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

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A zia "Lilly"

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Abstract

The aim of this thesis is to explore different approaches to perform a simulation of the dispersion of a tracer. In particular, after a first part focused on the analysis of the state of the art, a Lagrangian approach is used to develop a simplified model, which is then validated through a comparison with a Gaussian one.

The main goal is to verify that the concentration field resulting from the Lagrangian dispersion model in ideal conditions (i.e. homogeneous and isotropic turbulence, constant and uni-dimensional wind field) is validated with the one derived analytically using a Gaussian approach.

A sensitivity analysis of the dispersion of the plume was performed, to identify the main factors contributing to the values of the dispersion of the tracer in the plume (i.e. σ_y and σ_z). This analysis showed that as wind velocity along x increases, the standard deviations along y (σ_y) and z (σ_z) decrease exponentially, instead by increasing the starting standard deviations for the velocities of the particles along y and z: σ_v and σ_w, σ_y and σ_z increase logarithmically.

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Chapter 1

Introduction

Nowadays, pollution has become a crucial problem for the planet and for life on it. In order to be able to deal with it, as human race, we need to properly understand its characteristics and its dynamics, to develop accurate models to reproduces and forecast its behavior in the future, and to test strategies to mitigate it.[1]

The slow evolution of the Earth, has gradually changed the atmosphere making it an ideal environment for human, animal and plant life. However the rapid industrial revolution of the last centuries, has determined deep changes of the atmosphere state. Human activities have released large quantities of substances not present in the original state into the atmosphere or have drastically increased those already existing. As consequence, the composition of the atmosphere is progressively and rapidly changing, endangering life on the planet itself. This phenomenon is called contamination of the atmosphere or *air pollution.*

The protection of the environment as a whole and particularly the proper management of air quality, which is one of its main aspects, has grown in interest lately.
To quantify the state of air pollution, a series of elements defined as pollutants are introduced. The observable basis for defining air quality is the measurement of the concentration of a certain pollutant. If this element is above the quality standards, i.e. it assumes values over a threshold, it determines an unacceptable state of air quality or an episode of pollution. From a technical point of view, air pollution is the situation in which substances (gases of various types, aerosols, and particles of various grain sizes) are present in the atmosphere at concentrations higher than those naturally present in the air, with poten-

tially harmful effects on human health, quality of life, flora, fauna, landscape, materials, artefacts and works of art. Using this definition, air pollution is determined not only by human causes but it is also due to natural ones, such as the eruption of a volcano.

During the years, laws related to the control of air quality standards have been introduced everywhere, and have been based on the existence of limits on the concentrations of pollutants which should not be exceeded anywhere. However, if direct measurement of concentrations is the only method to obtain information on such pollutants levels, air quality control can only be performed at specific points that align with measurement stations of different detection networks across the country. Such a small number certainly does not allow an accurate picture of the space-time distribution of the concentration of various pollutants of interest. To make progress, it is necessary to simulate the dispersion of pollutants in the atmosphere through mathematical models. These are, in general, tools that seek to reconstruct the concentration state of various pollutants in a space-time calculation domain of interest as faithfully as possible.[2]

By itself, this modelling approach has no limitations in providing indications at every point in the territory, but the problem is how realistic the model's forecast is. It is evident that the model, as such, will always be an approximation of reality and therefore its predictions will always be in disagreement with what is measured. This disagreement can be quantified in statistical terms and such statistical indicators can be useful to compare the performance of different models applied to the same reality. It should be noted, however, that practically every model presents a greater or lower degree of calibration (tuning) that allows it to adapt somewhat to measurements. A possible strategy for using models would be:

- Apply the model to a given reality that is to be examined without any tuning;
- Compare the results obtained with the measurements taken by a detection network present in the territory or with the results of appropriate experimental campaigns;
- Calibrate the model so that the discrepancies between the model and measurements for the spatio-temporal domain considered fall below a predetermined level.

At this point, the model can be considered calibrated for that reality, and its predictions can be realistically viewed as a fairly realistic representation of reality itself.[2]

Modelling the dispersion of a pollutant is by no means a trivial operation. Indeed, the relation between emissions and concentrations is not simple. It would be if the atmosphere were an ideal container in which an instantaneous and homogeneous mixing of the different species of pollutants was possible. In this case called $E(g \cdot s^{-1})$ the emission of generic pollutant, $C_R(g \cdot m^{-3}s^{-1})$its concentration emission rate in air and $V(m^3)$ its volume in atmosphere, between E and C_R would exist the simple relation of direct proportionality: $C_R = E/V$. However, this model is profoundly distant from reality, as the emissions are carried by air masses in rapid and turbulent motion, typical of the Atmospheric Boundary Layer (ABL), which cannot be captured by the previously introduced proportionality relation.
The ability to estimate concentrations resulting from a given emission scenario is a key element in understanding air pollution and in developing any environmental remediation policy. This ability is therefore the essential link between the work of those involved in emissions and the work of those studying the damages caused by air pollution. This discipline can be referred to as the generic term Air Pollution Dispersion Modeling, which is the main focus of this study. Different approaches can be used to model the dispersion of a tracer, the most important are: Eulerian, Lagrangian and Gaussian models, and will be described in the next chapter. Dispersion models are used to explain how the concentration of a certain tracer varies in space and time, once the initial condition of the atmosphere and the source are known. The space in question is ABL and has specific properties.

The ABL is the lowest layer of the Earth's atmosphere, extending from the Earth's surface up to a height of a few kilometers. The ABL is a thin layer of air that interacts directly with the Earth's surface and is affected by its properties, such as temperature, moisture, and roughness. It is characterized by turbulent flows, which are caused by the interaction between the air and the Earth's surface. The turbulence in the ABL is important for mixing heat, moisture, and pollutants, and is responsible for the dispersion of pollutants from sources at or near the Earth's surface.

The height of the ABL varies depending on a number of factors, including the time of the day, the season, and the weather conditions. During the day, the ABL tends to be

deeper, as solar radiation heats the Earth's surface, causing the air to rise and mix with the air aloft (few kilometers). At night, the ABL tends to be shallower, as the Earth's surface cools and the air becomes more stable(few hundred meters).

The ABL is also characterized by the presence of various layers, each one with distinct properties. The surface layer is the lowest layer of the ABL and is directly affected by the properties of the Earth's surface. Above the surface layer there is the mixed layer, where turbulent mixing is strong and the properties of the air are relatively uniform. Above the mixed layer we find the free atmosphere, where the air is not directly influenced by the Earth's surface and is characterized by its stability and low turbulence.[1]

Chapter 2

Air Pollution Modelling

Pollutants dispersion models are mathematical tools that are used to simulate and predict the dispersion of pollutants in the atmosphere. These models are essential for understanding how pollutants move through the atmosphere and how they impact air quality in different regions. Overall, dispersion models are an important tool for understanding and managing the impacts of pollutants on the environment and public health. They allow scientists and policymakers to make informed decisions about how to mitigate the negative impacts of air pollution, and to develop effective strategies for improving air quality.

Pollutants dispersion models are based on the mathematical equations that describe the movement and transformation of pollutants in the atmosphere. These models take into account a range of factors that affect the dispersion of pollutants, including wind speed and direction, atmospheric stability and the physical and chemical properties of the pollutants themselves.

There are a variety of pollutants dispersion models available, ranging from simple empirical models to complex physics-based models. Each model has its own strengths and weaknesses and the choice of model will depend on the specific application and the available data. Air pollution models usually take as input different elements, such as:

- the geographical structure of the territory
- the emissions to be considered
- the physical characteristics of the ABL

and provide in output the space-time distribution of the concentration of the various pollutants under study.

