 %.

Lagrangian Representation

Solution for a continuous point source:

$$C(x,y,z) = \frac{S}{2\pi\, u\, \sigma_y\, \sigma_z} \exp\left(-\frac{(y-y_s)^2}{2\sigma_y^2} - \frac{(z-z_s)^2}{2\sigma_z^2} \right)$$

where C: pollutant concentration (g/m^3)

S: emission rate (g/s)

u: wind speed (m/s)

y and z: crosswind distances from the plume centerline (m)

σ_y and σ_z: standard deviations of the concentration distribution (m)

Lagrangian Representation
Standard Deviation σ

The standard deviations (σ_y and σ_z) of the concentration distribution must be estimated.

Taylor's theorem (1922) states that near the source (t => 0) :

$$\sigma^2(t) = \overline{u^2}\, t^2$$

That is, the standard deviations near the source are proportional to time, i.e., to the distance from the source if the mean wind speed is constant ($x = u\ t$).

Lagrangian Representation Standard Deviation σ

Taylor's theorem states that far from the source (t => ∞) :

$$\sigma^2(t) = 2\overline{u^2}\, t_L\, t$$

where t_L is the lagrangian time scale (on the order of 1 min in the atmosphere, less near the surface). That is, the standard deviations far from the source are proportional to the square root of time, i.e., to the square root of the distance from the source if the mean wind speed is constant ($x = u\, t$).

Eulerian Representation

Eulerian representation of atmospheric dispersion (mass conservation of the pollutant concentration, *C*):

$$\frac{\partial C}{\partial t} + \frac{\partial (uC)}{\partial x} + \frac{\partial (vC)}{\partial y} + \frac{\partial (wC)}{\partial z} = 0$$

Accounting for turbulence:

$$\frac{\partial C}{\partial t} + \frac{\partial (\overline{u}\,\overline{C} + \overline{u'C'})}{\partial x} + \frac{\partial (\overline{v}\,\overline{C} + \overline{v'C'})}{\partial y} + \frac{\partial (\overline{w}\,\overline{C} + \overline{w'C'})}{\partial z} = 0$$

Accounting for continuity of momentum : $\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$

$$\boxed{\frac{\partial \overline{C}}{\partial t} + \overline{u}\frac{\partial \overline{C}}{\partial x} + \frac{\partial (\overline{u'C'})}{\partial x} + \overline{v}\frac{\partial \overline{C}}{\partial y} + \frac{\partial (\overline{v'C'})}{\partial y} + \overline{w}\frac{\partial \overline{C}}{\partial z} + \frac{\partial (\overline{w'C'})}{\partial z} = 0}$$

Reynolds-averaged Navier-Stokes Equations (RANS)

Molecular diffusion is represented by Fick's law: $F = -D_m \frac{\partial C}{\partial x}$

where F is the mass flux, D_m is the molecular diffusion coefficient, C is the concentration of the diffusing species and $(\mathrm{d}C/\mathrm{d}x)$ is the spatial concentration gradient.

By analogy, one may represent the turbulent term using a similar formulation:

$$\boxed{\overline{u'C'} = -K_{xx} \frac{\partial C}{\partial x}}$$

Thus, one introduces the turbulent diffusion coefficient K_{xx} (equivalent to D_m). However, D_m is a property of the diffusing species and medium of diffusion, whereas K_{xx} is a property of the flow (i.e., turbulence intensity)

Eulerian Representation

Thus, invoking analogy with Fick's law for the turbulent diffusion terms:

$$\overline{u'C'} = -K_{xx}\frac{\partial C}{\partial x}\ , \qquad \overline{v'C'} = -K_{yy}\frac{\partial C}{\partial y}\ , \qquad \overline{w'C'} = -K_{zz}\frac{\partial C}{\partial z}$$

$$\frac{\partial C}{\partial t} + \left(u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z}\right) - \left(\frac{\partial}{\partial x}K_{xx}\frac{\partial C}{\partial x} + \frac{\partial}{\partial y}K_{yy}\frac{\partial C}{\partial y} + \frac{\partial}{\partial z}K_{zz}\frac{\partial C}{\partial z}\right) = 0$$

One assumes:

- a constant mean wind (speed and direction) with direction along *x* (thus, $v = w = 0$)
- uniform (constant in space) and stationary (constant over time) atmospheric turbulence

Eulerian Representation

Eulerian representation of dispersion with a continuous emission source, S (en g/s), at steady-state ($\mathrm{d}C/\mathrm{d}t = 0$), assuming $v = w = 0$:

$$u \frac{\partial C}{\partial x} - \frac{\partial}{\partial x} K_{xx} \frac{\partial C}{\partial x} - \frac{\partial}{\partial y} K_{yy} \frac{\partial C}{\partial y} - \frac{\partial}{\partial z} K_{zz} \frac{\partial C}{\partial z} = S\ \delta(x - x_s)\ \delta(y - y_s)\ \delta(z - z_s)$$

where δ is the Dirac function:

$$\delta(x - x_s) = 0 \quad \text{for } x \neq x_s$$

$$\delta(x - x_s) = +\infty \quad \text{for } x = x_s$$

$$\int_{-\infty}^{+\infty} \delta(x - x_s)\,\mathrm{d}x = 1$$

S is the emission rate at location x_s, y_s, and z_s.

Eulerian Representation

Eulerian equation for stationary dispersion: Diffusion along the plume axis (along *x*) can be neglected, because it is negligible compared to advection by the mean wind (so-called slender plume approximation); $K_{xx} = 0$.

$$u\frac{\partial C}{\partial x} - \frac{\partial}{\partial y}K_{yy}\frac{\partial C}{\partial y} - \frac{\partial}{\partial z}K_{zz}\frac{\partial C}{\partial z} = S\ \delta(x - x_s)\ \delta(y - y_s)\ \delta(z - z_s)$$

$$C(x, y, z, t) = 0 \quad for \quad x, y, \text{and } z \to \infty$$

Solution: $$C(x, y, z) = \frac{S}{4\pi\ u\ t\ \sqrt{K_{yy}K_{zz}}}\exp\left(-\frac{(y - y_s)^2}{4K_{yy}t} - \frac{(z - z_s)^2}{4K_{zz}t}\right)$$

Eulerian and Lagrangian Representations Standard Deviations σ

This solution is a gaussian distribution, which may be expressed as follows:

$$C(x,y,z) = \frac{S}{2\pi\, u\, \sigma_y\, \sigma_z} \exp\left(-\frac{(y-y_s)^2}{2\sigma_y^2} - \frac{(z-z_s)^2}{2\sigma_z^2} \right)$$

where:

$$\sigma_y = \sqrt{2K_{yy}t}$$
$$\sigma_z = \sqrt{2K_{zz}t}$$

The eulerian representation is identical to the lagrangian representation far downwind from the source, i.e., the standard deviation of the gaussian concentration distribution is proportional to the square root of time (or distance).

Standard Deviation σ Evolution from the Source toward the Far Field

Near the source (near field), the lagrangian theory leads to the following relationship:

$$\sigma^2(t) = \overline{u^2}\, t^2$$

Far downwind from the source (far field), the lagrangian theory and the eulerian representation lead to the following relationship:

$$\sigma(t) = (\ 2\ K\ t\ )^{1/2}$$

Therefore, the standard deviation of the gaussian distribution, σ (lagrangian dispersion coefficient), increases faster near the source than far downwind from the source.

Standard Deviation σ
Evolution from the Source toward the Far Field

- Near the source, only the eddies smaller than the plume will disperse the plume material: relative dispersion.

The eddies larger than the plume will move it around: meandering.

Meandering + relative dispersion: absolute dispersion

- As the plume grows in size, there is a greater number of eddies that are smaller in size than the plume and, therefore, available to disperse the plume material.

- Once the plume size covers the entire spectrum of eddy sizes, relative dispersion becomes commensurate with absolute dispersion and lagrangian dispersion then becomes equivalent to eulerian dispersion.

