Numerical simulation of the diffusion process in the atmosphere using a particle Lagrangian Model

Thesis Presentation

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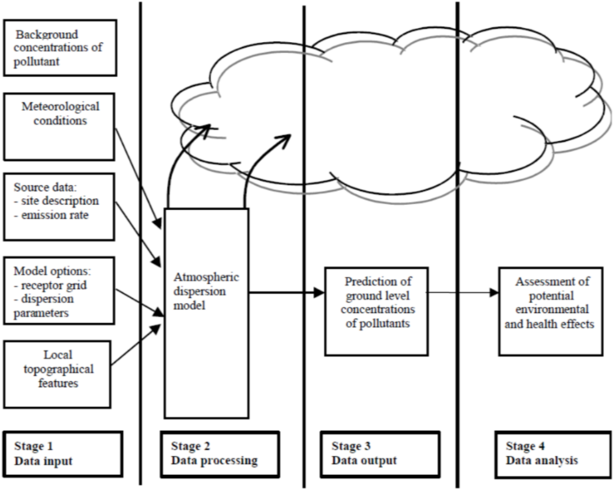
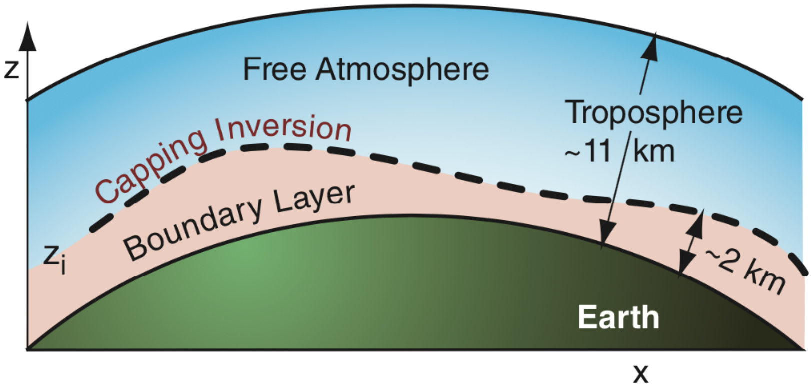
Bachelor's thesis under the supervision of Prof.Dino Zardi and dott.Sofia Farina

What is *Air Pollution* and why is it a problem?

Air Pollution model procedure



Atmospheric Boundary Layer



Types of air dispersion models

Based on the type of analytical approach used:

- Statistical models
- Deterministic models, divided into 2 classes: stationary and dynamic

Based on spatial scale:

- Short-range models: the order of 10km
- Mesoscale models: the order of 100 km
- Long-range models: very large areas up to thousands of kilometers from the source

Other elements used to discriminate models:

- The mathematical algorithm used to evaluate a specific phenomenon (finite differences, Montecarlo method, Gaussian method, etc.)
- The method of spatial description of the phenomenon (Eulerian, Lagrangian, two-dimensional, three-dimensional, etc.)
- The treatment of aspects of particular importance (orography, chemistry, photochemistry, etc.)

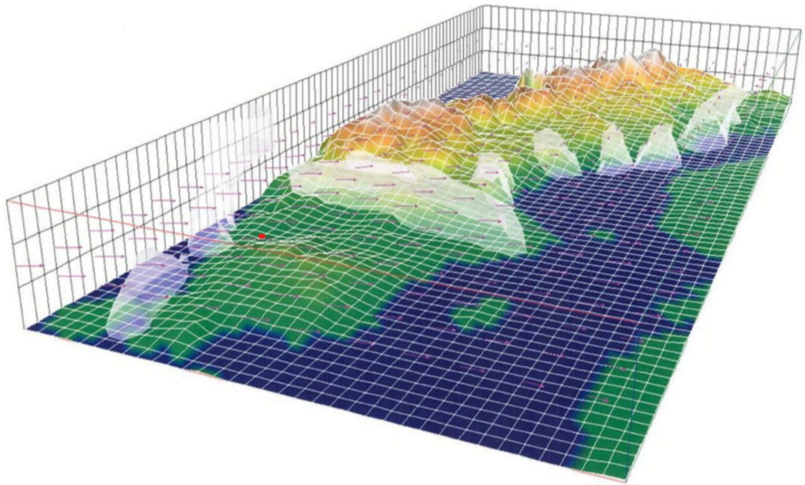
Eulerian model

- Solve numerically the atmospheric transport equation in a fixed coordinate frame.
- Theoretical basis are the equations which describe the instantaneous mass balance of pollutants. For example:

$$\frac{\partial c}{\partial t} + \left\{ \frac{\partial (c \cdot u)}{\partial x} + \frac{\partial (c \cdot v)}{\partial y} + \frac{\partial (c \cdot w)}{\partial z} \right\} = S + R + T \tag{1}$$

