Lesson 3 TRANSPORT AND DISPERSION OF AIR POLLUTANTS

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- 3.1. Atmospheric stability
- 3.2. Stability and plume behavior
- 3.3. Dispersion modeling



Pollutants enter the atmosphere in a number of different ways. For example, wind blows dust into the air. Automobiles, trucks and buses emit pollutants from engine exhausts and during refueling. Electric power plants, along with home furnaces, give off pollutants as they try to satisfy mankind's need for energy.

One method of pollution release from stationary point sources has received more attention than any other: **stacks**. As the exhaust gases and pollutants leave a stack, they mix with ambient air describing a **plume.** As the plume travels downwind, the plume diameter grows and it progressively spreads and disperses.



"Smoke plume from chimney of power plant" by Pöllö licensed under CC BY 3.0



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Gases leaving the tops of stacks rise higher than the stack top when they are either of lower density than the surrounding air (**buoyancy rise**) or ejected at a velocity high enough to give the exit gases upward kinetic energy (**momentum rise**).





After this initial stage, the **dispersion of pollutants** in the atmosphere is the result of the following three mechanisms: 1) general air motion that transports pollutants downwind, 2) turbulent velocity fluctuations that disperse pollutants in all directions and 3) diffusion due to concentration gradients.

Turbulence is highly irregular motion of the wind.

There are basically two different causes of turbulent eddies: **mechanical turbulence** and **convective turbulence**. While both of them are usually present in any given atmospheric condition, either mechanical or convective turbulence prevails over the other.

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Mechanical turbulence is caused by physical obstructions to normal flow such as mountains, building, trees,... The degree of mechanical turbulence depends on wind speed and roughness of the obstructions.

Convective turbulence results from different heating-cooling of surfaces and air masses. The higher the temperature difference, the greater the turbulence is.

Atmospheric eddies cause a breaking apart of atmospheric parcels which mixes polluted air with relatively unpolluted air, causing polluted air at lower and lower concentrations to occupy successively larger volumes of air. Thus, the level of turbulence in the atmosphere determines its dispersive ability.

Top Atmospheric Boundary Layer



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Most turbulent and pollutant dispersion processes occur in the **Atmospheric Boundary Layer** (ABL). ABL is the bottom layer of the troposphere.

- Its **thickness** is \approx **1000** m, but quite variable (100 m- 4000 m) in time and space.
- The configuration of the **flow** is quite variable too: **laminar** during night-time hours and **turbulent** during daytime.
- It can be divide into two layers, namely: **Surface Boundary Layer** (SBL) and **Planetary Boundary Layer** (PBL)

The ABL is the most important layer with respect to air pollution. Almost all of the airborne pollutants emitted into the ambient atmosphere are transported and dispersed within the ABL.



3.1. ATMOSPHERIC STABILITY

of the One most important characteristics in intensity of turbulence in the atmosphere is its stability. Stability is the tendency to resist vertical motions or to suppress existing turbulence). The atmospheric stability is related to the variation with altitude of temperature, pressure and humidity.





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Holding other conditions constant, the temperature of air increases as atmospheric pressure increases and conversely decreases as pressure decreases. With respect to the atmosphere, where air pressure decreases with rising altitude, the normal temperature profile of the troposphere is one where temperature decreases with height. An air parcel that becomes warmer than the surrounding air begins to expand and cool. As long as the parcel's temperature is greater that the surrounding air, the parcel is less dense than the cooler surrounding air. Therefore, it rises, or is buoyant. As the parcel rises, it expands thereby decreasing its pressure and, therefore, its temperature decreases as well. The initial cooling of an air parcel has the opposite effect.



Assuming that:

- 1. The air parcel is a relatively well-defined body of air that it does not mix with the surrounding air
- The exchange of heat between the air parcel and its surrounding is minimal: it does not gain or lose heat (adiabatic process) and,
- 3. This raising (falling) air parcel cools (heats) without reaching its dew point, that is, without saturation, any water in it remains in a gaseous state (**dry air**).

Likewise, the rate of cooling (or warming) of the air parcel forced to rise or descend is about -9.76 (+9,76) °C·km⁻¹. This is the **dry adiabatic profile** or **dry adiabatic lapse rate (DALR).**

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Warm air rises and cools, while cool air descends and warms

The extent to which an air parcel rises or falls depends on the relationship of its temperature to that of the surrounding air.