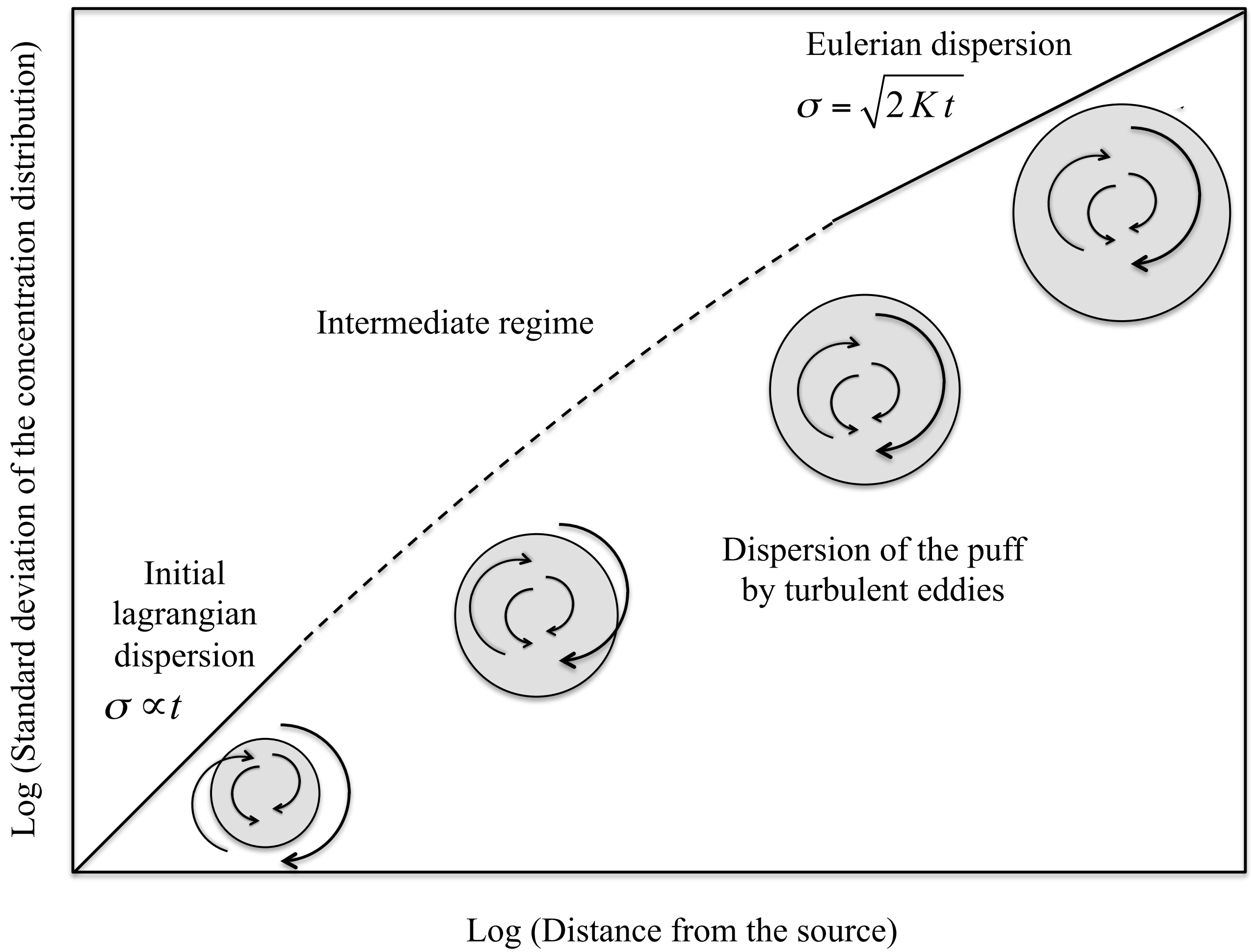
Standard Deviation σ
Relative versus Absolute Dispersion

The ratio of peak (instantaneous) versus time-averaged concentrations provides information on the relative dispersion versus absolute dispersion characteristics of the plume.

At 6 km from a source, Gifford (1960) estimated ratios of 2 to 3 for averaging times of 30 to 140 min.

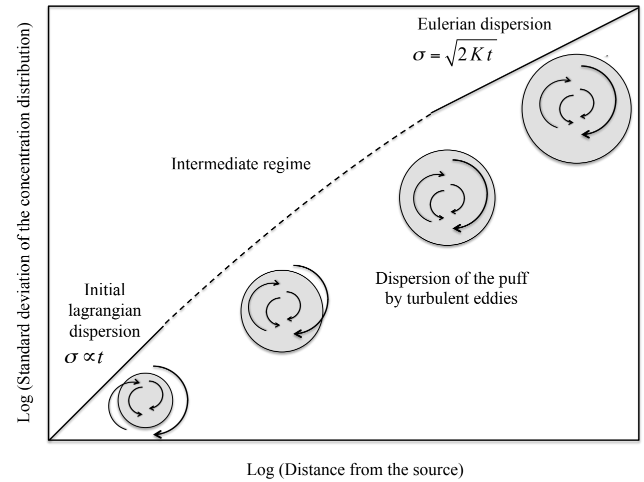
Ratios are greater near the source and tend toward 1 as the downwind distance increases, i.e., as lagrangian and eulerian dispersion become equivalent.

Standard Deviation σ
Evolution from the Source toward the Far Field



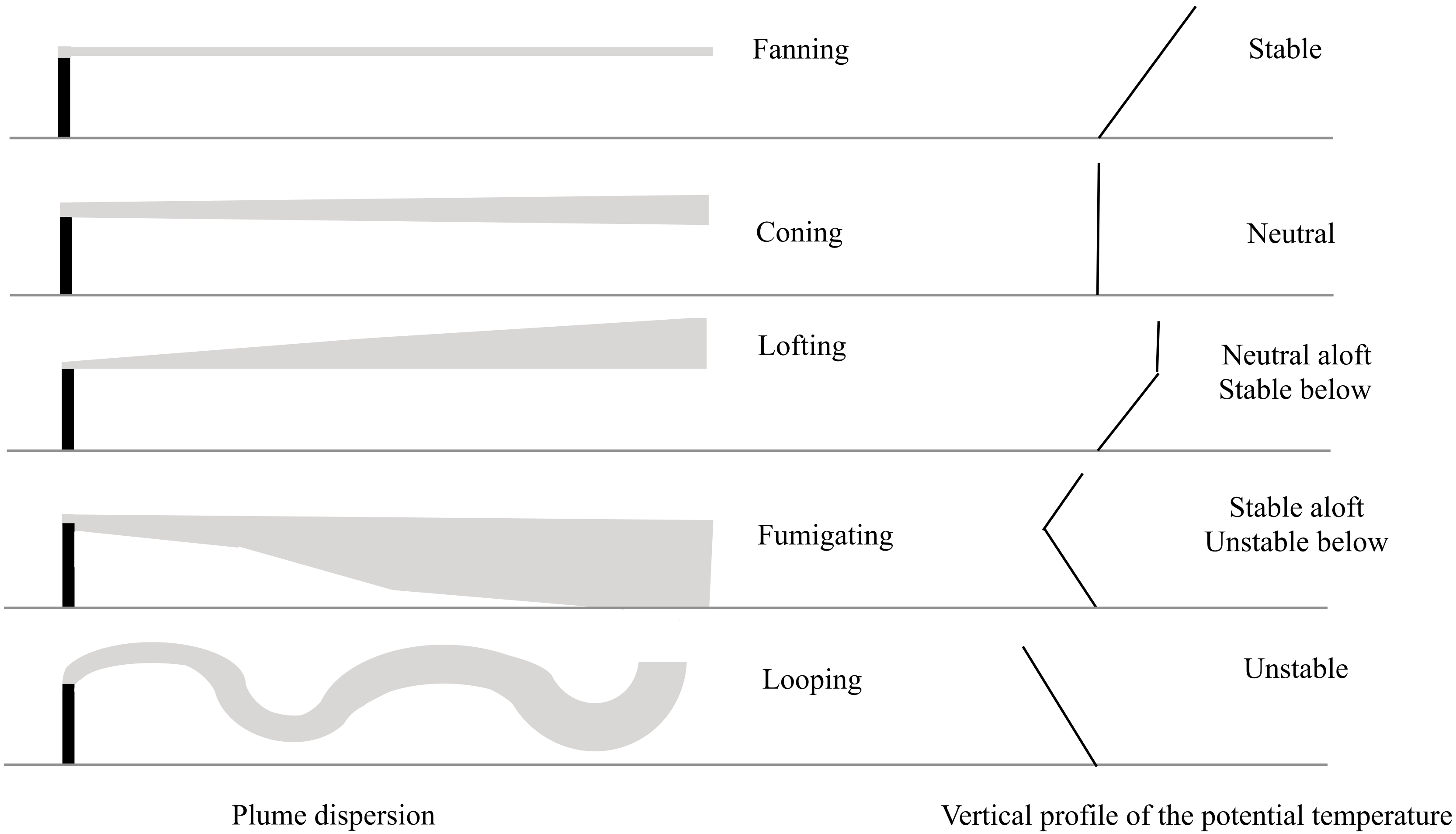
Standard Deviation σ Evolution from the Source toward the Far Field

Since the atmosphere is not a stationary and homogeneous medium, the evolution of the standard deviations may differ significantly from this theoretical representation.