- Equations are solved discretizing the partial derivatives on a 3D grid using numerical methods
- Non-steady 3D models that require high computing resources
- Useful for studying the dispersion of pollutants over long distances and for long-term predictions

Eulerian Model



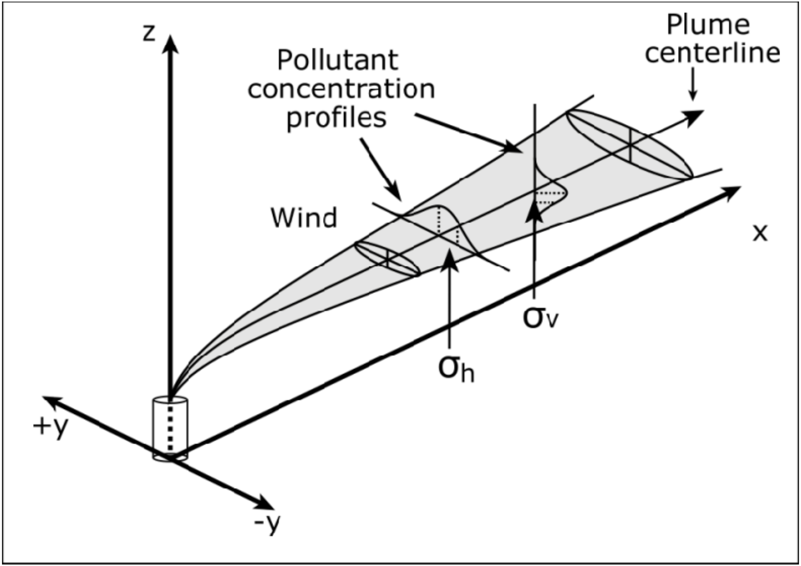
Gaussian Model

Based on mathematical solutions of the equations for the evolution of the concentration of pollutants that are obtained under several assumptions:

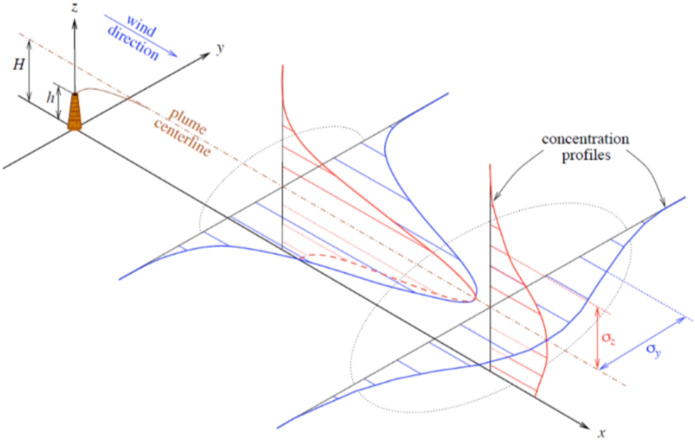
- Steady state conditions
- Wind speed, direction and diffusion characteristics of the plume are constant
- Conservation of mass, i.e. no chemical transformations take place
- Cannot work in calm wind conditions $\geq 1m/s$
- Variations in topography, turbulence and chemical reactions are neglected
- No memory of the contaminants released during the previous hour(s)

The results are realistic only in specific and close-to-ideal cases and should be used in conjunction with other models and with actual measurements of pollutant concentrations for more accurate predictions.

Gaussian Model



Gaussian Model



Gaussian Model: Mathematical description

We find, with some mathematical treatment, that the solution of the simplified equation in an infinite space devoid of obstacles has a Gaussian form and it reads:

$$\overline{\mathrm{c}}(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z\overline{u}} \exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{(z-H)^2}{2\sigma_z^2}\right) \tag{2}$$