The accuracy of these models depends on the quality and quantity of the input data, as well as the assumptions and simplifications used in the model. Taking into consideration the characteristics of the ABL is essential to have a model closer to reality. In fact, the ABL can be seen as a huge chemical reactor, in which chemical-physical reactions take place.[1]

2.0.1 General characteristics of a simulation model

When a substance is released into the atmosphere, it disperses and dilutes in the surrounding air volume, depending on atmospheric conditions. This means that the substance can be found in other locations after a certain amount of time with a different concentration level. The objective of air pollution dispersion models is to predict the concentration field of a substance: $C(x, y, z, t)$ in all points of space and time. To achieve this, it is necessary to take into account a number of specific phenomena that occur during the transport of the substance in the atmosphere, such as:

- Physical phenomena (transport, diffusion, plume rise, etc.);
- Chemical-atomic phenomena (chemical reactions, radioactive decay, etc.);
- physic-chemical phenomena (deposition, etc.).

Based on the type of analytical approach used, there are two main models used for the analysis of pollution:

- Statistical models
- Deterministic models.

Statistical models rely on past data measured by monitoring stations to predict future concentrations of pollutants at those same stations. *Deterministic* models, on the other hand, are based on cause-and-effect relationships between emissions, meteorology, and pollutant concentrations. Deterministic models can be either stationary or dynamic and can operate at different spatial scales. Statistical models are limited in their ability to

study and predict pollution phenomena and will not be discussed further. Deterministic models, however, will be the focus of the discussion, as they are more general and widely applicable, with different models designed for different spatial and temporal scales. Indeed they can be divided into 2 classes: *stationary* and *dynamic* models. Stationary models simplify the temporal evolution of a pollution phenomenon by treating it as a sequence of almost stationary states, but this reduces their generality and applicability. Dynamic models, on the other hand, treat the phenomenon's evolution dynamically.
Stationary models are often used for their simplicity and cost-effectiveness and are generally useful for analyzing relatively simple realities. Another important element of distinction between models is the spatial scale, which refers to the distance from the source within which the model can describe the phenomenon. There are three classes of models based on these parameters:

- Short-range models: the description of the dispersion of pollutants up to distances of the order of tens of kilometres
- Mesoscale models: the order of 100 km
- Long-range models: very large areas up to thousands of kilometers from the source

Models can also be distinguished based on their complexity, with complex models taking into account more phenomena than simple models. Finally, other elements used to discriminate models when the description of the model goes into greater detail are:

- 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.)

After explaining the general characteristics of dispersion models, the three main approaches (i.e. Eulerian, Gaussian and Lagrangian) will be presented in the following sections.

2.1 Eulerian and Gaussian model

The Eulerian model is a mathematical framework for studying the dispersion of pollutants in the atmosphere. This model considers the movement of air and pollutants as a continuous flow through a fixed grid of points in space and time.
In the Eulerian model, the atmosphere is divided into a three-dimensional grid or mesh, and pollutant concentrations are calculated at each point on the grid over time. The model accounts for the transport of pollutants due to advection (air movement) and diffusion (random movement of particles due to thermal energy).[3]

The Eulerian model is particularly useful for studying the dispersion of pollutants over long distances and for long-term predictions. According to this approach, the dynamics of the dispersion of chemical pollutants are described with a fixed spatial reference system of orthogonal Cartesian coordinates that are connected to the Earth's surface. This is the usual way in which the transfer of heat and mass phenomena are treated in Physics, and in the case of Micrometeorology, it is also the conventional way used to mathematically describe meteorological fields. The Eulerian method seeks to formulate the main statistical variables related to the concentration of different pollutants based on the statistical properties of Eulerian velocities of the fluid, i.e., velocities measured at a fixed point of the ABL. A formulation of this type is very useful not only because Eulerian statistics are easily measurable with the normal instruments used in meteorology but also because the mathematical expressions that derive from it are immediately applicable in situations where there is the presence of chemical reactions.[2]

Unfortunately, the Eulerian approach also presents serious obstacles. The first obstacle lies in the fact that the mathematical model to which this approach gives rise does not allow sufficiently general and immediately usable analytical solutions. The second obstacle, instead, is connected with the closure problem, which can make it difficult to realistically represent the dispersion of pollutants in a strongly convective ABL. In addition, it should be noted that an Eulerian-type model usually appears as a partial differential equation that requires a numerical solution, and the numerical algorithms used can heavily influence the final results.

Gaussian models, instead, are based on mathematical solutions of the equations for the evolution of the concentration of pollutants that are obtained under several assumptions. The Gaussian approach is based on the assumption that the dispersion of pollutants is subject to the laws of turbulence, which cause the pollutant to spread in a roughly bell-shaped curve, the Gaussian distribution.

The dispersion of the pollutant is influenced by several factors, including wind speed and direction, atmospheric stability, and the height of the release point.

The model calculates the pollutant concentration at various distances and directions from the source using a series of mathematical equations that take these factors into account. The output of the model is usually presented in the form of a contour map showing the predicted pollutant concentration at various locations.

A schematic of the plume diffusion can be seen in the following figure:

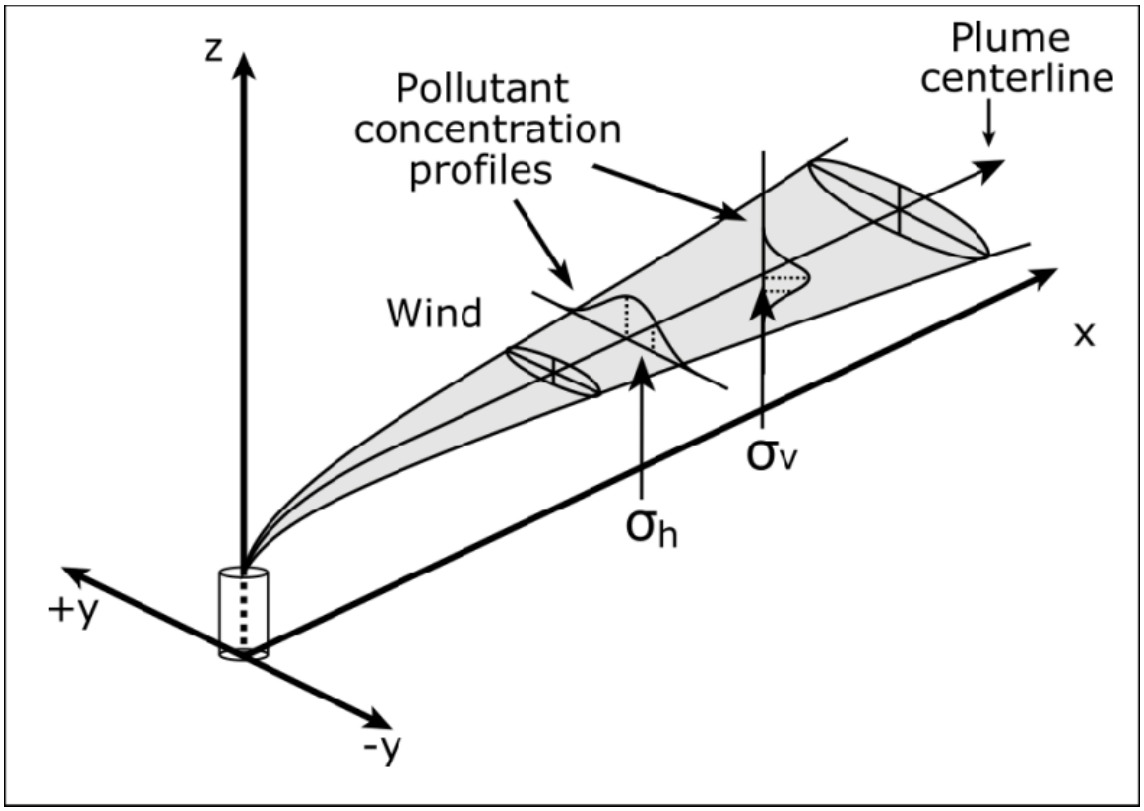


Figure 2.1: Structure of the dispersion plume described by orthogonal axis system[4]

The Gaussian model is widely used in air pollution modeling because it is relatively simple to use and provides a good approximation of the dispersion of pollutants in many situations. However, it has several limitations as the analytical solutions only exist for idealised and extremely simplified cases, including the assumption of a single point source,

stationary meteorological and emission conditions and the neglect of variations in topography, turbulence and chemical reactions. Overall, the Gaussian model is a useful tool for predicting the dispersion of pollutants in the atmosphere, but its results are realistic only in specific and close-to-ideal cases. It should be used in conjunction with other models and with actual measurements of pollutant concentrations for more accurate predictions.