Nevertheless, it is important to note the transition from a near-source lagrangian dispersion regime (which depends on the distance from the source and is used in near-source models) to an eulerian dispersion (which is independent from the distance from the source and is used in urban and regional dispersion models).

Plume Dispersion
as a Function of Atmospheric Stability



Atmospheric Dispersion Models

Lagrangian dispersion models (use of σ dispersion coefficients)

- Gaussian plume models
- Gaussian puff models
- Lagrangian “particle” models

Eulerian dispersion models (use of K dispersion coefficients)

- Chemical-transport models
- Computational fluid dynamics (CFD) models

Hybrid models

- Combination of lagrangian models imbedded within an eulerian model

Gaussian Models

Gaussian models can be used to simulate atmospheric dispersion of non-reactive air pollutants near their source of emission.

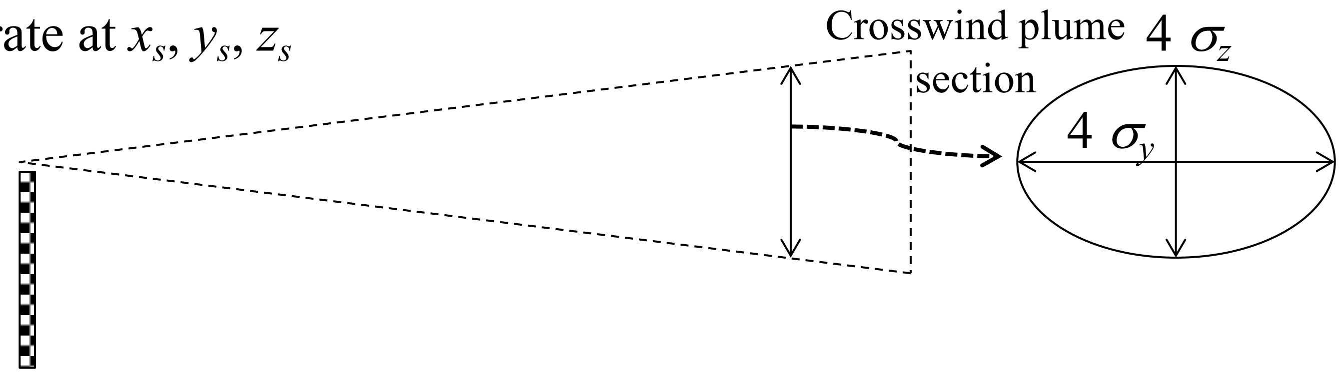
The two main categories are:

- Stationary plume models*
- Puff models (which may be non-stationary)

* Stationary: the inputs (emission, meteorology) are constant over time (generally with an hourly time step) and, for meteorology, spatially uniform.

Gaussian Plume Models

S: emission rate at x_s, y_s, z_s



The concentrations of the air pollutants in the plume are represented by the following equation:

$$c(x,y,z,t) = \frac{S}{2\pi\, u\, \sigma_y\, \sigma_z} \exp\left(-\frac{(y-y_s)^2}{2{\sigma_y}^2} - \frac{(z-z_s)^2}{2{\sigma_z}^2} \right)$$

The ellipse ($4\sigma_y$, $4\sigma_z$) contains 95.4 % of the gaussian plume material;

The ellipse ($2\sigma_y$, $2\sigma_z$) contains 68.2 % of the gaussian plume material

Plume Rise

Plume height:

$$z_{s,f} = z_s + \Delta z_s$$

where Δz_s is the plume rise above the source height z_s; $z_{s,f}$ is the final plume height following plume rise

Several formulas are available to calculate the plume rise:

- Briggs
- Holland
- Carson et Moses
- Concawe
- …

The Briggs formula is the most widely used in gaussian plume models

Plume Rise

Briggs plume rise formula

$$\Delta z_s = \left(\frac{3F_a\,x}{0.36u^2} + 4.17\frac{F_b\,x^2}{u^3}\right)^{1/3}$$

$$F_a = \frac{T}{T_s} v_i^2 \frac{d_s^2}{4}$$

$$F_b = g\,v_i \frac{d_s^2}{4}\left(\frac{T_s - T}{T_s}\right)$$

$$x_t = 49\,F_b^{5/8} \text{ for } F_b \le 55$$

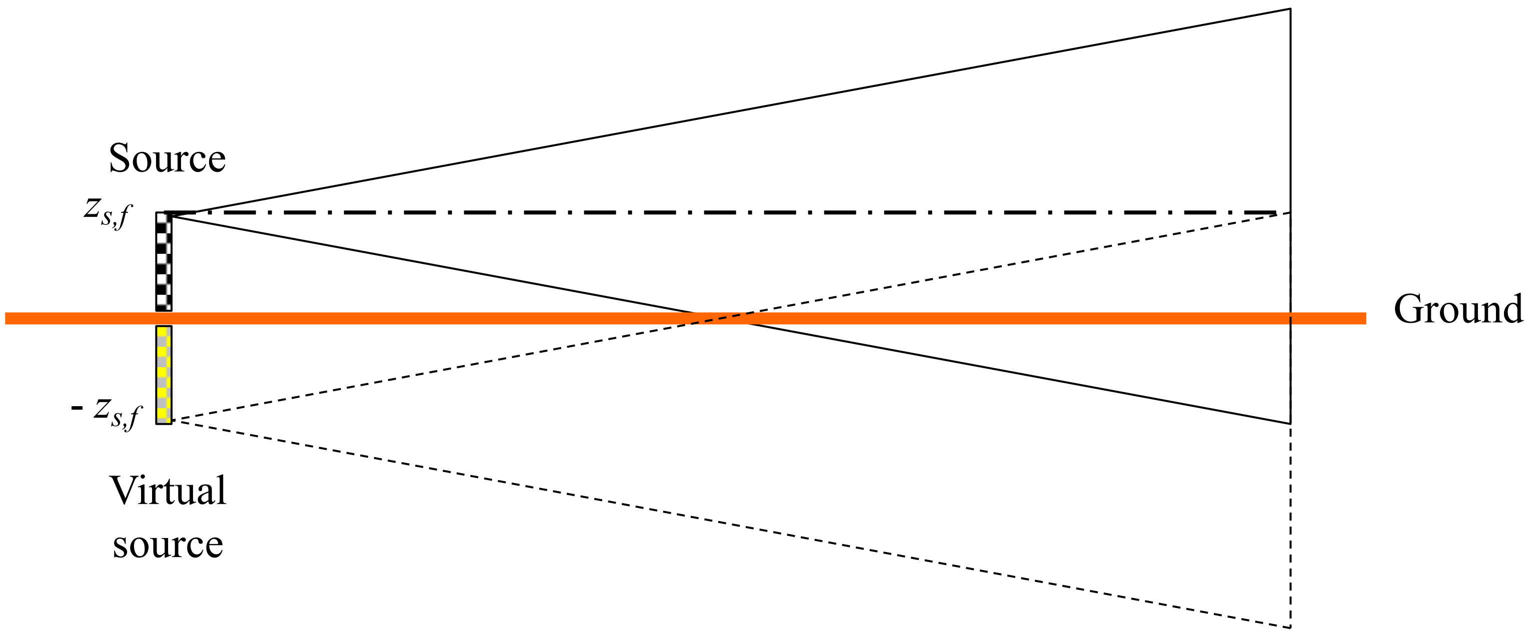
$$x_t = 119\,F_b^{2/5} \text{ for } F_b \ge 55$$