Thus, the **degree of stability** of the atmosphere can be determined from comparing the DALR and the **environmental lapse rates.**



Comparing the temperature of the parcel to that of the surrounding environment, it is seen that in rising from *a* to *b*, the parcel undergoes the temperature change of the DALR. Since the rate of the surrounding environment is steeper than the DALR (**superadiabatic**), at *b* the parcel is warmer than the environment b', and the resulting acceleration is upward. The parcel will continue to rise. This atmosphere is enhancing the vertical motion (**unstable**).



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However, when the lapse rate of the surrounding environment is not as steep as the dry adiabatic lapse rate (**subadiabatic**), in the forced ascent of the air parcel up the slope from *a* to *b* it cools less than the DALR; thus, at *b* parcel is cooler than the environment *b*`, therefore, it will sink back to its original level. This atmosphere resists upward or downward motion (**stable**).



Temperature

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When the lapse rate of the surrounding environment is the same as the dry adiabatic lapse rate (adiabatic), the vertical movement is neither encouraged nor hindered. The atmosphere is in a state of neutral stability.



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Summing up, according to the vertical temperature profiles there are three categories of stability:

• Neutral conditions $\Gamma_{env} = \Gamma_{DALR}$ Occur on windy days or when there is a cloud cover such as that

strong heating or cooling of the earth's surface does not occur.

✓ Mechanical turbulence

• Unstable conditions $\Gamma_{env} > \Gamma_{DALR}$

Develop on sunny days with low wind speeds.

- ✓ Mechanical turbulence + thermal induced turbulence
- Stable conditions $\Gamma_{env} < \Gamma_{DALR}$

Occur at night when there is little or no wind.

✓ Mechanical turbulence + thermal induced turbulence



When air temperature increases with altitude an **inversion** occurs. Inversions are directly related to pollutant concentrations in the ambient air, since they inhibit vertical movements and the dispersion of air pollutants. The most common inversion type is **radiation inversion** and occurs when the earth's surface cools rapidly.



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3.2. STABILITY AND PLUME BEHAVIOUR

The stability of the air (vertical air movement) together with the horizontal air flow influences the behavior of plumes from stacks. Thus, watching smoke plumes provides a clue to the turbulence of the atmosphere, and knowing the stability yields important information about the dispersion of pollutants.

Next figure depicts early morning conditions. The winds are light, and a radiation inversion extends from the surface to above the height of the stack. In this **stable** environment, there is little up and down motion, so the smoke spreads horizontally rather than vertically. The smoke plume resembles the shape of a fan: **fanning**

¹⁹ smoke plume.



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Later in the morning, the surface air warms quickly and destabilizes as the radiation inversion gradually disappears In **neutral** conditions, the **coning smoke plume** occurs.

If daytime heating of the ground continues, the depth of atmospheric instability increases. Light-to-moderate winds combine with rising and sinking air to cause the smoke to move up and down in a wavy pattern, producing a **looping smoke plume**.

While **unstable** conditions are generally favorable for pollutant dispersion, momentarily high-ground level concentrations can be registered if the plume loops downward to the surface: **fumigation**.



"Atmosphere fanning" by Saperaud licensed under Public Domain

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"Atmosphere conning" by Saperaud licensed under Public Domain





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A major problem for pollutant dispersion is an **inversion** layer, which acts as a barrier to vertical mixing. The height of the stack in relation to the height of the inversion layer influence ground-level pollutant concentrations during an inversion.

When conditions are unstable above an inversion the release of a plume above the inversion results in effective dispersion without noticeable effects on ground level concentrations around the source. This condition is known as **lofting**.





"Atmosphere lofting" by Saperaud licensed under Public Domain

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If the plume is released under an inversion layer, a serious air pollution situation could develop. As the ground warms in the morning, air below an inversion layer becomes unstable. When the instability reaches the level of the plume that it is still trapped below the inversion layer, the pollutants can be rapidly transported down toward the ground. This is known as **fumigation**.