2.2 Semi-empirical equation of dispersion in the atmosphere

Considering a single pollutant of the gaseous type, neglecting the molecular diffusivity, and applying the conservation of the mass of the pollutant, we obtain the following equation:

$$\frac{\partial c}{\partial t} + \left\{ \frac{\partial (c \cdot u)}{\partial x} + \frac{\partial (c \cdot v)}{\partial y} + \frac{\partial (c \cdot w)}{\partial z} \right\} = S + R + T \tag{2.1}$$

Where:

- c is the concentration of the pollutant
- u, v and w are the wind speeds in the x, y and z directions, respectively
- S is the source term
- R is the removal term
- T is term that takes into account chemical transformations and more

The right hand-side of 2.1 is the total derivative. If we are interested in N different pollutants, for the i-th generic pollutant it is possible to write the relative instantaneous conservation equation, which is reduces to the following partial differential equation:

$$\begin{aligned} \frac{\partial c_i}{\partial t} + \frac{\partial (c_i u)}{\partial x} + \frac{\partial (c_i v)}{\partial y} + \frac{\partial (c_i w)}{\partial z} = K_i \left[\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial^2 c_i}{\partial z^2} \right] + \\ + R_i(c_1, c_2, ..., c_n, T) + S_i(x, y, z, t) \end{aligned} \tag{2.2}$$

where the term c_i represents the instantaneous concentration of the i-th pollutant at the point P(x,y,z) at time t. The spatial coordinates referred to in this equation are those of a standard orthogonal Cartesian system fixed with respect to the ground, and time is relative to an arbitrary initial instant t_0. In equation 2.2, K_i represents the molecular diffusivity of the i-th species, while R_i and S_i symbolically represent the chemical kinetics involving

species i and all source terms (production or destruction), respectively. Essentially, 2.2 states that the Eulerian variation in time of the instantaneous concentration of pollutant i depends on:

- The instantaneous transport carried out by the instantaneous wind field, of which u, v, and w are the relative Cartesian components;
- Molecular diffusion, represented by the first term on the right-hand side of 2.2;
- The chemical reactivity of the i-th species with respect to other substances present in the air;
- The source term S_i, which represents the rate of production or destruction (e.g. radioactive decay) at point P at time t for species i.

If in the instantaneous model molecular diffusion, chemical reactions and the source term are neglected, equation 2.2 is transformed as follows:

$$\frac{\partial c}{\partial t} + \frac{\partial (c_i \cdot u)}{\partial x} + \frac{\partial (c_i \cdot v)}{\partial y} + \frac{\partial (c_i \cdot w)}{\partial z} = 0 \tag{2.3}$$

We can apply the *Reynolds hypothesis*, which states that each instantaneous component of the wind can be considered as the superposition of a slowly varying mean component and a seemingly random fluctuation caused by vortices of various sizes. According to such hypothesis, equation 2.2 states that a puff released at a point undergoes two different types of transport: regular transport due to the mean velocity of the wind, and irregular transport due to turbulent structures. In the case of a smoke plume, this is the process responsible for the irregularity of its shape when observed up close and for the spreading of smoke around the plume's center of mass. Thus, this is a convective transport process that has many similarities with the disorderly motion characteristic of irregular diffusion, hence it is called turbulent diffusion.

If we consider a certain distribution of wind speed as a function of time and take a time interval called *Reynolds Average Time* (RAT). In RAT we can calculate the mean value, called $\overline{u}$. We can also find for each instant of time the deviation from the mean value(u': fluctuation term), found as the difference between u and $\overline{u}$. The value of u and c will then

be determined for each instant of time by:

$$\begin{aligned} u &= u' + \overline{u} \\ c &= c' + \overline{c} \end{aligned} \tag{2.4}$$

This procedure, at the basis of the treatment of turbulence, is called *Reynolds Decomposition.*

The Reynolds-average of the equation 2.2 reads:

$$\frac{\partial \overline{c_i}}{\partial t} + \sum_{j=1}^{3} \left(\overline{u_j} \frac{\partial \overline{c_i}}{\partial x_j} \right) = \overline{S_c} - \sum_{j=1}^{3} \left(\frac{\partial \overline{\mathrm{c_i' u_j'}}}{\partial x_j} \right) + K_i \frac{\partial^2 \overline{c_i}}{\partial x_j^2} + \overline{R_i} \tag{2.5}$$

The second term on the left-hand side represents the regular transport of a pollutant due to the average motion of the atmosphere, and is usually referred to as the *advective term*, while the second term of the right-hand side of the equation keeps into account the irregular transport due to turbulent structures present in the ABL. Therefore, it is a flux term and is usually referred to as the *diffusive term.* The third term on the right-hand side is for molecular diffusion and the R_i term describes the chemical reactions taking place in the interaction between the pollutant and the atmosphere.
In order to find a concentration field that is a solution for the equation, some others assumptions and simplifications are made, in particular: the chemical reaction term is ignored because we assume that the chemical species does not modify the motion field; molecular diffusion is negligible compared to the other terms.

The turbulent diffusion is generally treated introducing parameterizations, and the most simple one is the so called $K-$closure, which reads:

$$\overline{\mathrm{c_i' u_j'}} = -\sum_{k=1}^{3} K_{jk} \frac{\partial c_i}{\partial x_k} \tag{2.6}$$

Where $[K_{jk}]$ is *turbulent diffusion tensor.* Assuming for simplicity that the matrix is diagonal:

$$\overline{\mathrm{c_i' u_j'}} = -K_{jj} \frac{\partial c_i}{\partial x_j} \tag{2.7}$$

We get:

$$\frac{\partial \overline{c_i}}{\partial t} + \sum_{j=1}^{3} \left(\overline{u_j} \frac{\partial \overline{c_i}}{\partial x_j} \right) = \sum_{j=1}^{3} \left\{ \frac{\partial}{\partial x_j} \left[K_{jj} \frac{\overline{\partial c_i}}{\partial x_j} \right] \right\} + \overline{S_c} \tag{2.8}$$

This equation is called the *semi-empirical equation of dispersion in the atmosphere.*

2.2.1 Gaussian Modelling

To solve the above equation analytically, some assumptions are made, and in particular:

- the source is a one point-source
- the contaminant is emitted at a constant rate (the coefficients K_{jj} are constant) at a certain point of the domain: $\vec{x} = (0, 0, H)$, where H is the height of the source
- the wind velocity has just one component different from zero: $\vec{u} = (u, 0, 0)$

If we consider the right hand-side of 2.8, the first term vanishes because c is steady, while in the right hand-side summation only the term along x remains because the wind speeds along y and z are zero. In order to find the solution, the the following considerations can be made:

- the solution is steady-state
- the eddy diffusivity (K) changes along x only
- the wind velocity is sufficiently high that diffusion in x direction is smaller than advection, so the first term of :

$$\frac{\partial \overline{\mathrm{c'u'}}}{\partial x} + \frac{\partial \overline{\mathrm{c'u'}}}{\partial y} + \frac{\partial \overline{\mathrm{c'u'}}}{\partial z} \tag{2.9}$$

  is negligible; turbulence is important in the direction perpendicular to the wind, while parallel the important term is advection
- the variations in topography can be neglected
- contaminant does not penetrate the ground

We finally find, with some mathematical treatment, that the solution of the simplified equation has a Gaussian form and it reads:

$$\overline{\mathrm{c}}(x, y, z) = \frac{Q}{2\pi\sigma_y\sigma_z\overline{u}} \exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{(z-H)^2}{2\sigma_z^2} \right) \tag{2.10}$$

Where

$$\begin{aligned}\sigma_y &= \left(\frac{2x}{\overline{u}}K_{yy}\right)^{\frac{1}{2}} \\ \sigma_z &= \left(\frac{2x}{\overline{u}}K_{zz}\right)^{\frac{1}{2}}\end{aligned} \tag{2.11}$$

Q is the mass quantity of pollutant released in $[g]$ and x is the distance from the source in $[m]$.

The solutions of the diffusion equation described above, in the idealized situations to which they refer, depict the dispersion of pollutants essentially in an infinite space devoid of obstacles. However, in reality, if one considers an emission at a height of H (for example, a chimney), the effect of the ground will be negligible up to distances from the chimney such that $\sigma_z < H$, but it will become important at greater distances. 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, it is possible to correct the previous formulas by superimposing the effect of a fictitious image source placed at a height equal to $(-H)$ onto the actual source. In this case, equation 2.10 is transformed into the following relationship:

$$\overline{\mathrm{c}}(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z\overline{u}}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\cdot\left\{\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right)+\exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right)\right\} \tag{2.12}$$

The last term on the right side is the second artificial released, placed at $z - H$ height. In the scenario where there are multiple walls, we require an infinite number of images to resolve the problem. These images must be placed symmetrically in relation to all walls. The placement of these images can continue indefinitely, and for every new image, there is a new reflection. This can be expressed mathematically as $m = (-\infty, +\infty)$. So the equation 2.12 will become:

$$\begin{aligned}\overline{\mathrm{c}}(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z\overline{u}}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\cdot \\ \sum_{m=-\infty}^{m=+\infty}\left\{\exp\left(-\frac{(z+2mh_i-H)^2}{2\sigma_z^2}\right)+\exp\left(-\frac{(z+2mh_i+H)^2}{2\sigma_z^2}\right)\right\}\end{aligned} \tag{2.13}$$

Where h_i is the height from ground level to bottom of the inversion aloft.

This equation will be used in the computational part of the thesis to simulate the dispersion of a pollutant and the final result will be compared with that of the Lagrangian model.[2]

2.3 Lagrangian Model

The Lagrangian model is a mathematical framework for simulating the dispersion of pollutants in the atmosphere. Unlike the Eulerian model, which assumes that the atmosphere is divided into a fixed grid, the Lagrangian model tracks the motion of individual particles or air parcels as they move through the atmosphere. A schematizaton of these approaches is reported in figure 2.2 .

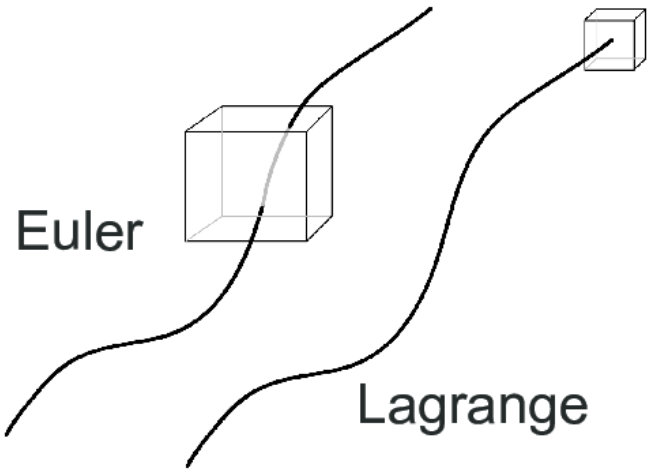


Figure 2.2: Lagrangian models involve tracking parcels of air that move with the wind and keeping a record of the pollutants they contain. On the other hand, Eulerian models utilize a fixed grid system for integrating the mass-balance equation.[5]

The Lagrangian approach is based on the advection-diffusion equation, which describes the transport of pollutants due to air movement and the random movement of particles due to thermal energy. The model calculates the trajectory of individual particles based on their initial position and velocity, and atmospheric conditions such as wind speed and direction.

Lagrangian modelling is particularly useful for simulating the behavior of pollutants in complex, turbulent environments, such as near the surface or in urban areas. It can also be used to study the transport of pollutants on short time scales and to track the dispersion of individual plumes or emissions.

To simulate the dispersion of pollutants with the Lagrangian model, several input parameters are required, including the initial position and velocity of the particles, the emission rate and location, and atmospheric conditions. The model then calculates the movement of individual particles over time, allowing researchers to track the dispersion of pollutants

and estimate their impact on human health and the environment.

In summary, the Lagrangian model is a powerful tool for simulating the dispersion of pollutants in the atmosphere, especially in complex and turbulent environments. It provides detailed information about the behavior of individual particles and enables researchers to develop effective strategies to mitigate the effects of pollution on human health and the environment.

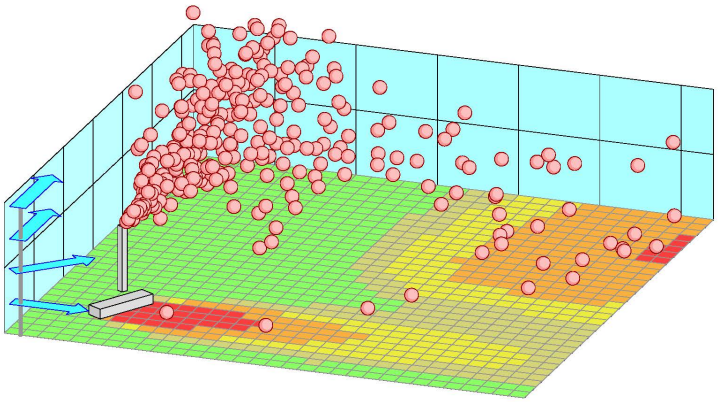


Figure 2.3: Schematic representation of the approach used in a Lagrangian Dispersion Model: the generated concentration field on the ground is illustrated with different colors: brighter colors more intense field. Wind directions are shown as blue arrows.[6]

As it can be seen from the Figure 2.3, the Lagrangian dispersion of a plume represented as a set of particles in two different ways: a point source at a certain height (like a chimney) and a continuous source on the ground (like a street).

2.3.1 Mathematical Analysis of Lagrangian Model

Lagrangian particle dispersion models (LPDM) are being increasingly used to simulate the dispersion of air pollutants across different temporal and spatial scales and stability conditions. These models aim at determining the concentration of pollutants at any given point in space and time after emission.