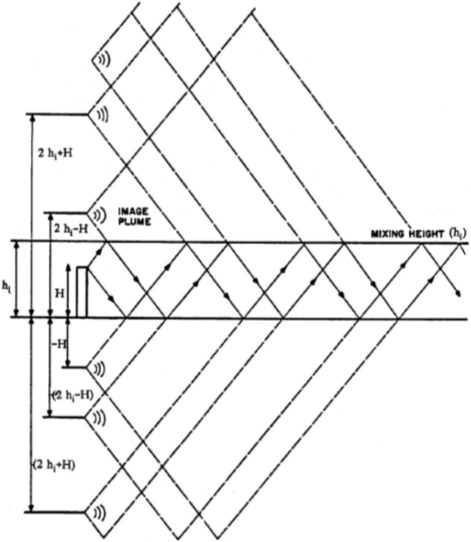
In the idealized situation where the ground is flat and does not absorb the pollutant but simply acts as a barrier that reflects it upward, we can use the method of image sources:

$$\overline{\mathrm{c}}(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z\overline{u}} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \cdot \left\{\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right)\right\} \tag{3}$$

With infinite image sources:

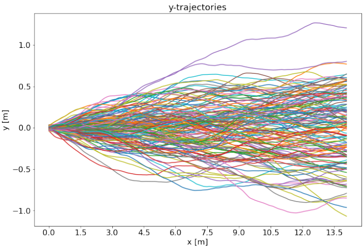
$$\overline{\mathrm{c}}(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z\overline{u}} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \cdot \sum_{m=-\infty}^{m=+\infty} \left\{\exp\left(-\frac{(z+2mh_i-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+2mh_i+H)^2}{2\sigma_z^2}\right)\right\} \tag{4}$$

Gaussian Model: image sources

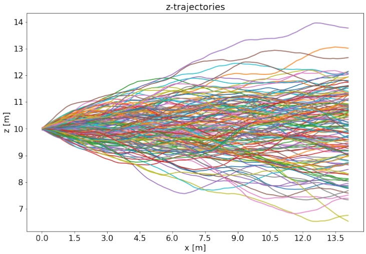


Lagrangian Model

Lagrangian particle models evaluate the trajectories of single particles that are emitted by different sources in the atmosphere.
The particle is immersed in a turbulent fluid and as a consequence also its motion will be turbulent. Then, its motion can be seen as the superposition of a mean and a turbulent motion.
The trajectory of each particle is partly calculated in a deterministic way and partly in a stochastic way.

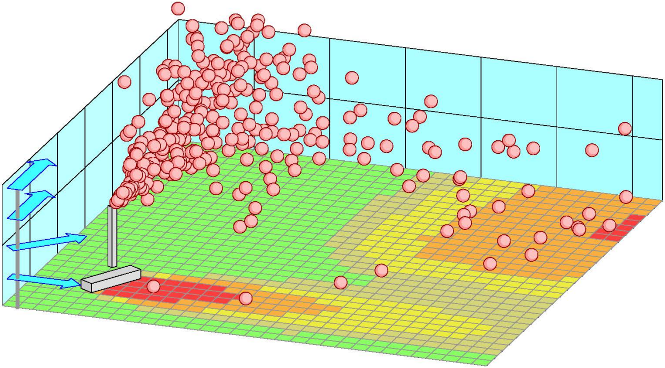


(a) spatial evolution of particles along y



(b) spatial evolution of particles along z

Lagrangian Model



Schematic representation of the approach used in a Lagrangian Dispersion Model. The generated concentration field on the ground is illustrated with different colors: brighter colors more intense field. Wind directions are shown as blue arrows.

Lagrangian Model: Mathematical analysis

The equations for a single particle model are:

$$\begin{cases} du_i & = -\frac{u_i}{T_L}dt + \sqrt{C_0\epsilon}dW(t) \\ dx_i & = u_i dt \end{cases} \tag{5}$$

Where C_O is the constant of the Langevin equation, T_L is the Lagrangian integral time scale, ϵ is the coefficient of dissipation rate of the turbulent energy, $dW(t)$ is the increment of a Wiener process.
This equation was used in the computational part of the thesis.

Utilized Data

An ideal situation is modelled: the wind blows steadily only along x, so $\vec{v} = (u, 0, 0)$ the source is only one and a point source, the emission rate(Q) is constant and variations in topography, turbulence and chemical reactions are neglected. The LPDM was implemented using the following values:

$nstep$	$T_L[s]$	$dt[s]$	C_0	N	$U[m/s]$	$Q[g/s]$	$pblh[m]$	$he[m]$
1000	0.47	$T_L/100$	4	20000	3	3	15	10

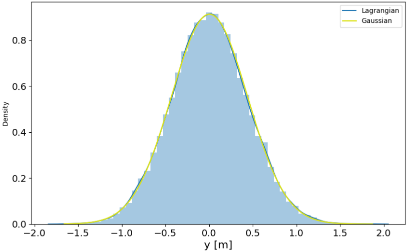
Utilized data

the values of standard deviations for the initialization of position and velocity of the particles are reported in table 2.