If the air below the inversion is neutral, vertical movements are blocked and the plumes are trapped below this layer. This is **trapping** (not shown). It should therefore be apparent why taller chimneys have replaced many of the shorter ones. Although these tall stacks can prevent fumigation and trapping, thus improving the air quality in their immediate area, they may also contribute to larger scale problems by allowing the pollutants to be swept great distances downwind.





"Atmosphere fumigation" by Saperaud licensed under Public Domain

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3.3. DISPERSION MODELING

Air quality modeling is the necessary substitute for ubiquitous air quality monitoring, which is impossible. It is also necessary for predicting the impacts from potential emitters, simulation of ambient concentrations under different policy options, determining the relative contributions from different sources,...

Air quality models (AQM) are tools to research the relations between the emission of pollutants and/or precursors and the ambient air concentration.



Applications

At a **local level** AQM can be used to design stacks, to select a placement for a new source, to verify that before issuing a permit, a new source will not exceed ambient air quality standards,...

At a **regional level**, AQM are useful as prediction tools (for example, to estimate the future pollutant concentrations from multiple sources after a regulatory program), to give a measure of the expected effectiveness of various options in reducing harmful exposures to humans; for urban planning and policies on zoning, traffic routes,...

Additionally, AQM are helpful tools at the **continental** and **global scale** for the estimation of transboundary transport; for developing long-term air pollution control policies,... and so on

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Input data

The required model inputs are the following:

- Emissions data: distribution of the sources and emission rate
- **Meteorological data**: wind speed and direction, temperature, pressure and vertical mixing.
- Chemical transformations and deposition processes



"North Europe wind speed sample" by Johnjsturman licensed under Public Domain



Classification

According to their **approach**, dispersion models can be classified into two types:

Physical models or dynamic models simulate the physical and chemical processes that affect air pollutants as they disperse and react on a reduced scale. Simulation is carried out in prototypes such as wind tunnels or hydrodynamical channels.

Mathematical models or numerical simulation models consist of a set of equations that interpret and predict pollutant concentrations due to transport and dispersion.

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There are four generic types of mathematical models:

- 1. Models based on statistical treatment of databases
- 2. Models based on random trajectories
- 3. Pure advection models: Box models
- 4. Diffusion models are based on the solution of transport equations. According to the method of solution they are subclassified into:
 - Gaussian plume model (analytical solution)
 - K models (numerical solution)

Rapid advances in high performance computing hardware and software are leading to increasing applications of numerical simulation models.



1. MODELS BASED ON STATISTICAL TREATMENT OF DATABASES

These models are based on statistical techniques to analyze and adjust the interrelationship between atmospheric conditions and air quality (AQ).



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They can be used to study the meteorological conditions and processes that affect the AQ in an area. Moreover, they are very useful for real-time forecasting of AQ.



velocity:

Where: x(t) = position at time t $x(t - \Delta t)$ = position of the particle in the previous time interval (t-1) $u\Delta t$ = displacement from *t*-1 to *t*

The **position** of each particle is calculated by using the semi-random

 $x(t) = x(t - \Delta t) + u\Delta t$

These models are particularly useful for simulating short-term releases from sources with highly variable emission rates in complex dispersion scenarios.

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2. MODELS BASED ON RANDOM TRAJECTORIES

These models characterize air pollution by calculating the statistics of the trajectories of a large number of fictitious particles.

Particle motion is produced by semivelocities generated random using Monte Carlo techniques.

The velocity of the particles accounts for two components:

	$u = \overline{u} + u'$
Where:	<i>u</i> = semi-random velocity [L·T ⁻¹]
	$\overline{\mathbf{u}}$ = mean wind velocity [L·T ⁻¹]
	<i>u</i> '= pseudo-random velocity [L·T ⁻¹]

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3. PURE ADVECTION MODELS

To conduct a dispersion study over a large area like a city where a number of point-sources, linear-sources, area-sources and diffuse sources coexist, each one releasing pollutants with a different emission rate, non diffusive or pure advection models are used.

The **simplest box model** assumes that the volume of the atmospheric air of the study area is inside the volume of a 3D box.