Δz_s: Plume rise (m)
x: Horizontal distance from the source (m)
u: Horizontal wind speed at source height (m/s)
v_i: Initial flue gas vertical velocity (m/s)
d_s: Diameter of the source (m)
T_s: Flue gas temperature (K)
T: Ambient temperature (K)
F_a: Dynamic term ($m^4\ s^{-2}$)
F_b: Buoyancy term ($m^4\ s^{-3}$)
g: Gravitational constant (9.81 $m\ s^{-2}$)
x_l: Distance at which the final plume rise is calculated

Gaussian Plume Model
Reflection at the Ground

The reflection of a plume at the ground is represented in the gaussian formula by adding a virtual source, which is the mirror image of the actual source with respect to the ground:

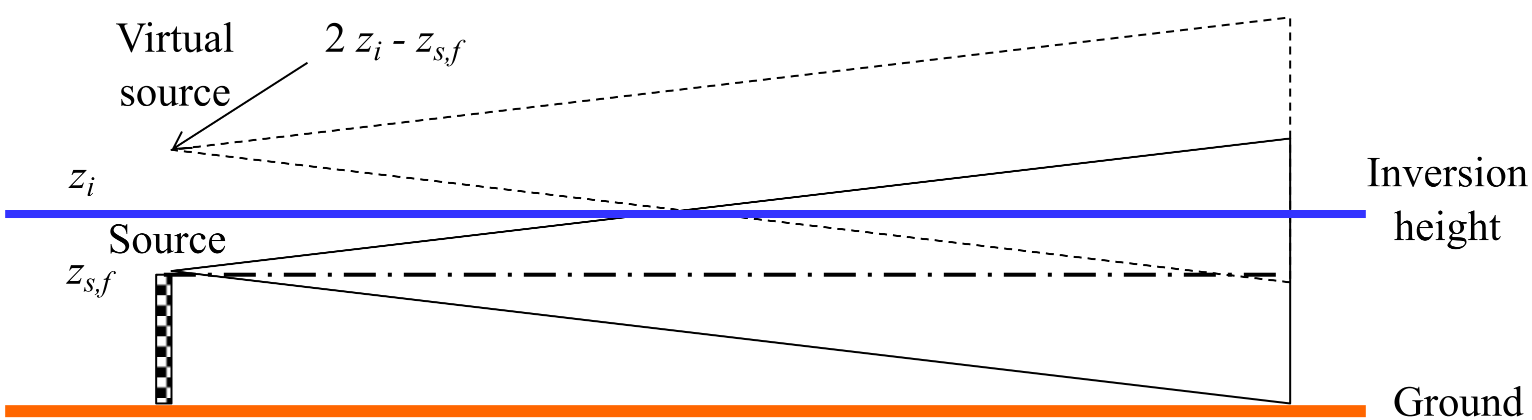
$$C(x,y,z,t) = \frac{S}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left(\exp\left(-\frac{(z-z_{s,f})^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+z_{s,f})^2}{2\sigma_z^2}\right)\right)$$



Gaussian Plume Model
Reflection at the Temperature Inversion Height

The reflection of a plume at the bottom of the temperature inversion is represented in the gaussian formula by adding a virtual source, which is the mirror image of the actual source with respect to the temperature inversion height:

$$C(x,y,z,t) = \frac{S}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left(\exp\left(-\frac{(z - z_{s,f})^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + z_{s,f} - 2z_i)^2}{2\sigma_z^2}\right)\right)$$



Gaussian Plume Model
Reflection at the Ground and at the Inversion Height

The reflection of a plume at the ground and at the bottom of the temperature inversion can be represented jointly in the gaussian formula by adding a set of virtual sources, which leads to the following formula:

$$C(x,y,z,t) = \frac{S}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \sum_{-N_r}^{+N_r} \left(\exp\left(-\frac{(z - z_{s,f} + 2N_k z_i)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + z_{s,f} - 2N_k z_i)^2}{2\sigma_z^2}\right) \right)$$

An acceptable solution is obtained with N = 1, and a very accurate solution is obtained with N = 5.

Atmospheric Stability
Pasquill Classification

- Atmospheric stability[a] is related to turbulence.
- It can be calculated via the Monin-Obukhov length or the Richardson number.
- Empirically, it can be estimated from information that is readily available: time of day, cloudiness, and wind speed.

Wind speed ($m\ s^{-1}$) at 10 m	Day			Night	
	Solar radiation[b]			Cloudiness[c]	
	Strong	Moderate	Weak	≥ 4/8	≤ 3/8
< 2	A	A or B	B	F	F
2 to 3	A or B	B	C	E	F
3 to 5	B	B or C	C	D	E
5 to 6	C	C or D	D	D	D
> 6	C	D	D	D	D

(a) Stability categories: A (very unstable), B (unstable), C (moderately unstable), D (neutral), E (stable), F (very stable).
(b) Solar radiation: strong (> 700 $W\ m^{-2}$), moderate (between 350 and 700 $W\ m^{-2}$), weak (< 350 $W\ m^{-2}$)
(c) Cloudiness: fraction of the sky covered by clouds.

Atmospheric Stability
Vertical Temperature Gradient

- Atmospheric stability[a] is related to turbulence
- Empirically, it can also be estimated from the vertical gradient of the ambient temperature, if it is available over a sufficient altitude difference (about 100 m)

Atmospheric stability category	**Vertical temperature gradient (°C / 100 m)**
A	$\Delta T/\Delta z < -1.9$
B	$-1.9 < \Delta T/\Delta z < -1.7$
C	$-1.7 < \Delta T/\Delta z < -1.5$
D	$-1.5 < \Delta T/\Delta z < -0.5$
E	$-0.5 < \Delta T/\Delta z < 1.5$
F	$1.5 < \Delta T/\Delta z$

(a) Stability categories: A (very unstable), B (unstable), C (moderately unstable), D (neutral), E (stable), F (very stable).

Atmospheric Stability
Richardson Number

- A formulation of the bulk Richardson number based on vertical measurements of temperature and wind speed is as follows:

$$\mathrm{Ri_b} = \frac{g}{T(z_1)} \frac{\dfrac{(T(z_2) - T(z_1))}{z_2 - z_1}}{\left(\dfrac{u(z_2) - u(z_1)}{z_2 - z_1}\right)^2}$$

where $T(z)$ is the temperature (in K) at height z, $u(z)$ is the wind speed (in m/s) at height z and g is the gravitational constant (9.81 m/s^2).

Atmospheric Stability
Richardson Number

- Atmospheric stability is related to turbulence
- It can be calculated via the Richarson number (over a significant height difference)

Atmospheric stability category	**Bulk Richardson number**[a]
A	$Ri_b < -0.86$
B	$-0.86 < Ri_b < -0.37$
C	$-0.37 < Ri_b < -0.10$
D	$-0.10 < Ri_b < 0.053$
E	$0.053 < Ri_b < 0.134$
F	$0.134 < Ri_b$

(a) The observed temperature must be corrected using a vertical gradient of -1 ° C / 100 m to obtain the potential temperature.