In LPDM, the concentration field is interpreted as an ensemble average. The fundamental relationship involves the emitted mass Q at time $t = 0$, the probability that a particle that was initially at location x_0 at time t_0 arrives at location x at time t: $P(x, t|x_0, t_0)$, and the concentration at time t and location x is:

$$C(x, t) = QP(x, t|x_0, t_0) \tag{2.14}$$

To calculate the probability, a large number of particles are released and their trajectories are tracked to determine how many of them arrive at a small volume surrounding x at time t. Particle movement occurs without a grid and is determined by the first two or three moments of the Probability Density Function (PDF) of wind velocity at the location of the particle, which are obtained through measurements or parameterizations that correspond to the specific stability conditions, site type, and time and space scales considered. LPDMs are based on two main hypotheses. First, the turbulent flux is a statistical set of similar fluxes that satisfy the same boundary conditions. Second, the velocity evolution of a fluid particle can be considered a Markov process. The evolution of a tracer can be studied by simulating multiple trajectories of particles without solving the equations of motion. The number of particles released simultaneously determines the order of the statistical model that can be estimated, with single particle models calculating the mean concentration and multi-particle models calculating the variance. In LPDM, particles are assumed to move with the same velocity as the fluid element (passive tracer) in high Reynolds number flows where the effects of molecular diffusion and viscosity can be neglected. Additionally, the correlation time of accelerations between two instants is low in high Reynolds number flows, making velocity increments independent when their time separation is greater than the temporal Kolmogorov microscale. Hence, if ΔT lies in the inertial subrange, the velocity increments can be considered as a Markov process.
The Langevin stochastic differential equation (SDE) for the turbulent velocity can be written as follows:

$$du_i = a_i(\vec{u}, \vec{x}, t)dt + b_{ij}(\vec{u}, \vec{x}, t)dW_j \tag{2.15}$$

and is coupled to the equation for the position $x(t)$:

$$dx_i(t) = u_i dt \tag{2.16}$$

where $a_i(\vec{u}, \vec{x}, t)$ is the drift coefficient, a deterministic term, $b_{ij}(\vec{u}, \vec{x}, t)$ is the diffusion coefficient and dW_j is the increment of a Wiener process whose distribution is $G(0, dt)$. Hence $b_{ij}(\vec{u}, \vec{x}, t)dW_j$ is the stochastic term. In multiple dimensions $dW_i(t)$ and $dW_j(t)$ are statically independent for $i \neq j$ and $t \neq s$:

$$\begin{aligned} \overline{dW_j(t)} &= 0 \\ \overline{dW_i(t)dW_j(s)} &= \delta_{ij}\delta(t-s)dt \end{aligned} \tag{2.17}$$

Where δ_{ij} is the Kronecker delta and $\delta(t-s)$ is the Dirac delta function.
Substituting every solution of 2.15 into 2.17 , a random trajectory is obtained, and so, to generate a numerical sample of trajectories, we can use finite increments ΔU, Δx, and Δt instead of infinitesimal increments du, dx, and dt.
Corresponding to the Langevin SDE is the Fokker-Planck equation:

$$\frac{\partial P_L}{\partial t} + \frac{\partial}{\partial x_i}(u_i P_L) = -\frac{\partial}{\partial u_i}(a_i P_L) + \frac{\partial^2}{\partial u_i \partial u_j}(B_{ij} P_L) \tag{2.18}$$

Where $B_{ij} = \frac{1}{2} b_{ik} b_{kj}$ and $P_L(\vec{u}, \vec{x}, t; \vec{u_0}, \vec{x_0}, s)$ the Lagrangian Velocity Density Probably Function.The ensemble average of P_L over an Eulerian distribution P_E of initial states gives:

$$P_E(\vec{u}, \vec{x}, t) = \int P_L(\vec{u}, \vec{x}, t; \vec{u_0}, \vec{x_0}, s) P_E(\vec{u_0}, \vec{x_0}, s) d\vec{u_0} d\vec{x_0} ds \tag{2.19}$$

Eq.2.18 is linear in P_L and hence it is satisfied also by P_E:

$$\frac{\partial P_E}{\partial t} + \frac{\partial}{\partial x_i}(u_i P_E) = -\frac{\partial}{\partial u_i}(a_i P_E) + \frac{\partial^2}{\partial u_i \partial u_j}(B_{ij} P_E) \tag{2.20}$$

Eq.2.20 must satisfy the following physical constraints:

- Solution has to be compatible with Eulerian equations:

$$\frac{\partial c}{\partial t} + \vec{\nabla} \cdot (\vec{u}_E c) = 0 \tag{2.21}$$

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\vec{u}_E \rho) = 0 \tag{2.22}$$

$$\frac{\partial \vec{u}_E}{\partial t} + (\vec{u}_E \cdot \vec{\nabla}) \vec{u}_E = \frac{d\vec{u}_E}{dt} \tag{2.23}$$

  These are continuity equations for the concentration c and density ρ; we neglected the diffusivities of c and ρ.

- Direct and inverse diffusion are equivalent: $P_E(\vec{u}, \vec{x}, t) = P_E(\vec{u}, \vec{x}, -t)$, that is, symmetrical by time reversal.

- Well-mixed condition: the particles are initially uniformly distributed (well-mixed), they must remain so during the flow evolution; tracer PDF is the same as air PDF after having reached stationarity. It ensures that the tracer is mixed with the surrounding air by the turbulence.

Now we have to determine the coefficients b_{ij} and a_i of 2.15. We can start from the

Lagrangian velocity structure function from the Kolmogorov theory of local isotropy in the inertial sub range:

$$D^L(\tau) = C_0 \epsilon \tau \tag{2.24}$$

Where ϵ is the coefficient of dissipation rate of the turbulent energy and $\tau = t' - t$. The velocity structure function can be defined also as auto-function in terms of time:

$$D^L(\Delta T) = \overline{(\vec{u}(t+dt) - \vec{u}(t))^2} = \overline{(du)^2} \tag{2.25}$$

The mean operator on the set was used.
When the Langevin equation's average of $dui(t)$ is substituted, the following results are obtained by applying Eq.2.17 and only taking into account terms of the order of dt:

$$\overline{d\vec{u}^2} = \overline{(a(\vec{x})dt + b(\vec{x})dW)^2} = b^2(\vec{x})\overline{dW^2(t)} = b^2(\vec{x})dt = C_0\epsilon(\vec{x})dt \tag{2.26}$$

Therefore, introducing the further hypothesis that $b(\vec{x}, \vec{u}) = b(\vec{x})$, we have:

$$b(\vec{x}) = \sqrt{C_0\epsilon(\vec{x})} \tag{2.27}$$

We can also derive another formulation for the coefficient b. Expanding the square of 2.25:

$$\begin{aligned} D^L(\tau) &= \overline{(u(t+\tau) - u(t))^2} \\ &= \overline{u^2(t+\tau)} - 2\overline{u(t+\tau)}u(t) + \overline{u^2(t)} \end{aligned} \tag{2.28}$$

We assume that the turbulence is stationary in small space-time regions so that the temporal Lagrangian autocorrelation function:

$$R(t,\tau) = \frac{\overline{u(t)u(t+\tau)}}{\overline{u^2}(t)} \tag{2.29}$$

is only function of τ and also $\sigma_u^2 = \overline{u^2(t+\tau)} = \overline{u^2(t)}$. For a Markov process we have:

$$R(\tau) = e^{-\tau/T_L} \tag{2.30}$$

Where T_L is the Lagrangian time scale, i.e. the characteristic time until turbulent velocities are correlated or, equivalently, the time scale of the vortexes with autocorrelation function