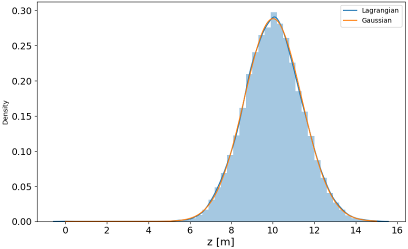
$\sigma_v[m/s]$	$\sigma_w[m/s]$	$\sigma_y[m]$	$\sigma_z[m]$
0.05	0.5	0.02	0.02

Standard deviations for initializing particle velocities and positions

Validation of Lagrangian Model

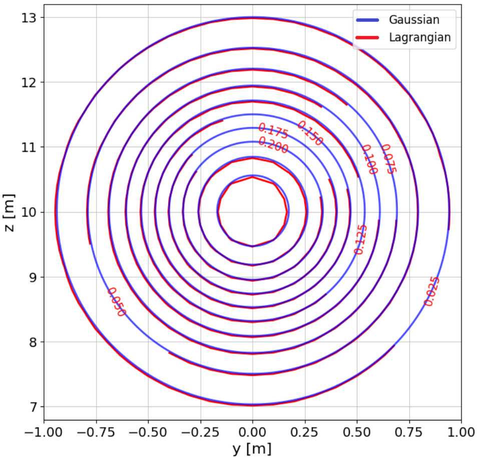


(a) comparison between the two distributions along y



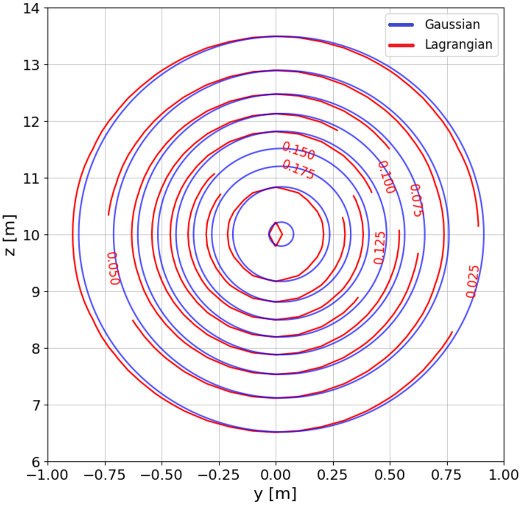
(b) comparison between the two distributions along z

Validation of Lagrangian Model



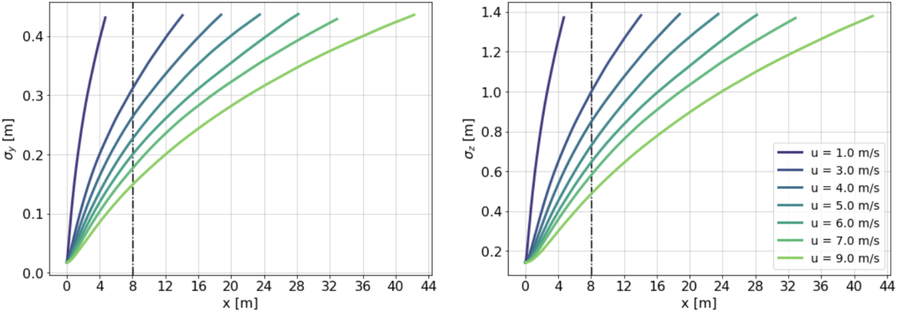
Comparison between Gaussian and Lagrangian concentration fields as function of y and z: red line is used for the Lagrangian field, while blue line is used for the Gaussian one; the numbers above the curves represent the concentration values of isolines in g/m^3

Sensitivity Analysis: Different value of N



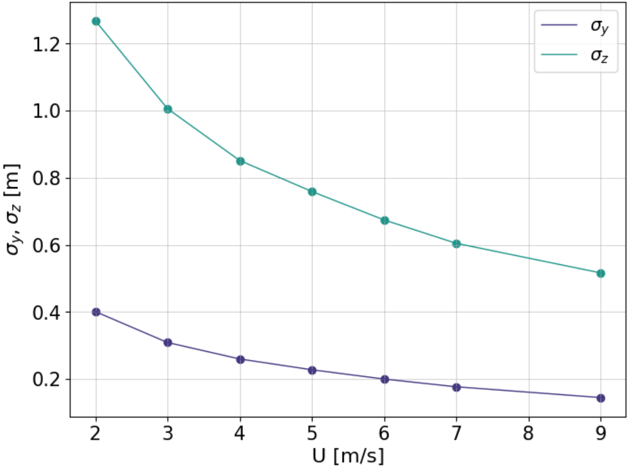
Comparison between Gaussian and Lagrangian concentration fields with N=200

