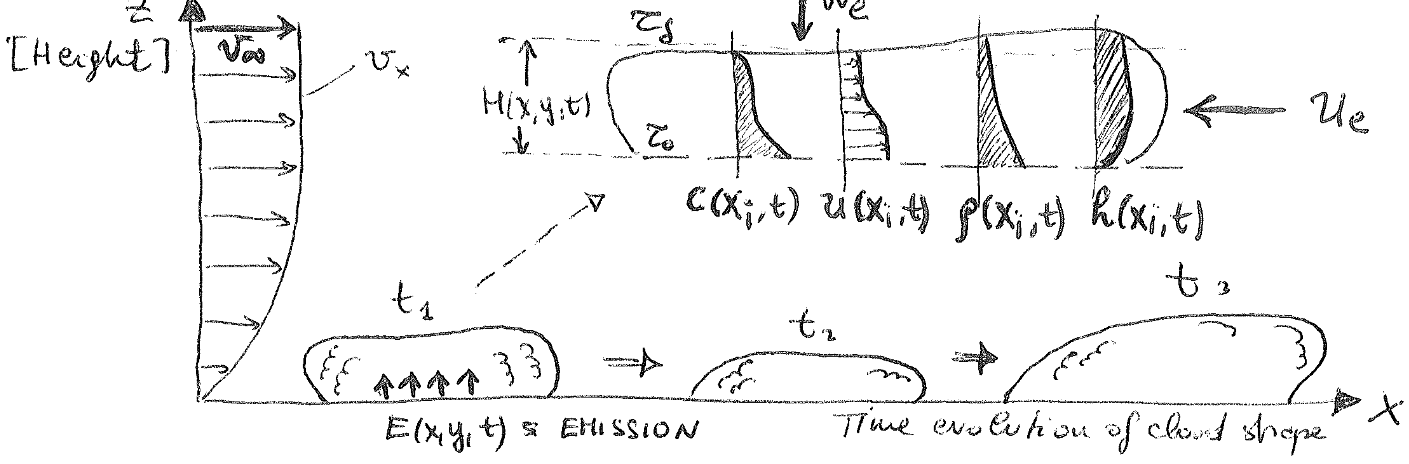
ATMOSPHERIC DISPERSION OF HEAVY GASES

The general physical problem of interest in this Section is the dispersion (by mixing with atmospheric air) of a mass of heavy gas that is released during a finite time period into the atmospheric boundary layer.

Different from a neutral gas (which does not alter the behavior of the air, hence the name "passive contaminant"), a heavy gas will spread under the influence of gravity (being denser than the ambient air) and this influence will affect its advection and dispersion by the atmospheric turbulence.

A schematic of the typical development and evolution of a heavy gas "cloud" is the following:



where :

- $E(x,y,t)$ is the rate at which the heavy gas is issued from the cloud source
- $C(x,y,z,t) \equiv C(x_i,t)$ is the local concentration of the heavy gas
- $\rho(x,y,z,t)$ its density
- $h(x,y,z,t)$ its enthalpy (equivalent to the total heat content within the cloud)
- $u(x,y,z,t)$ the gas velocity profile within the cloud
- u_e, W_e are the entrainment velocities (in the horizontal and vertical directions, respectively), with which atmospheric air is entrained inside the cloud through the front (and side) boundaries - u_e - and through the top boundary - W_e - of the cloud.
- τ_0, τ_δ are the shear stresses generated at the cloud bottom and top surfaces, respectively.

Typically, the phase during which the cloud is formed has a small duration compared to the time during which the cloud travels to the maximum distance exposed to the threshold value of gas concentration of interest.