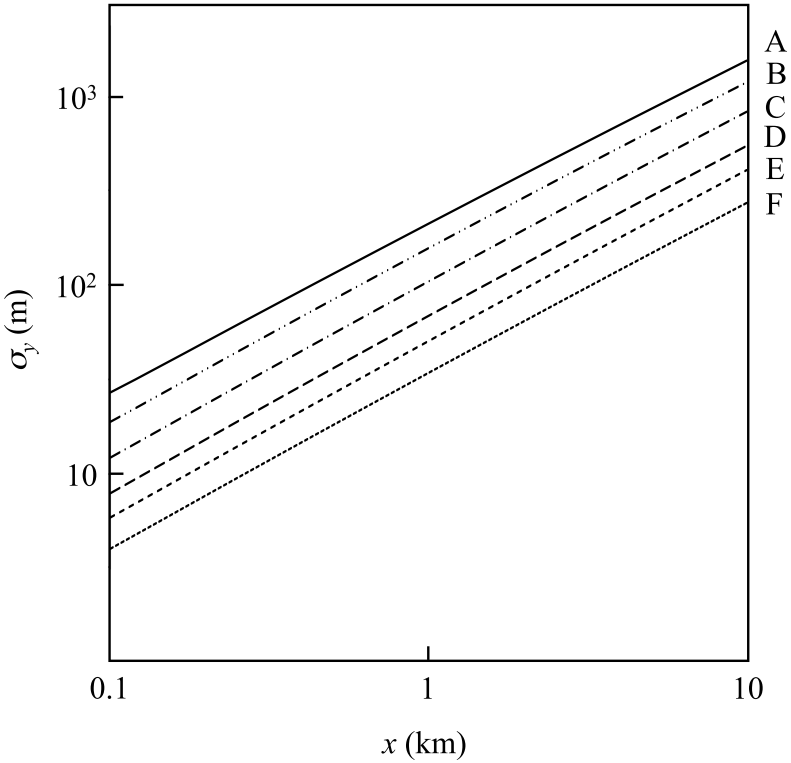
Pasquill stability classes

A: very unstable, B: unstable, C: moderately unstable, D: neutral, E: stable, F: very stable

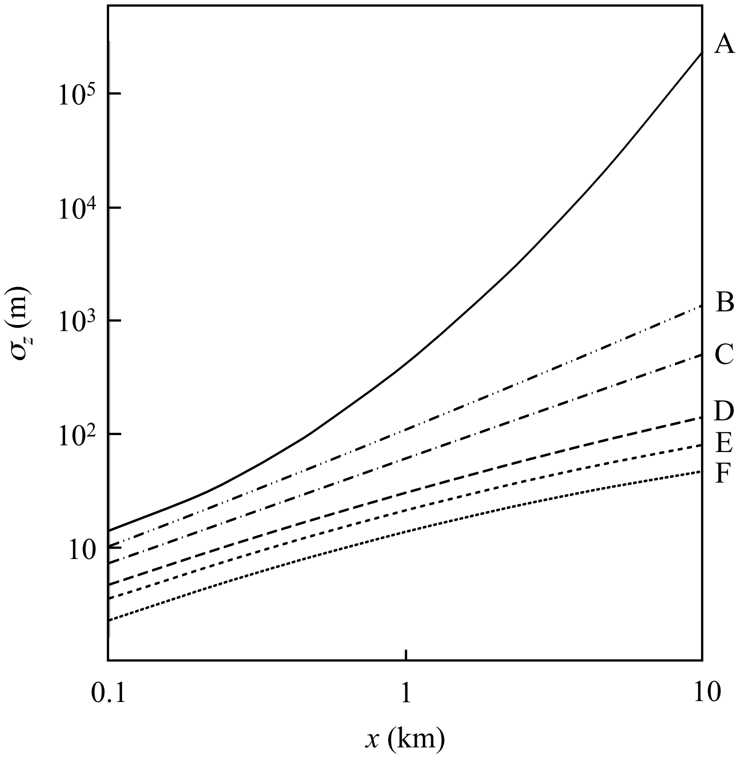
Gaussian Plume Models
Empirical Dispersion Coefficients

Pasquill-Gifford-Turner (PGT) dispersion coefficients

Horizontal dispersion



Vertical dispersion



A: very unstable, B: unstable, C: moderately unstable, D: neutral, E: stable, F: very stable

Source: D.B. Turner, « Workbook of Atmospheric Dispersion Estimates » (1970)

Gaussian Plume Models
Empirical Dispersion Coefficients

Dispersion coefficients: Analytical formulas of Pasquill-Gifford

Pasquill-Gifford						
Stability	$\sigma_y = \exp\left(a_y + b_y \ln(x) + c_y (\ln(x))^2\right)$			$\sigma_z = \exp\left(a_z + b_z \ln(x) + c_z (\ln(x))^2\right)$		
	a_y	b_y	c_y	a_z	b_z	c_z
A	-1.104	0.9878	-0.0076	4.679	-1.172	0.2770
B	-1.634	1.0350	-0.0096	-1.999	0.8752	0.0136
C	-2.054	1.0231	-0.0076	-2.341	0.9477	-0.0020
D	-2.555	1.0423	-0.0087	-3.186	1.1737	-0.0316
E	-2.754	1.0106	-0.0064	-3.783	1.3010	-0.0450
F	-3.143	1.0148	-0.0070	-4.490	1.4024	-0.0540

A: very unstable, B: unstable, C: moderately unstable, D: neutral, E: stable, F: very stable

Gaussian Plume Models
Empirical Dispersion Coefficients

Dispersion coefficients: Analytical formulas of Briggs-McElroy-Pooler

Briggs-McElroy-Pooler		
Stability	σ_y	σ_z
Rural conditions		
A	$0.22\,x\,(1 + 0.0001\,x)^{-1/2}$	$0.20\,x$
B	$0.16\,x\,(1 + 0.0001\,x)^{-1/2}$	$0.12\,x$
C	$0.11\,x\,(1 + 0.0001\,x)^{-1/2}$	$0.08\,x\,(1 + 0.0002\,x)^{-1/2}$
D	$0.08\,x\,(1 + 0.0001\,x)^{-1/2}$	$0.06\,x\,(1 + 0.0015\,x)^{-1/2}$
E	$0.06\,x\,(1 + 0.0001\,x)^{-1/2}$	$0.03\,x\,(1 + 0.0003\,x)^{-1}$
F	$0.04\,x\,(1 + 0.0001\,x)^{-1/2}$	$0.016\,x\,(1 + 0.0003\,x)^{-1}$
Urban conditions		
A & B	$0.32\,x\,(1 + 0.0004\,x)^{-1/2}$	$0.24\,x\,(1 + 0.001\,x)^{1/2}$
C	$0.22\,x\,(1 + 0.0004\,x)^{-1/2}$	$0.20\,x$
D	$0.16\,x\,(1 + 0.0004\,x)^{-1/2}$	$0.14\,x\,(1 + 0.0003\,x)^{-1/2}$
E & F	$0.11\,x\,(1 + 0.0004\,x)^{-1/2}$	$0.08\,x\,(1 + 0.00015\,x)^{-1/2}$

A: very unstable, B: unstable, C: moderately unstable, D: neutral, E: stable, F: very stable

Gaussian Plume Models
Simple Chemistry

The formulation of the gaussian plume model applies to chemically inert species (i.e, non-reactive). However, it is possible to add a term to account for a first-order loss term (i.e. proportional to the air pollutant concentration) to the gaussian equation; then, one obtains the following equation, which holds for a first-order chemical kinetics (i.e., the oxidant concentration, [X], is assumed to be constant):

$$C(t) = C_0 \exp\left(-k\,[\mathrm{X}]\,t\right) = C_0 \exp\left(-k'\,t\right)$$

$$C(x,y,z) = \frac{S}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left(\exp\left(-\frac{(z - z_{s,f})^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + z_{s,f})^2}{2\sigma_z^2}\right)\right) \exp\left(-k' t\right)$$

Gaussian Plume Models
Rain Scavenging (Washout)

It is also possible to add a term to the gaussian equation to account for the scavenging of air pollutants by rain using a first-order loss term (i.e. proportional to the air pollutant concentration) that includes an empirical scavenging rate coefficient, Λ (s^{-1}); then, one obtains the following equation:

$$C(t) = C_0 \exp\left(-\Lambda t\right)$$

$$C(x,y,z) = \frac{S}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left(\exp\left(-\frac{(z - z_{s,f})^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + z_{s,f})^2}{2\sigma_z^2}\right)\right) \exp\left(-\Lambda t\right)$$

Gaussian Plume Models
Dry Deposition

Dry deposition is more difficult to represent in the gaussian dispersion formula, because it affects the concentrations of the pollutant near the surface rather than the concentrations throughout the plume. The most appropriate representation consists in treating dry deposition as a partial absorption at the surface:

$$C(x,y,z) = \frac{S}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left(\exp\left(-\frac{(z - z_{s,f})^2}{2\sigma_z^2}\right) + \alpha_d \exp\left(-\frac{(z + z_{s,f})^2}{2\sigma_z^2}\right)\right)$$

$$\alpha_d = 1 - \frac{2 v_d}{v_d + \left(u z_{s,f} \sigma_z^{-1}\right)\left(\frac{d\sigma_z}{dx}\right)}$$

where v_d is the dry deposition velocity; for $\alpha = 1$, there is no dry deposition ($v_d = 0$) and for $\alpha = -1$, there is complete dry deposition of plume material in contact with the surface

Gaussian Plume Models
Limitations

- Gaussian models have limitations that result from the hypotheses associated with their formulation:

  - They do not apply far from sources (appropriate if $x < 50$ km).