Sensitivity Analysis: Different wind speeds



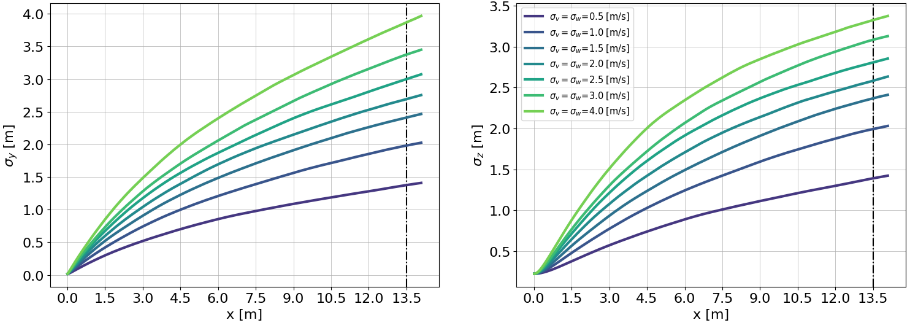
Standard deviations for different wind speeds along x

Sensitivity Analysis: Different wind speeds



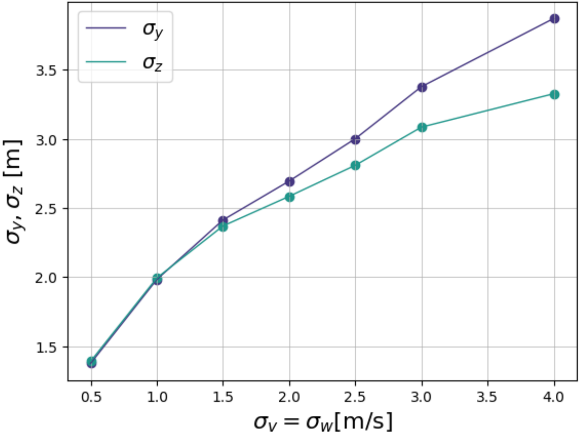
Standard deviations for a fixed value of $x = 8m$.

Sensitivity Analysis: Different values of σ_v and σ_W



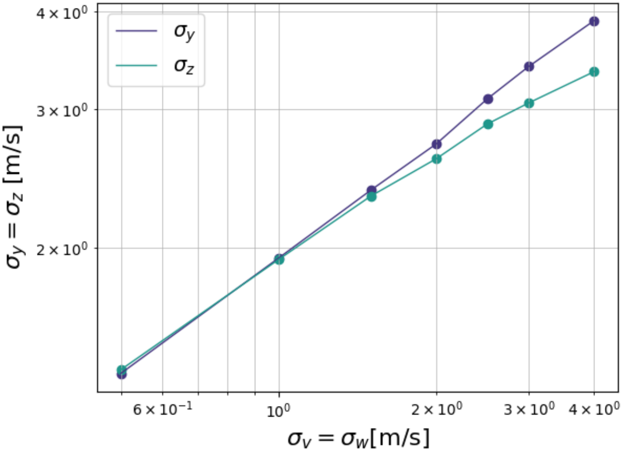
Standard deviations for different values of σ_v and σ_w

Sensitivity Analysis: Different values of σ_v and σ_W



Standard deviations for a fixed value of $x = 13.5m$.

Sensitivity Analysis: Different values of σ_v and σ_W



logarithmic scale of standard deviations for a fixed value of $x = 13.5m$

Conclusions

- Under ideal conditions, the concentration field obtained from the Lagrangian dispersion model was qualitatively verified to be consistent with the analytical result obtained from the Gaussian approach.
- Sensitivity analysis showed that increasing the velocity of the wind along x led to a decrease in the standard deviations along y and z exponentially, while increasing the starting standard deviations for the velocities of particles along y and z led to an increase in σ_y and σ_z logarithmically.
- Being able to model the concentration field of a tracer and to know its distribution on the ground in different meteorological conditions is crucial if we want to understand how a pollutant is spread from, for example, a chimney of a waste-to-energy plant through ABL.
- Lagrangian model provides a powerful tool for understanding the behavior of pollutants in the atmosphere.

Conclusion: Coati's Fire