$R(\tau)$:

$$T_L = \int_0^\infty R(\tau) d\tau \tag{2.31}$$

So at first-order of Taylor series approximation the 2.30 become:

$$R(\tau) = e^{-\tau/T_L} \approx 1 - \frac{\tau}{T_L} + O(\tau^2) \tag{2.32}$$

Therefore the equation 2.28 can be written as:

$$\begin{aligned} D^L(\tau) &= 2\sigma_u^2 - 2\sigma_u^2 R^{(L)}(\tau) = 2\sigma_u^2 - 2\sigma_u^2 e^{-\tau/T_L} \\ &\approx 2\sigma_u^2 - 2\sigma_u^2 \left(1 - \frac{\tau}{T_L}\right) = \frac{2\sigma_u^2 \tau}{T_L} \end{aligned} \tag{2.33}$$

and from $D^L(\tau) = b^2 dt$ we have:

$$b = \sqrt{\frac{2\sigma_u^2}{T_L}} \tag{2.34}$$

Finally putting the expression for b 2.27 together with 2.34 gives:

$$\epsilon = \frac{2\sigma_u^2}{C_0 T_L} \tag{2.35}$$

In stationary turbulence, i.e. $P_E(\vec{u}, \vec{x}, t) = P_E(\vec{u}, \vec{x})$, the Fokker-Planck equation 2.18 can be integrated and, for a given PDF, the term $a_i(x, u)$ calculated as:

$$a_i = \frac{C_0 \epsilon}{2P_E} \frac{\partial P_E}{\partial u_i} + \frac{\phi i}{P_E} \tag{2.36}$$

Where the function ϕ_i must satisfy the following equation:

$$\frac{\partial \phi_i(\vec{u}, \vec{x})}{\partial u_i} = -\frac{\partial P_E}{\partial t} - \frac{\partial u_i P_E}{\partial x_i} \tag{2.37}$$

Therefore a_i depends on the choice of PDF. It is important to observe that the well mixed condition guarantees that the solution to the Fokker-Planck equation is consistent with

the Eulerian equations. So the final equations for a single particle model are:

$$\begin{aligned} du_i &= a_i(\vec{u},\vec{x})dt + \sqrt{C_0\epsilon(\vec{x})}dW_j \\ dx_i &= u_i dt \\ a_i(\vec{u},\vec{x}) &= \frac{C_0\epsilon(\vec{x})}{2P_E(\vec{u},\vec{x})}\frac{\partial P_E(\vec{u},\vec{x})}{\partial u_i} + \frac{\phi_i}{P_E(\vec{u},\vec{x})} \\ \phi_i &= -\frac{\partial}{\partial x_i}\int_{-\infty}^{u_i} u_i P_E(\vec{u},\vec{x})du_i \end{aligned} \tag{2.38}$$

Where the last equation for ϕ_i is the integral version of 2.37. The selection of PDF for Eulerian turbulent velocities is a critical aspect of Lagrangian modelling. The form of P_E is based on the prevalent turbulence characteristics. A Gaussian PDF can be fully characterized by the mean and standard deviation, while non-Gaussian PDFs require higher order moments for complete description. However, for actual atmospheric PDFs, their non-Gaussian form can generally be sufficiently approximated by incorporating moments up to the third or fourth order. In situations of homogeneous and isotropic turbulence, as in our computational model, the Gaussian PDF is a suitable choice due to its natural fit.

$$P_E(\vec{x},\vec{u}) = \frac{1}{\sqrt{2\pi^3 detC_u}}e^{\frac{1}{2}(u_i C_{ij}^{-1}u_j)} \tag{2.39}$$

Where C_u is covariance matrix of velocities. In homogenic and isotropic condition is diagonal and $C_{ij} = C = \sigma^2$. Therefore:

$$P_E = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{u^2}{2\sigma^2}} \qquad\qquad \frac{\partial P_E}{\partial u} = -\frac{u}{\sigma^2}P_E \tag{2.40}$$

and plugging in 2.36 for the coefficient a:

$$a_i = -\frac{C_0\epsilon}{2\sigma^2}u_i + \frac{\phi_i}{P_E} \tag{2.41}$$

The solution for a_i is not unique, but in homogeneous and isotropic turbulence, the correct choice is $\phi = 0$. So using 2.35 gives:

$$du_i = -\frac{u_i}{T_L}dt + \sqrt{C_0\epsilon}dW(t) \tag{2.42}$$

This equation will be used in the computational part of the thesis.[2]

Chapter 3

Results

3.1 Validation of Lagrangian Model

A Lagrangian model was implemented and then validated with the Gaussian solutions using Python. 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 explained in the previous section 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

Table 3.1: parameters utilized

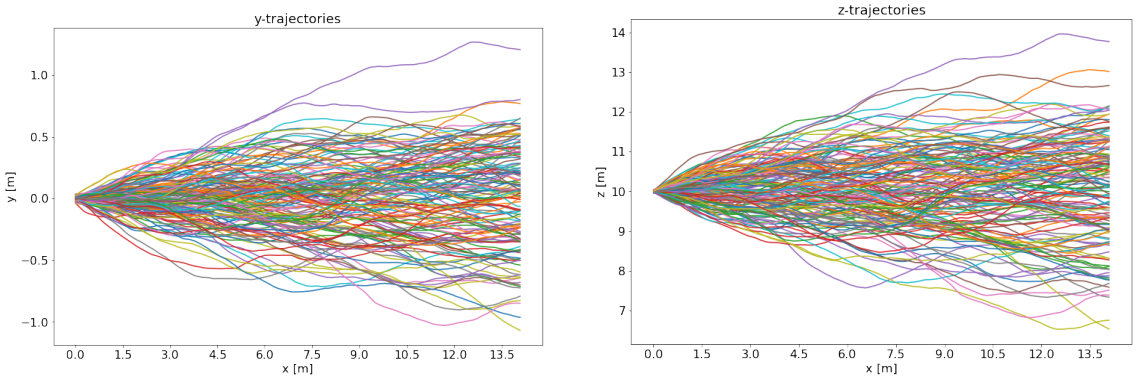
Where $nstep$ is the number of steps that the motion of the particle is integrated, T_L is the Lagrangian integral time scale, dt is the time increment, C_0 is the constant of the Langevin equation, N is the number of particles followed, U is the mean wind only along x, Q is the constant emission rate, $pblh$ is the upper boundary of our domain, he is the height of the source. Furthermore, the values of standard deviations for the initialization of position and velocity of the particles are reported in table 3.2.

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

Table 3.2: Standard deviations for initializing particle velocities and positions

Where σ_v and σ_w are the standard deviations of the velocities along y and z respectively and σ_y and σ_z the standard deviations for positions along y and z.

In figures 3.1 the typical evolution of the position of the particles along y and z can be observed.



(a) spatial evolution of particles along y

(b) spatial evolution of particles along z

Figure 3.1: Spatial evolution of particles

It can be seen from the images how the particle distribution varies with increasing distance from the source. Particularly, the standard deviations along y and z: (σ_y, σ_z) rise as the distance do, while the mean value of the ensemble along y and z remains almost constant as can be noted from the images:

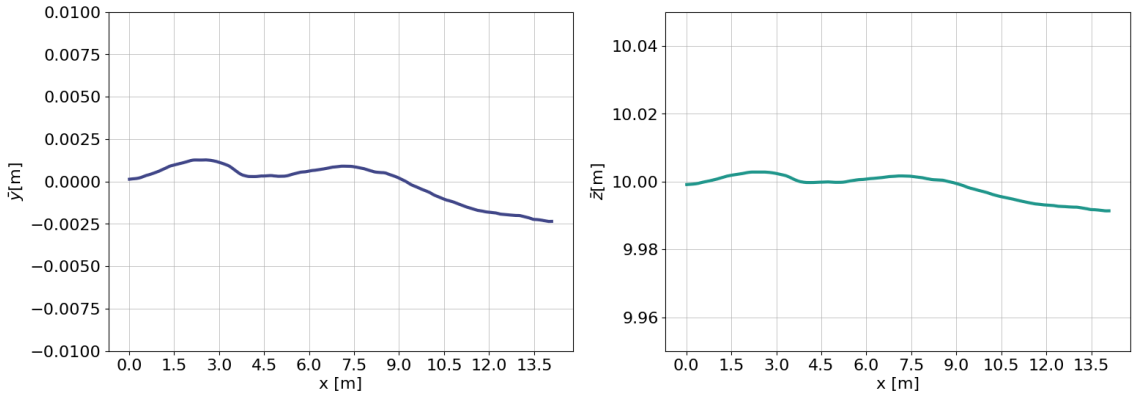


Figure 3.2: mean value of ensemble along y and z

Along z the mean value is centered at a height of 10 m from the ground corresponding to the height of the source .