The heavy gas cloud is three-dimensional and highly transient. Because of this, a model to predict accurately momentum, mass and energy transfer processes within the cloud (which are of interest because it's these processes that control the evolution of the cloud and its dynamics) is extremely complex and difficult to develop. Indeed, the cloud evolution is characterized by several distinct stages:

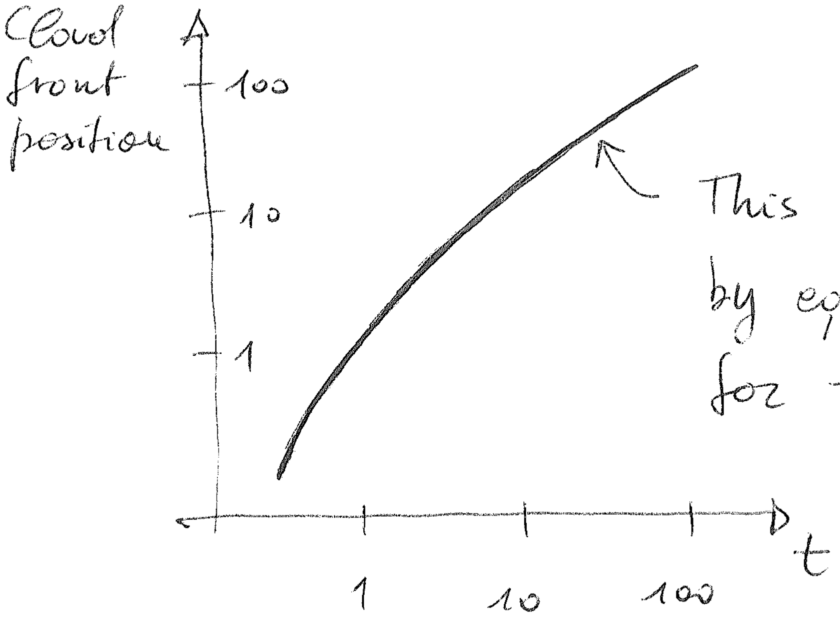
1) Emission from a source : the heavy gas is released into the atmosphere, and forms a cloud that has similar vertical and horizontal dimensions in the vicinity of the source (especially in the case of fast release of large amounts of gas). The behaviour of the gas cloud immediately after release is relatively independent of the characteristics of the ambient atmospheric air (e.g. wind field).

modelled as a gravity-driven intrusion of the heavy gas into the surrounding air. The transient gravity front that forms can be modelled as a quasi-steady flow in which the buoyancy spreading forces are balanced by the inertial forces. Under such assumptions, the velocity of the front is calculated from the relation:

$$\boxed{u_f = C_E \cdot \sqrt{g' \cdot H}} \quad [1]$$

g' = REDUCED GRAVITY $= \frac{\rho_c - \rho_a}{\rho_a} \cdot g$

which is obtained from the Bernoulli equation in the case of balance between the potential energy and the kinetic energy of the cloud with negligible viscous dissipation effects.



This curve is well predicted by eq. [1] with $C_E = 1.16$ for $t > 20T$, where $T = \frac{V^{1/6}}{\sqrt{g'}}$ is the characteristic time-scale of the cloud release (V is the cloud volume)

2) Buoyancy - dominated flow regime: close to the source, the cloud develops under the combined contribution of buoyancy forces, inertial forces and ambient air motions. In this stage, the cloud "slumps" (to slump = to fall or sink suddenly) because it is still heavy and spreads over the ground driven by gravity. During this process of slumping and lateral spreading, the cloud's shape resembles that of an expanding vortex ring. It has been proven that slumping and lateral spreading lead to entrainment of large amounts of ambient air (up to ten times the initial mass of the cloud): This implies that the density ratio between the cloud (not so heavy, anymore) and the ambient air is reduced by a factor of ten, namely that strong dilution takes place (dilution factor of ten to one hundred).