  - They apply to flat terrain: approximations can be made to treat specific cases (e.g., hill), but they cannot treat certain configurations (e.g., street-canyon).

  - They apply to simple meteorological conditions: they can take into account the effect of an elevated inversion layer, but they cannot treat wind shear for example.

Lagrangian Models

- Lagrangian models, as gaussian models, calculate air pollutant concentrations with respect to a reference system that follows the trajectory of the mean wind. However, the hypothesis of stationary conditions (i.e., constant wind speed and direction) is no longer necessary.

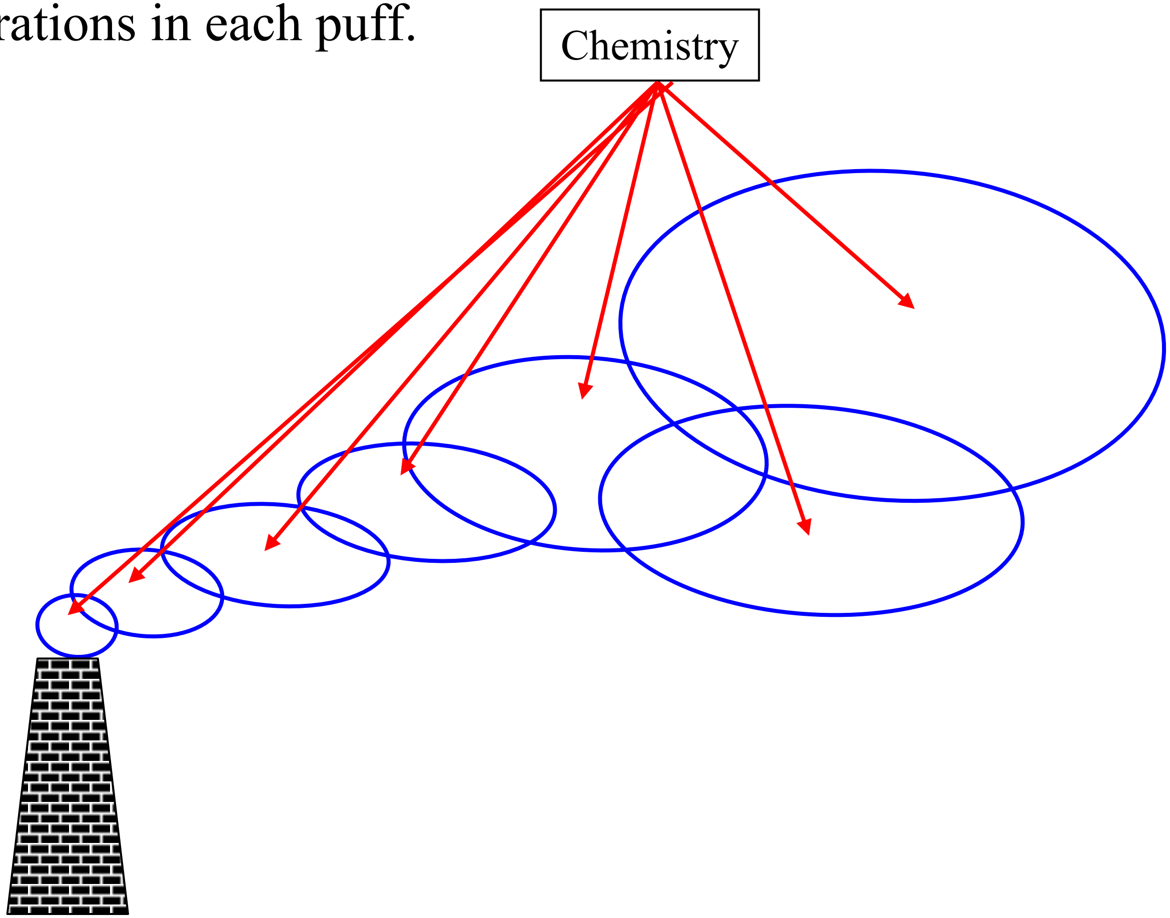
- There are two major categories of lagrangian models:
  - 2D Gridded lagrangian models with an expanding grid positioned crosswind
  - Lagrangian puff and "particle" models

Lagrangian Puff Models

- Puff and "particle" lagrangian models can handle complex wind fields, such as wind shear, because distinct puffs or "particles" can follow different trajectories.
- Individual puffs may use gaussian concentration profiles; however, the puff ensemble, which constitutes the plume, does not necessarily show gaussian concentration profiles because of the different trajectories followed by the individual puffs. Some approximations must be made for the atmospheric chemistry because average concentrations are typically assumed for each individual puff.
- "Particle" models cannot treat chemistry because there is no air volume associated with the "particles".

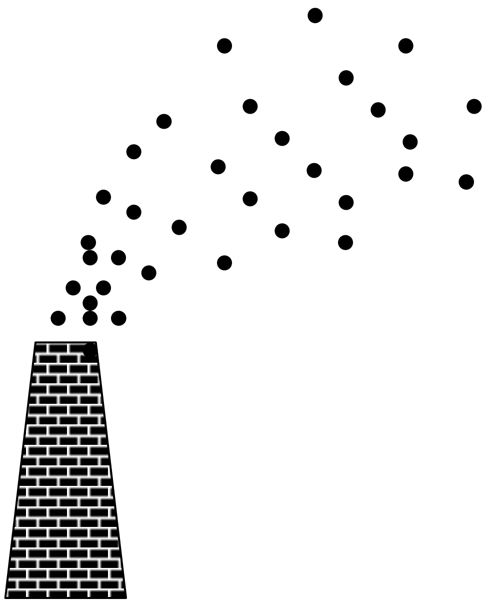
Lagrangian Puff Models

- Puff model: the chemistry may be treated using spatially-averaged concentrations in each puff.



Lagrangian “Particle” Models

- “Particle” model: the dispersion under complex configurations (e.g., buildings, complex terrain) can be treated if the wind field and turbulence are provided (for example, from a computational fluid mechanics simulation).