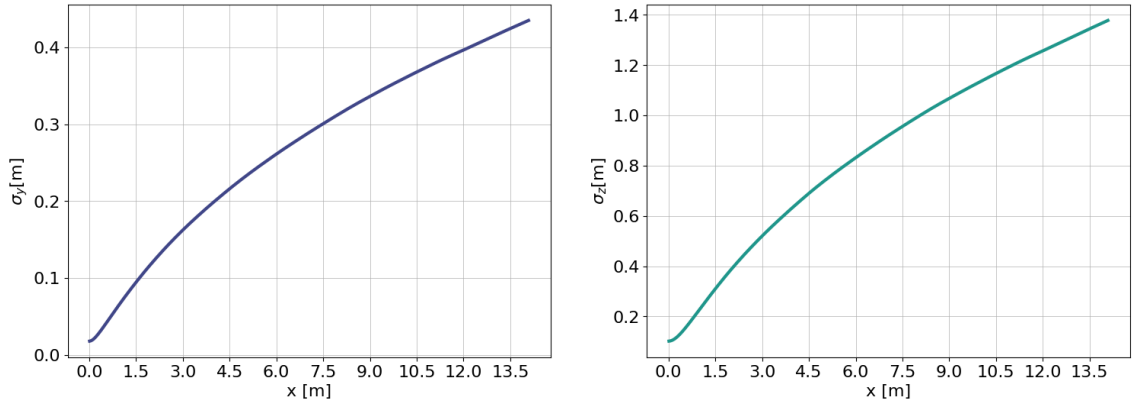


Figure 3.3: standard deviations along y and z

The Gaussian model assumes a Gaussian distribution of pollutant concentration, while the Lagrangian model tracks the movement of individual particles in the atmosphere. In idealized conditions, as we have already mentioned in the previous section, these models can be compared to evaluate their effectiveness in predicting pollutant dispersion. We can now do a qualitative analysis of what the two models match. Then the PDF are plotted as a function of y and z:

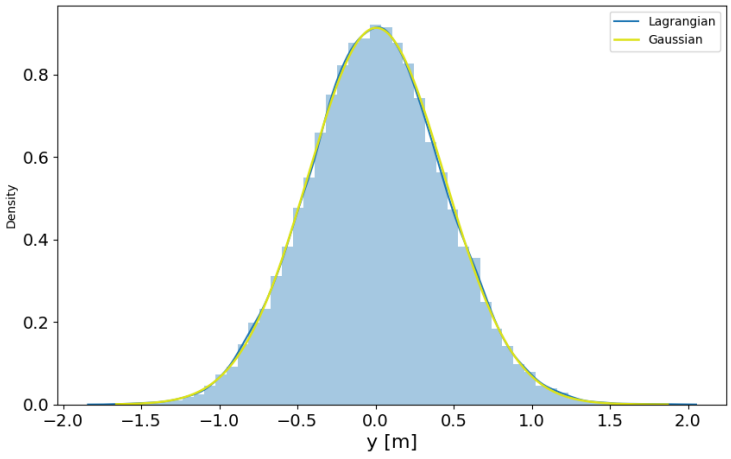


Figure 3.4: comparison between the two distributions along y

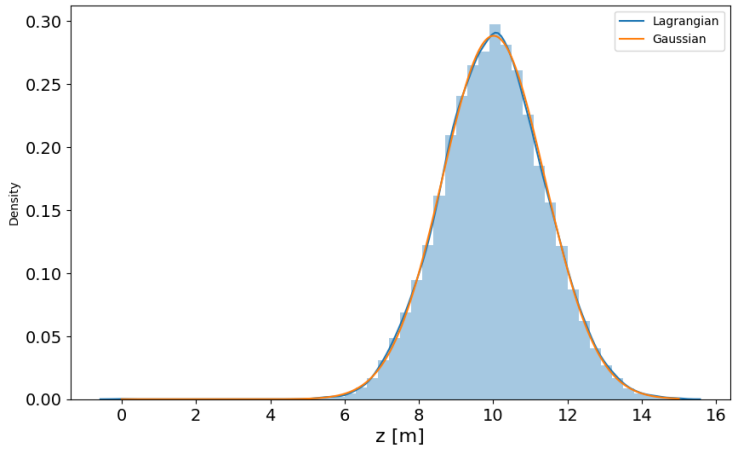


Figure 3.5: comparison between the two distributions along z

It can be seen from figure 3.5 that the distributions along z are centered at $z = 10m$, indeed this is the height of the source. With a very large number of particles ($N = 20000$), the two PDF along y and z coincide.

It is also possible to see the Lagrangian evolution in space of the pollutant in terms of concentration with graphs that represent the various concentrations with different colors at a distance of $13m$ from the source:

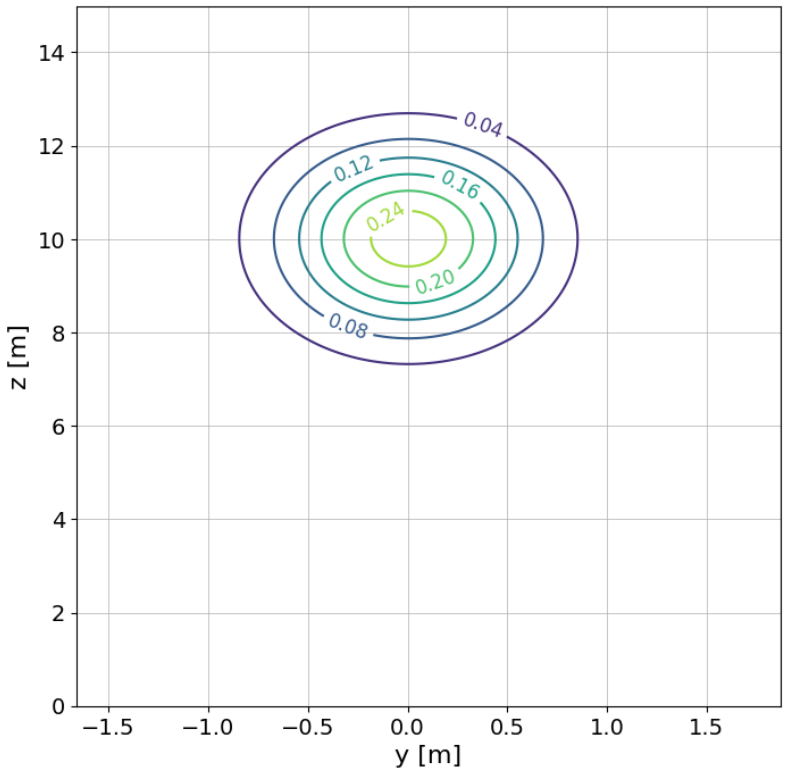


Figure 3.6: Concentration field in function of y and z, the value of concentration fields is written above the curves in g/m^3