It also makes the following simplifying assumptions:



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- 1. The city is a rectangle with dimension $W(\Delta x)$ and $L(\Delta y)$
- 2. Complete mixing of pollutants up to *zi* is produced. It considers the diurnal variation of mixed layer height *zi*.
- 3. The turbulence is strong enough that the pollutant concentration is *C* uniform in the whole volume of air over the city.
- 4. The wind blows in **x** direction with velocity **u**. This velocity is constant and is independent of time, location or elevation.
- 5. The concentration of pollutant entering the city is constant and equal to C_b (background concentration). The same applies for the concentration above the mixing layer C_a .
- 6. The air pollution emission rate of the city is Q_a . It is constant and unchanging with space and time.
- 7. Pollutants are inert and long-lived in the atmosphere.





Parameters of the Box model

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The general mass balance equation is:

$$\Delta x \, z_i \, \frac{\partial C}{\partial t} = \, \Delta x \, Q_a + \, u \, z_i \, (C_b - C) + \Delta x \, \frac{\partial z_i}{\partial t} \, (C_a - C)$$

Whe $\Delta x \, z_i \frac{\partial C}{\partial t}$

rate of change of mass within the box

 $\Delta x \ Q_a$ sum of the emission rates at which the pollutant mass is added

$$u z_i (C_b - C)$$
 concentration change due to
horizontal advection

$$\Delta x \frac{\partial z_i}{\partial t} (C_a - C) \qquad \text{concentration change due to variations} \\ \text{in mixing height and vertical advection}$$



Assuming steady-state emissions and atmospheric conditions:

$$\frac{\partial C}{\partial t} = \frac{\partial z_i}{\partial t} = 0 \quad \longrightarrow \quad C = \quad \frac{\Delta x}{z_i} \frac{Q_a}{u} + C_b$$

Further simplifications can be made for negligible background concentrations:

C = steady-state concentration [M·L⁻³]

 Q_q = area emission rate [M·L⁻²·T⁻¹]

u= mean wind speed [L·T⁻¹]

 z_i = mixing height [L]

 Δx = distance over which emissions take place [L]

$$C = \frac{\Delta x}{z_i} \frac{Q_a}{u}$$

Where:

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4. DIFFUSION MODELS

These models describe how the emission, chemistry, transport and deposition processes determine the atmospheric concentrations of pollutants based on the **continuity equation.**

Because of the complexity and variability of the processes involved, the continuity equation cannot be solved exactly. Thus, it is necessary to use **approximations** to convert the complex atmosphere into a model system which lends itself to a solution.

The **integral approach** reduces the problem to a system of differential equations by making some simplifications (Gaussian plume models); whereas the **numerical approach** divides the domain into grids of discrete elements and then uses several methods to solve the equation over the full domain (K models).



Gaussian plume model

The Gaussian plume model is the most common air pollution model for estimating concentrations from point sources downwind.

Employing a three-dimensional axis of downwind (*x*), crosswind (*y*), and vertical (*z*) with the origin at the effective height of emission, it assumes that the time-averaged plume concentrations from a continuously emitting plume, at each downwind distance, have independent **Gaussian distributions** both in the horizontal and the vertical.



"Gaussian 2d" by Kghose licensed under CC BY-SA 3.0



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In its simplest form, it also assumes the following:

- Concentrations are proportional to the emission rate
- Pollutants are diluted by the wind at the point of the emission at a rate inversely proportional to the wind speed, which is constant both in time and height
- They do not undergo chemical reactions or other removal processes
- Pollutant material reaching the ground or the top of the mixing height as the plume grows is reflected back to the plume centerline.

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Thus, the concentration *C* resulting at a receptor (*x*, *y*, *z*) from a point source with a continuous and constant emission rate based on a coordinate scheme with the origin located at the effective height (0, 0, *H*) and the x-axis in the wind direction, is given by the following equation: $1(y^2 - z^2)$

$$\bar{C}(x,y,z) = \frac{Q}{2\pi \sigma_y \sigma_z \bar{u}} e^{-\frac{1}{2} \left(\frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right)}$$

C= concentration $[M \cdot L^{-3}]$ Q= emission rate $[M \cdot T^{-1}]$ σ_y and σ_z = standard deviation of horizontal and vertical distribution of plume concentration [L] u= wind speed $[L \cdot T^{-1}]$ x and y= downwind and crosswind distances [L] z= receptor height above ground [L] H= effective height of emission [L]

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PLUME RISE

Although the plume originates at a stack height h, it rises to an additional height Δh owing to the buoyancy of the hot gases and the momentum of the gases leaving the stack. This is referred to as plume rise. Consequently, the plume appears as if it is originated as a point source at an effective stack height H.