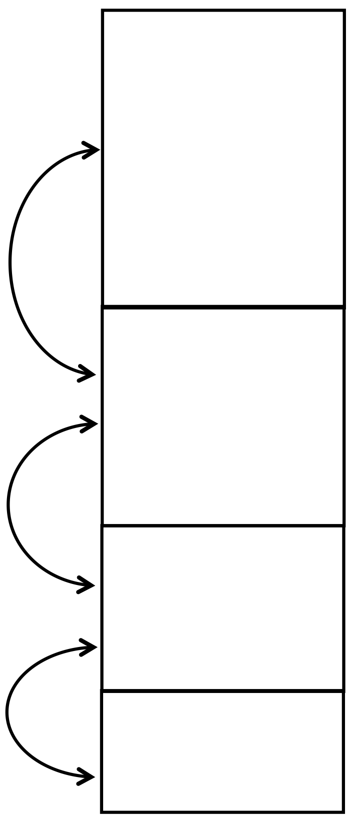


Eulerian Models
The Chemical-Transport Equation

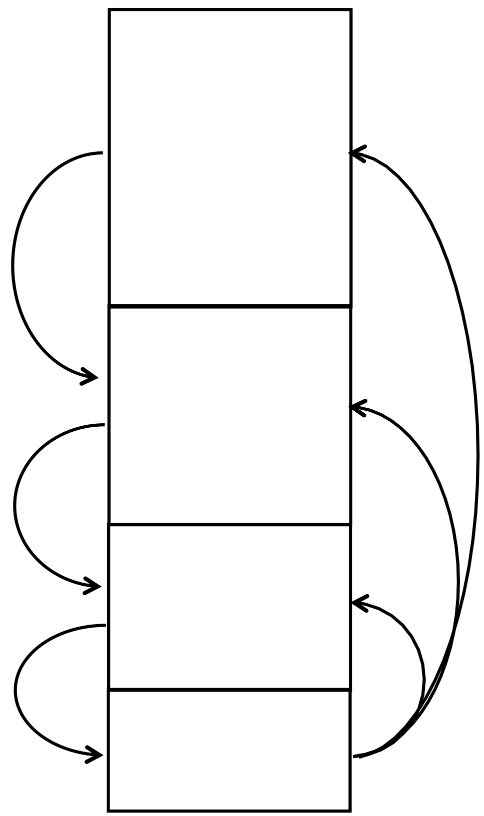
- The chemical-transport equation (also called the atmospheric diffusion equation or the mass conservation equation) does not have an analytical solution except for very simple cases (for example in the case of a steady-state gaussian plume) that are typically not representative of the atmosphere at regional or global scales. Therefore, a numerical solution is needed. It is generally solved via a discretization of the chemical-transport equation.

$$\frac{\partial C}{\partial t} = -\nabla(\underline{u}C) + \frac{\partial}{\partial x} K_h \frac{\partial C}{\partial x} + \frac{\partial}{\partial y} K_h \frac{\partial C}{\partial y} + \frac{\partial}{\partial z} K_z \frac{\partial C}{\partial z} + S - \Lambda C$$

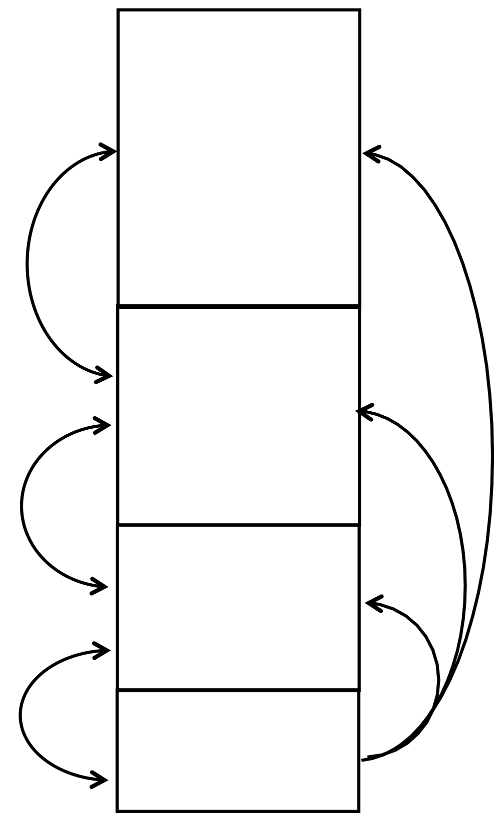
Eulerian Models
Various Representations of Vertical Dispersion



K-type turbulent diffusion

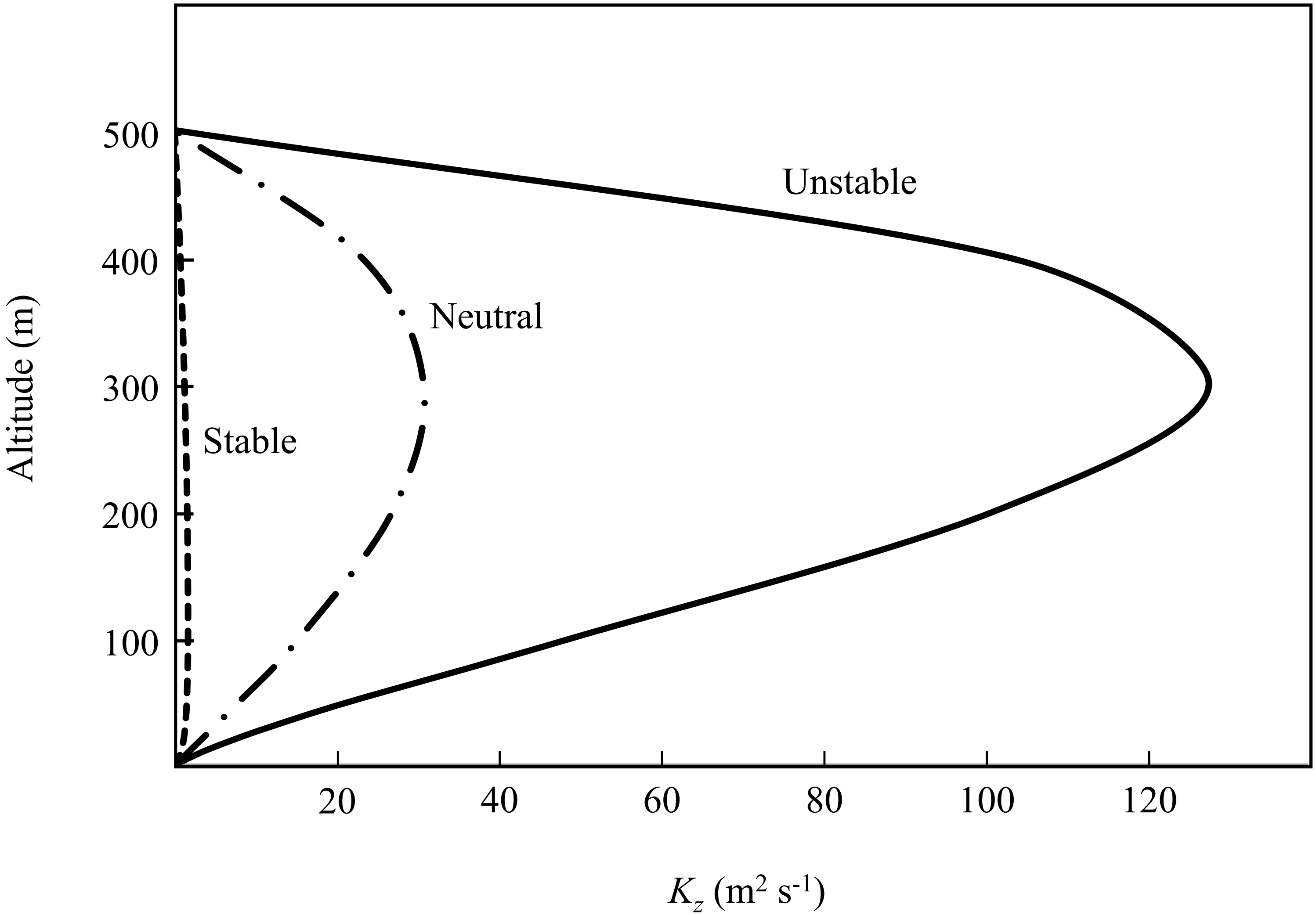


Asymmetric convective mixing
(ACM)



Asymmetric convective mixing
with K-type diffusion (ACM2)

Eulerian Models
Representation of Vertical Dispersion (K_z)



Eulerian Models
Representations of Horizontal Dispersion

- There are three major approaches to treat horizontal dispersion:

  - No horizontal dispersion: one considers that numerical diffusion due to the advection algorithm is sufficient to create horizontal dispersion

  - Smagorinsky algorithm (or similar)

$$K_{h,Smagorinsky} = 0.16\left(S_\Gamma^2 + S_\Lambda^2\right)^{\frac{1}{2}}\left(\Delta x\right)^2$$

$$S_\Gamma = \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) \qquad S_\Lambda = \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)$$

  - Unif algorithm (or similar)

$$K_{h,Unif} = 2000\left(\frac{4000}{\Delta x}\right)^2$$

Eulerian Models
Representations of Horizontal Dispersion

- **Smagorinsky algorithm**
  - The dispersion coefficient is proportional to the horizontal grid surface area, X^2.
  - Numerical diffusion increases with the grid size.
  - Therefore, the Smagorinsky algorithm leads to an increase in horizontal dispersion as the grid resolution becomes coarser.