The process of lateral spreading is typically

As far as dilution is concerned, the main observable that needs to be modelled is air entrainment into the heavy gas cloud. In particular the flow rate of entrained air must be modelled. Referring to the schematic of page 1, such flowrate can be expressed as:

$$[2] \quad \boxed{Q_e = u_e \cdot A_f + w_e \cdot A_t} \quad [m^3/s]$$

where $u_e \cdot A_f$ is the horizontal entrainment rate (with A_f the surface area through which air is entrained horizontally with velocity u_e) and $w_e \cdot A_t$ is the vertical entrainment rate (with A_t the surface area through which air is entrained vertically with velocity w_e).

Estimates for u_e and w_e are:

$$\boxed{u_e = C_e \cdot u_f} \rightsquigarrow u_e \propto u_f$$

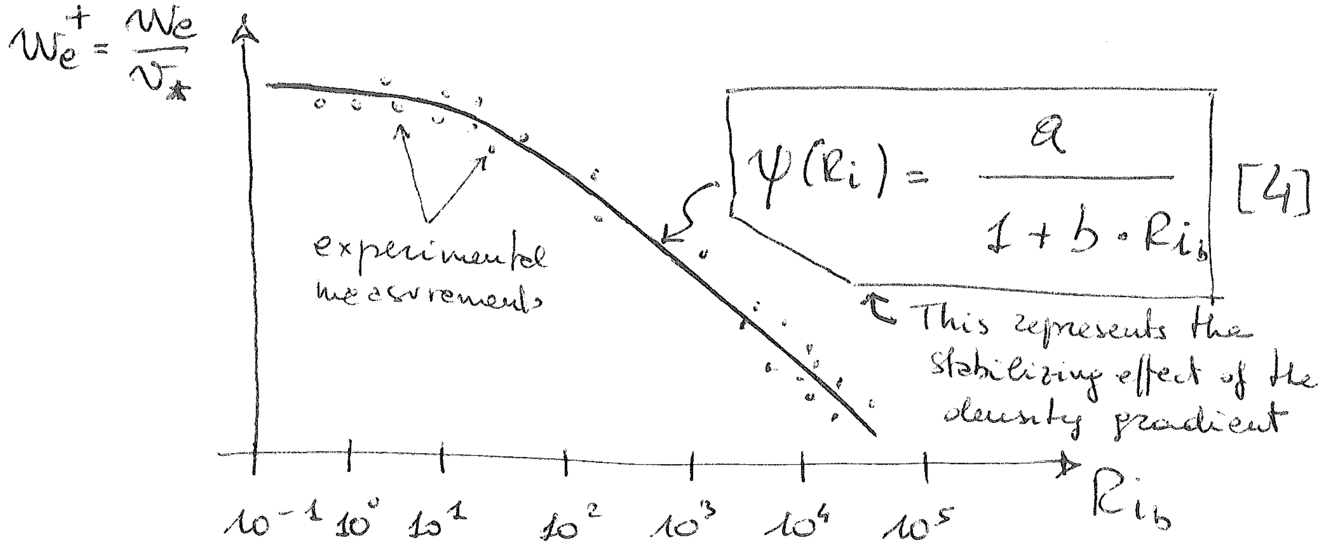
$$\boxed{w_e = v_* / \Psi(Ri_b)}$$

[3]

with v_* = friction velocity

Ψ = function of the bulk Richardson

The correlation of the vertical entrainment velocity with the bulk Richardson number, validated by experimental results, is:



$$\psi(Ri) = \frac{a}{1 + b \cdot Ri_b}$$ [4]

where a and b are empirical constants.

3) Stably-stratified flow regime: This flow regime represents an intermediate stage of the gas dispersion process, between the buoyancy-dominated flow regime and the latter stages where dispersion becomes passive. This regime is characterized by the persistence of a lateral gravity-driven flow in the cross-wind direction but also by vertical density stratification, which damps turbulent mixing.

The lateral gravity-driven flow can be described by a stably-stratified cloud embedded in the ambient air flow driven by the mean wind velocity. Therefore, eq. [1] can still be used to compute the front velocity.