The effective height of emission is obtained by adding the plume rise to the physical height of the stack:

$$H = h + \Delta h$$

There are numerous methods for calculating the plume rise. Algorithms developed by Briggs determine Δh as a function of atmospheric stability:

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1) For unstable and neutral stability categories (A-B-C and D)

$$\Delta h = 1.6 \, F^{1/3} \, x_f^{2/3} \, \frac{1}{\bar{u}}$$

F = Buoyancy flux parameter or floatation parameter [L⁴·T⁻³]

u = wind speed at the physical stack top [L·T⁻¹]

 x_f = distance from the stack to where the final plume rise occurs [L]

The value of **buoyancy flux** or **floatation** (F) is:

$$F = g v_s r_s^2 \frac{T_s - T_a}{T_s}$$

$$r_s = \text{inside stack-top radius [L]}$$

$$g = \text{acceleration due to gravity [L·T-2]}$$

$$v_s = \text{stack gas velocity [L·T-1]}$$

$$T_s = \text{stack gas temperature (K)}$$

$$T_a = \text{ambient air temperature (K)}$$



The horizontal distance from the stack to where the final plume rise occurs is assumed to be:

$$x_f = 49 F^{\frac{5}{8}}$$
 if $F < 55 \text{ m}^4 \text{s}^{-3}$
 $x_f = 119 F^{\frac{2}{5}}$ if $F \ge 55 \text{ m}^4 \text{s}^{-3}$

2) For stable categories (E and F):

$$\Delta h = 2.4 \, \left(\frac{F}{\bar{u} \, S}\right)^{1/3}$$

S is the stability parameter. It is calculated by $S = \frac{g}{T_a} \frac{\Delta T_a}{\Delta z} + 0.01^{\circ} \text{C/m}$

where $\Delta T_{\alpha} / \Delta_{z}$ is the change of ambient air temperature.

3) For calm conditions, the plume rise is:
$$\Delta h = \frac{5 F^{1/4}}{S^{3/8}}$$

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DISPERSION PARAMETERS

They are a measure of the atmospheric mixing capacity. The parameters σ_v and σ_z are found by the estimation from graphs, as a function of the **distance** between source and receptor (x), from the appropriate curve, one for each stability class (A-B-C-D-E).

Alternatively, σ_v and σ_z can be calculated using the following powerlaw expressions: Coefficients and exponents for dispersion parameters

$\sigma = \alpha r^p$	Stability	σ,		σ _z (0.5-5 km)		σ _z (5-50 km)	
$v_y - ux^2$	class	а	р	b	q	b	q
$\sigma_z = bx^q$	А	0.3658	0.9031	0.0003	2.1250		
- v- distance	В	0.2751	0.9031	0.0019	1.6021		
downwind (m)	С	0.2089	0.9031	0.2000	0.8543	0.5742	0.7160
	D	0.1474	0.9031	0.3000	0.6532	0.9605	0.5409
	E	0.1446	0.9031	0.4000	0.6021	2.1250	0.3979



PASQUILL STABILITY CATEGORIES

Pasquill advocated the use of fluctuation measurements for dispersion estimates but provided a scheme. The necessary parameters for the scheme consist on wind speed, insolation, cloudiness, which are basically obtainable from routine observations.

		Insolation	Night		
Surface wind speed (m·s ⁻¹)	strong	moderate	slight	thinly overcast or ≥4/8 low cloud	≤ 3/8 cloud
<2	А	A-B	В	-	-
2-3	A-B	В	С	Е	F
3-5	В	B-C	С	D	E
5-6	С	C-D	D	D	D
> 6	С	D	D	D	D

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WIND SPEED VARIATION WITH HEIGHT

Ordinary meteorological instrumentation includes wind measurements made at **10 m** above ground by using **anemometers**. Measurements above the surface can also be made by radiosondes, wind profilers or aircraft. Since operating the latter instruments is extremely expensive, attention has focused on **indirect determination** of upper-air wind speed.