Eulerian Models
Representations of Horizontal Dispersion

- **Unif algorithm**

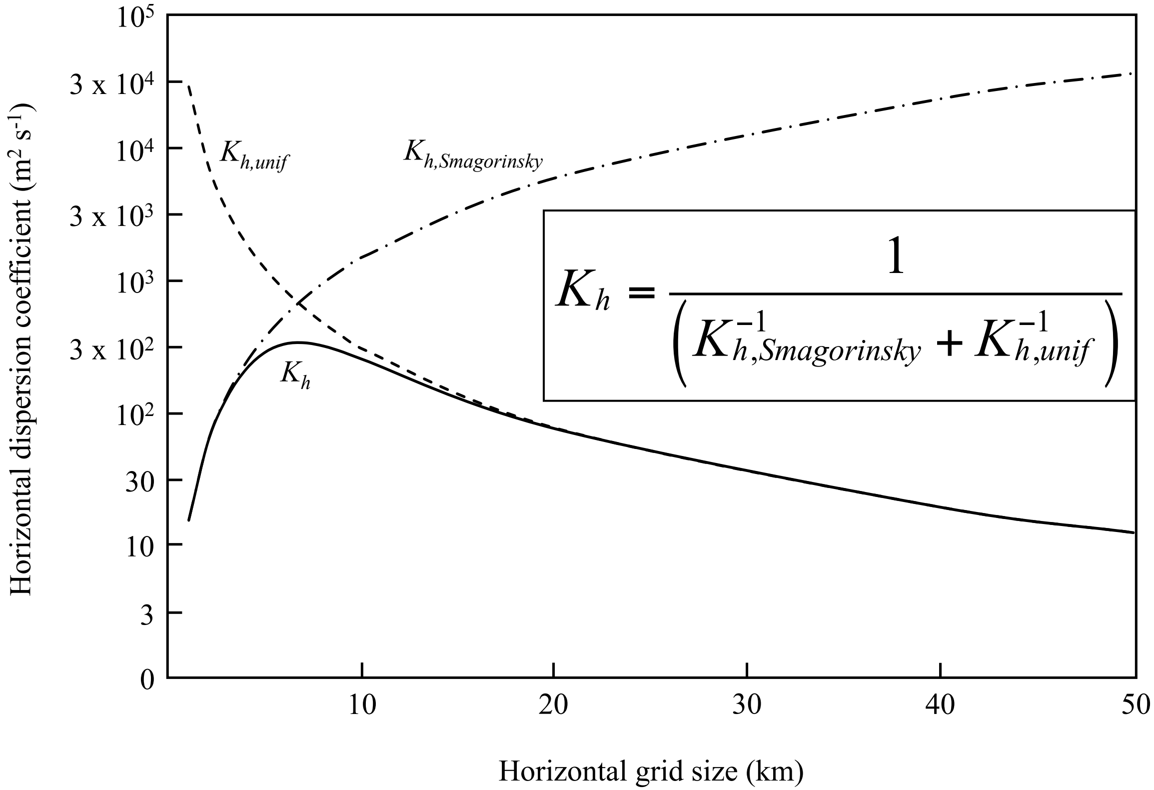
  - The dispersion coefficient is inversely proportional to the horizontal grid surface area: X^{-2}.

  - Numerical diffusion increases with the grid size.

  - Therefore, the Unif algorithm leads to an increase in horizontal dispersion as the grid resolution becomes finer.

Eulerian Models
Representations of Horizontal Dispersion

- Combining both formulations, using Unif for large grid sizes and Smagorinsky for small grid sizes, provides an optimal approach for horizontal dispersion in eulerian models.



Street-Canyon Models

- Street-canyon models represent the dispersion of air pollutants within a street canyon and the interactions between the street air volume and (1) the background urban air above roof level (represented by the vertical dispersion coefficient σ_w) and (2) the street-canyons located upwind and downwind.

$$u_s\, h_b\, W_s\, C_u + S\, L_s = u_s\, h_b\, W_s\, C + F_d\, L_s\,(W_s + 2\, h_b) + \frac{\sigma_w\, W_s\, L_s}{\sqrt{2}\,\pi}(C - C_b)$$

- Dimensions of the street canyon: L_s, W_s, and h_b
- Concentrations of the air pollutant: C, C_b (background air), and C_u (upwind)
- Meteorological conditions: u_s (horizontal wind speed within the street canyon) and σ_w (standard deviation of vertical wind speed at roof level)
- Dry deposition flux: F_d

Eulerian and Lagrangian Models
Hybrid (Plume-in-grid) Models

- If one wants to simulate background air pollution (urban or regional) and near-field pollution, one may construct a hybrid model, which simulates background air pollution in an eulerian grid system and the near-source air pollution with a lagrangian approach (using puffs, plumes or simple parameterizations) embedded within the eulerian model. This approach is called "plume-in-grid" (PinG) modeling (although it may actually use puff models to simulate the plumes) or multi-scale modeling.

- Hybrid models offer several advantages:
  - Representation of the near-source pollution at the sub-grid level
  - Correct treatment of atmospheric dispersion and chemistry for the plumes emitted from large point sources (stacks of power plants, cement plants, refineries…), volume sources (fugitive emissions from refineries, chemical plants…), and line sources (major roads and freeways, airplanes, ships, street canyons…).

Computational Fluid Dynamics (CFD) Models

- CFD models can provide a large array of parameterizations of turbulence with very fine spatial resolution and complex configurations:

  - *K*-theory
  - k-ε
  - k-ω
  - Large eddy simulation (LES)

Air Pollution Models

Gaussian plume models: near-source pollution

Lagrangian models: near-source and long-distance pollution for a limited number of sources

Eulerian models: urban background pollution up to regional, continental and global pollution for all sources (> 1 km resolution)

Street-canyon models: near-source pollution

Hybrid models (plume-in-grid): background pollution <u>and</u> near-source pollution

CFD models: near-source pollution with complex configurations

Gaussian Plume Models
Advantages and Shortcomings

Advantages:
- Simple analytical formulas
- Easy to develop a computer code
- Short computational times

Shortcomings:
- Only a few sources can typically be handled
- Constant atmospheric conditions (wind speed and direction, atmospheric stability) during a given period (typically 1 hour) and domain (< 50 km at most)
- Simple terrain (ideally flat, parameterizations available for simple configurations such as hills)
- Simple chemistry

Lagrangian Puff and “Particle” Models
Advantages and Shortcomings

Advantages:

- Simple analytical formulas (although some may use more advanced parameterizations)
- Short computational times compared to 3D gridded models
- Possibility to handle 3D flow fields
- Possibility to simulate long-range transport
- Possibility to handle comprehensive chemistry, but with some approximations

Shortcomings:

- Only a few sources can typically be handled

Eulerian Models
Advantages and Shortcomings

Advantages:

- 3D representation
- Comprehensive chemistry and deposition processes
- All sources can be handled
- Large domains can be simulated

Shortcomings:

- Limited spatial resolution (> 1 km): no near-source resolution
- Large computational times

Street-canyon Models
Advantages and Shortcomings

Advantages:
- Simple analytical formulas
- Easy to develop a computer code
- Short computational times

Shortcomings:
- Parameterized representations of the air flow
- Constant atmospheric conditions (wind speed and direction, atmospheric stability) during a given period (typically 1 hour) and domain (street network)
- Idealized representation of the building configuration (uniform building height and street width for a given street)
- Simple chemistry

Hybrid Models
Advantages and Shortcomings

Advantages:
- Those of the near-source models and those of the 3D eulerian models

Shortcomings:
- Greater computational times than the standard eulerian models, depending on the number of sources treated at the subgrid scale

CFD Models
Advantages and Shortcomings

Advantages:

- Navier-Stokes equations: good representation of the 3D flow
- Possibility to represent turbulence with various levels of detail (*K*-theory, k-ε, k-ω, LES, etc.)
- Complex configurations can be simulated (hills, buildings, etc.)
- Possibility to include comprehensive chemistry and deposition processes
- Several sources can be handled

Shortcomings:

- Very large computational times