As far as vertical mixing is concerned, eqns. [3] and [4] can be used: These two equations are rather accurate over a wide range of values for Rib, encompassing the majority of heavy gas dispersion scenarios of practical interest.

Note that air entrainment in the stably-stratified flow regime occurs primarily through the top of the cloud.

Also note that the suppression of turbulent mixing leads to a significant reduction of the cloud dilution compared to the buoyancy-dominated flow regime.

4) Passive turbulent dispersion regime: As the dispersion proceeds, the stable stratification decreases until the process can be represented as a

neutrally - buoyant cloud in a neutral or stratified ambient air flow. At this stage, dilution is such that the excess density of the heavy gas cloud has a negligible effect on dispersion and natural levels of turbulence are established again. The gas becomes a passive contaminant, whose dispersion is well described by Gaussian dispersion models.

In this flow regime, the dynamics of the cloud is controlled by ambient turbulence and, therefore, by the mean wind field. The velocity profile in a shear flow against a rough wall boundary (like the one generated by wind blowing near the ground) is determined from ;

$$\boxed{\frac{dv_x}{dz} = \frac{1}{K} \cdot \frac{v_*}{z} \cdot \psi_M\left(\frac{z}{L}\right)} \qquad [5]$$

where v_x is the mean wind velocity, $K \cong 0.4$ is the Von Karman constant, z is the vertical height and ψ_M is a function of the dimensionless quantity $\frac{z}{L}$.

The quantity z/L is a dimensionless height that provides a measure of the stability of the atmospheric flow at height z.

L is the OBUKHOV LENGTH, defined by:

$$\boxed{L \triangleq -\frac{\theta}{g} \cdot \frac{v_*^3}{w'\theta'} \cdot \frac{1}{K}} \quad [6]$$

where θ is the characteristic temperature of the boundary layer within the cloud, $\overline{w'\theta'}$ is the vertical turbulent heat flux. From eq. [6], the length L provides a measure of the height at which the production of turbulent Kinetic energy by buoyancy is equal to the production of turbulent Kinetic energy by the shearing action of the wind (buoyancy production of TKE = shear production of TKE).

Therefore L expresses the relative importance of shear and buoyancy in the production of energy, and can achieve values of order 1 to tens of meters. L is positive (negative) for stable (unstable) stratification, whereas it becomes infinite in the limit of neutral stratification (since $\overline{w'\theta'} = 0$).

Indeed, L is negative in the daytime (when $\overline{w'\theta'}$ is usually positive) while L is positive at night (when $\overline{w'\theta'}$ is usually negative). At dawn and dusk, $\overline{w'\theta'} \to 0$ and therefore $L \to \infty$.

Going back to eq. [5], when $L \to \infty$ then $\Psi_M = 1$ and one gets:

$$\frac{dv_x}{dz} = \frac{1}{K} \cdot \frac{v_*}{z} \Rightarrow \int_{v_x(z_0)}^{v_x(z)} dv_x = \frac{v_*}{K} \int_{z_0}^{z} z^{-1} dz$$

with z_0 = roughness height (approximately equal to one-tenth of the height of terrain roughness elements such as trees, crops, canopies, buildings).

Since $v_x(z_0)$ is assumed to be nearly zero, one gets:

$$\boxed{v_x(z) = \frac{v_*}{K} \ln(z/z_0)} \Rightarrow v_x^+ = \frac{1}{K} \ln\left(\frac{z}{z_0}\right)$$

Note that z_0 expresses the typical height of terrain elements on which the bulk aerodynamic drag can be exerted and act (below z_0, no aerodynamic drag is produced).