"Wind Profiler" by Epolk licensed under Public Domain via Wikimedia Commons



The mean wind speed is often represented as a power-law function of height by: $(z)^p$

$$u_z = u_{10} \left(\frac{z}{z_{10}}\right)^p$$

 u_z = wind speed at height z (m·s⁻¹) [L·T⁻¹) u_{10} = wind speed at the anemometer measurement height (10 m) [L·T⁻¹) z_{10} = 10 meters (m) [L)

The exponent p is an empirically derived coefficient that varies depending upon the atmospheric stability and surface roughness:

Stability class	Α	В	С	D	Ε	F	Rural/flatlands	p = 0.16
p	0.15	0.15	0.20	0.25	0.40	0.60	Downtown	p = 0.20 p = 0.4

Coefficients recommended by the EPA



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It is convention to locate the origin at the base of the stack (0,0, z-H) instead at the effective height. This latter scheme is more convenient for assessing the total concentration at a receptor from more than one source. Substituting this value into the general equation, it becomes:

$$\bar{C}(x, y, z) = \frac{Q}{2\pi \sigma_y \sigma_z \bar{u}} e^{-\frac{1}{2} \left(\frac{y^2}{\sigma_y^2} + \frac{(z-H)^2}{\sigma_z^2}\right)}$$

The preceding equation can be modified to take into account the reflection of pollutants back to the atmosphere, once the plume reaches ground level. The reflection at a distance *x* is equivalent to having a mirror image of the source.



Contribution of the real source

$$\frac{Q}{2\pi \sigma_y \sigma_z \bar{u}} e^{-\frac{1}{2} \left(\frac{y}{\sigma_y}\right)^2} e^{-\frac{1}{2} \left(\frac{z-H}{\sigma_z}\right)^2}$$

Contribution of the virtual source

$$\frac{Q}{2\pi\,\sigma_y\,\sigma_z\,\bar{u}}\,e^{-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2}e^{-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2}$$

As a result, the concentration equation for a source with reflection becomes:

$$\bar{C}(x,y,z) = \frac{Q}{2\pi \,\sigma_y \,\sigma_z \,\bar{u}} \,e^{-\frac{1}{2} \left(\frac{y}{\sigma_y}\right)^2} \left(e^{-\frac{1}{2} \left(\frac{z-H}{\sigma_z}\right)^2} + e^{-\frac{1}{2} \left(\frac{z+H}{\sigma_z}\right)^2}\right)$$

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Simplifications

Concentration at ground level

$$\bar{C}(x, y, 0) = \frac{Q}{\pi \sigma_y \sigma_z \bar{u}} e^{-\frac{1}{2} \left(\frac{y}{\sigma_y}\right)^2} e^{-\frac{1}{2} \left(\frac{H}{\sigma_z}\right)^2}$$

Concentration at ground level in the centerline:

$$\bar{C}(x,0,0) = \frac{Q}{\pi \sigma_y \sigma_z \bar{u}} e^{-\frac{1}{2} \left(\frac{H}{\sigma_z}\right)^2}$$

Maximum concentration and the distance to maximum concentration:

$$\bar{C}_{max}(x_{max},0,0) = \frac{2Q}{e \pi \bar{u} H^2} \frac{\sigma_z(x_{max})}{\sigma_y(x_{max})} \qquad \sigma_z(x_{max}) = \frac{H}{\sqrt{2}}$$





Almost all the regulatory models (stack design, impacts at short distances,...) recommended by the U.S Environmental Protection Agency (EPA) are Gaussian.

 AERMOD (American Meteorological Society/Environmental Protection Agency Regulatory MODel). This is a steady-state continuous plume-model.

http://www.epa.gov/ttn/scram/dispersion_prefrec.htm#aermod

•For non-steady-state conditions, the EPA recommends the **CALPUFF** modeling system, which is non-steady state **puff dispersion model** that simulates the effects of time and space-varying meteorological conditions on pollution transport and removal.

http://www.epa.gov/ttn/scram/dispersion_prefrec.htm#calpuff

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