For the vertical entrainment velocity, one can invoke Reynolds analogy to assume that:

$$\psi(Ri_b) \simeq \psi_M \Rightarrow \psi(Ri_b) = C_1 \cdot \psi_M$$

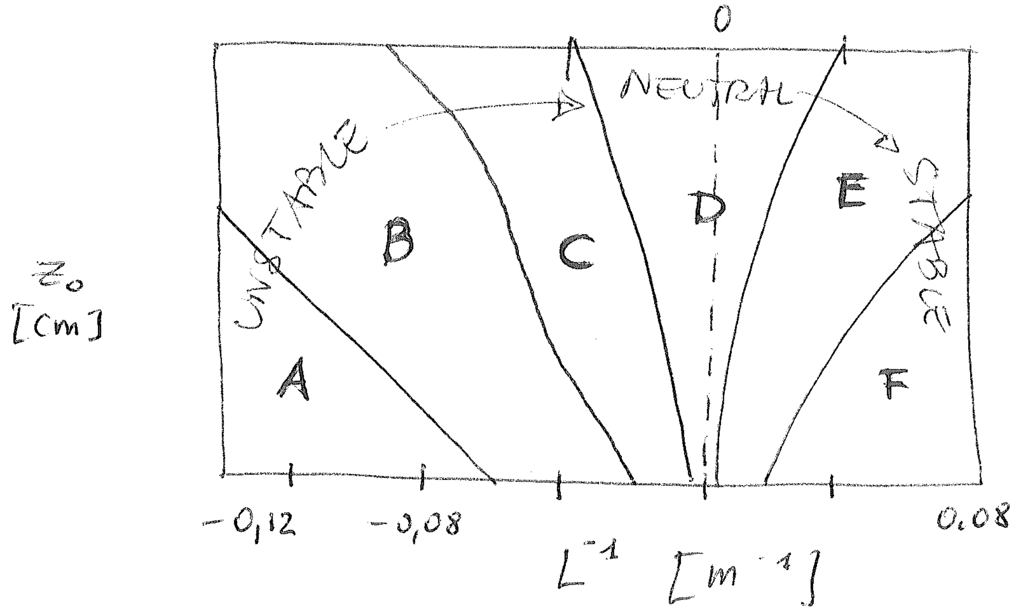
which yields $W_e = \frac{v_*}{\psi_M} \cdot \frac{1}{C_1}$ with $\frac{1}{C_1} = K$ (von Karman constant).

Namely:

$$\boxed{W_e = K \cdot \frac{v_*}{\psi_M}}$$

<u>DIGRESSION</u>: The Obukhov length L and the roughness height z_0 are used to classify atmospheric stability. The first atmospheric stability classification scheme was proposed by Pasquill in 1961:

CLASS A : extremely unstable
B : moderately unstable
C : slightly unstable
D : neutral
E : slightly stable
F : moderately stable



PASQUILL'S
STABILITY
CLASSES

The identification of the stability class is required by the so-called STABILITY-CLASS METHOD to calculate the <u>dispersion parameters</u> σ_y and σ_z, which represent the cross-wind and vertical standard deviations appearing in the equation of the gas concentration when it is treated as a passive contaminant.
In this latter case, the gas does not alter the density of the ambient air, has no effect on the flow and disperses in such a way that its concentration distribution can be represented, from a statistical point of view, by a Gaussian (bell-shaped) distribution. This is precisely what the gas does in the passive dispersion regime.

Skipping the derivation, it can be shown that the contaminant concentration distribution is given by:

Source emission strength [kg/s]

$$\boxed{C(x,y,z) = \frac{E}{v_x} \cdot g_y(x,y) \cdot g_z(x,z)}$$

mean wind velocity

with:

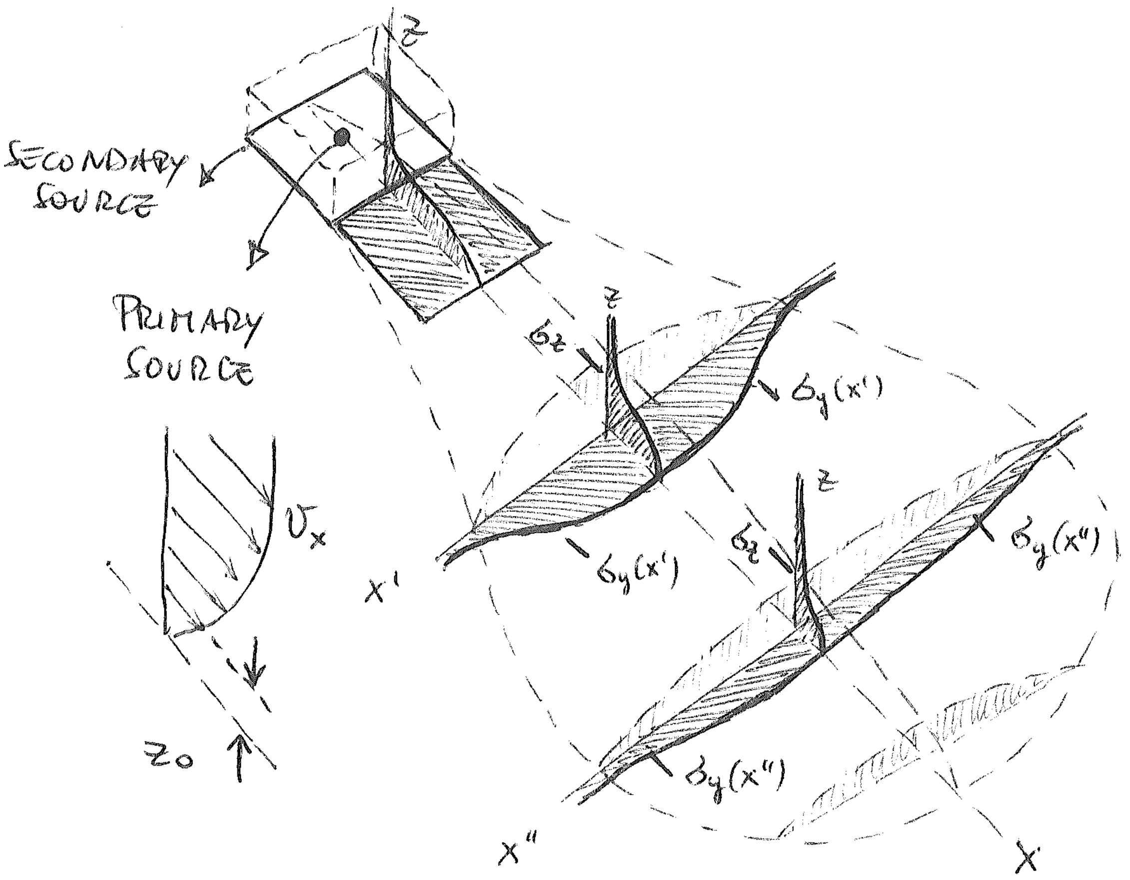
$$g_y(x,y) = \frac{1}{\sqrt{2\pi} \cdot \sigma_y(x)} \cdot \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y(x)}\right)^2\right]$$

$$g_z(x,z) = \frac{1}{\sqrt{2\pi} \cdot \sigma_z(x)} \cdot \left\{\exp\left[-\frac{1}{2}\left(\frac{z-h_s}{\sigma_z(x)}\right)^2\right] + \right.$$

$$\left. + \exp\left[-\frac{1}{2}\left(\frac{z+h_s}{\sigma_z(x)}\right)^2\right]\right\}$$

where h_s is a distance beneath the ground at which a mirror (fictitious) source of contaminant is ideally placed to model the trapping effect of the ground in case of ground emission.

The model of cloud dispersion that makes use of the above equations to calculate the concentration distribution of the gas inside the cloud can be rendered as follows;


z
SECONDARY SOURCE
PRIMARY SOURCE
z
σz
σy(x')
σy(x')
x'
z
σz
σy(x'')
σy(x'')
x''
x
vx
z0