The brighter (lighter) shades of color represent a higher concentration of the pollutant.The concentration field scales very quickly to zero, indeed moving both along y and along z by about 2 meters, the concentration becomes very low.
The Lagrangian concentration field can also be compared with the Gaussian one at a distance of $13m$ from the souce trough a plot:

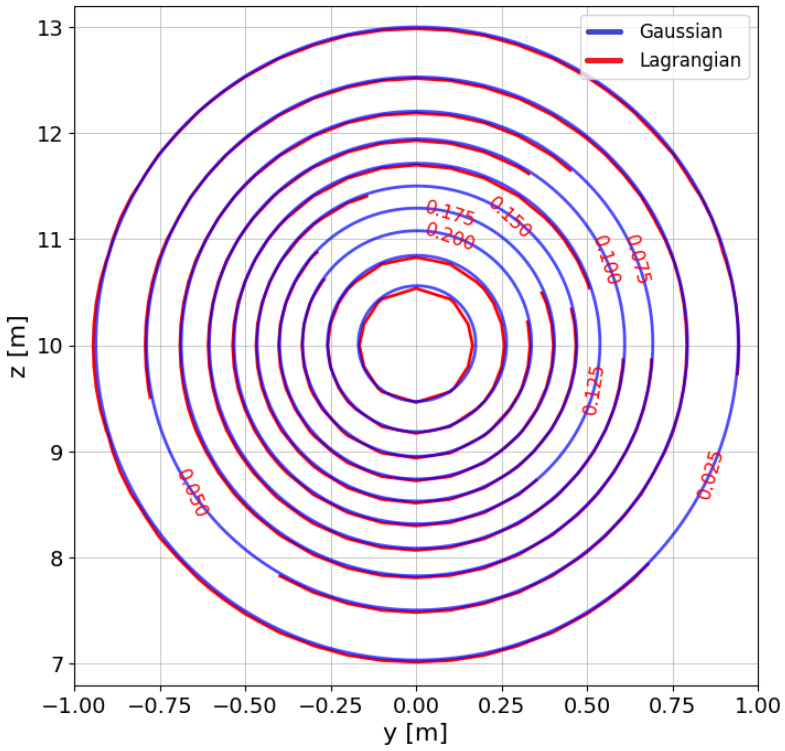


Figure 3.7: Comparison between Gaussian and Lagrangian concentration fields as function of y and z: red line is used for the Lagrangian field, while blue line is used for the Gaussian one; the numbers above the curves represent the concentration values of isolines in g/m^3

In the plot the blue line represents the Gaussian concentration field while the red line represents the Lagrangian one. The concentrations are written above the curves and are expressed in g/m^3.
As it can be observed in the plot, the concentration fields obtained with the Lagrangian and the Gaussian approach are alike, thus validating the Lagrangian model written from scratch.

3.2 Sensitivity analysis

In a Lagrangian model of pollutant dispersion, sensitivity analysis can be a powerful tool for understanding the behavior of pollutants in different environmental conditions.

Sensitivity analysis involves varying different model parameters and observing how the model output changes in response. This can help to identify which parameters are most critical for predicting the behavior of pollutants in different environmental conditions, and can aid in the development of more accurate and reliable models.

For example, sensitivity analysis can be used to study the effect of different atmospheric conditions on the dispersion of pollutants, such as wind speed, wind direction, temperature, and humidity. By varying these parameters and observing the resulting changes in pollutant concentrations, it is possible to determine which factors have the greatest influence on the dispersion of pollutants.

Sensitivity analysis can also be used to study the effect of different pollutant properties on their behavior in the atmosphere, such as particle size, density, and chemical composition. By varying these properties and observing the resulting changes in pollutant concentrations, it is possible to determine which properties have the greatest influence on the fate and transport of pollutants.

Overall, sensitivity analysis of Lagrangian models of pollutant dispersion can provide valuable insights into the behavior of pollutants in different environmental conditions and can aid in the development of more accurate and reliable models for predicting pollutant concentrations in the atmosphere.

First of all we can modify the number of particles to follow in the Lagrangian model and see how the means, standard deviations and concentrations vary.

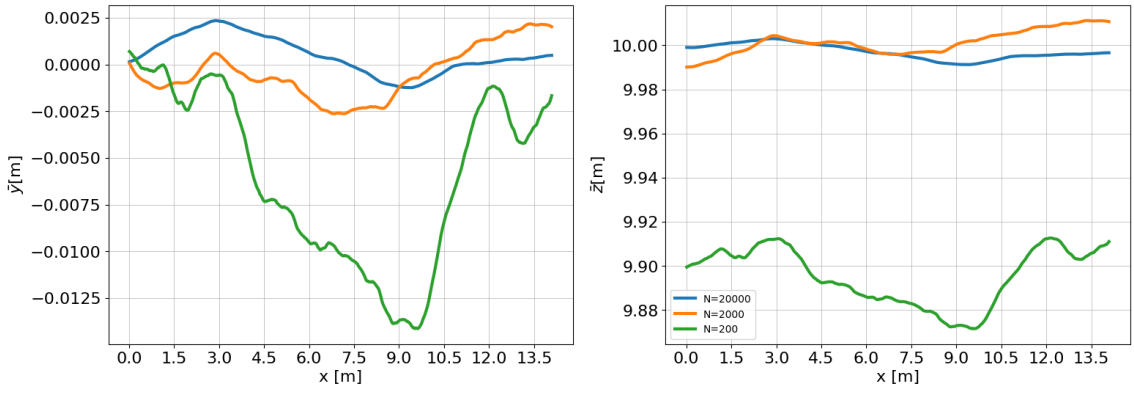


Figure 3.8: comparison of mean value with $N = 20000$, $N = 2000$, $N = 200$

And for standard deviations:

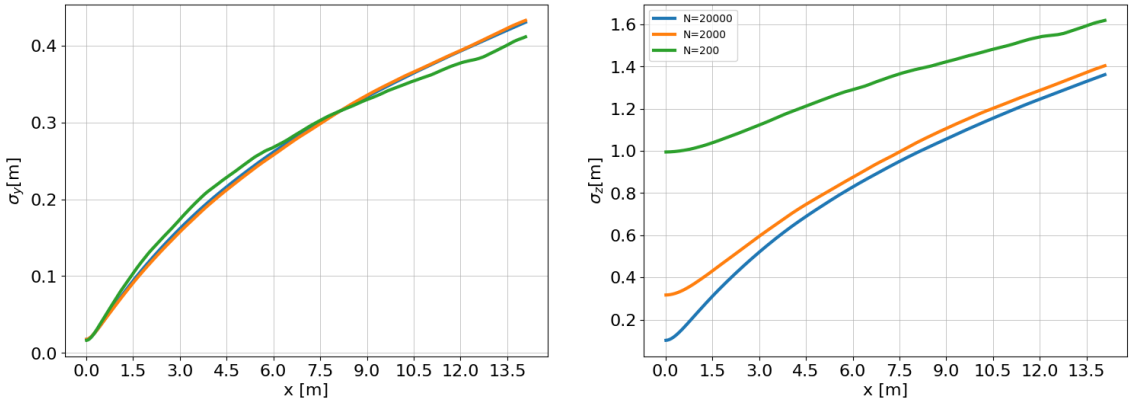


Figure 3.9: comparison of standard deviations with $N = 20000$, $N = 2000$, $N = 200$

we can see that the more the number of particles N decreases, the more the fluctuations of the ensemble average value increase. Indeed we can expect that the more the points increase the more the mean value will tend to the expectation value. As we expect also in standard deviations we have the same behavior.

We can plot the Gaussian and Lagrangian concentration field at a distance along x from the source of $13m$ with $N = 200$.

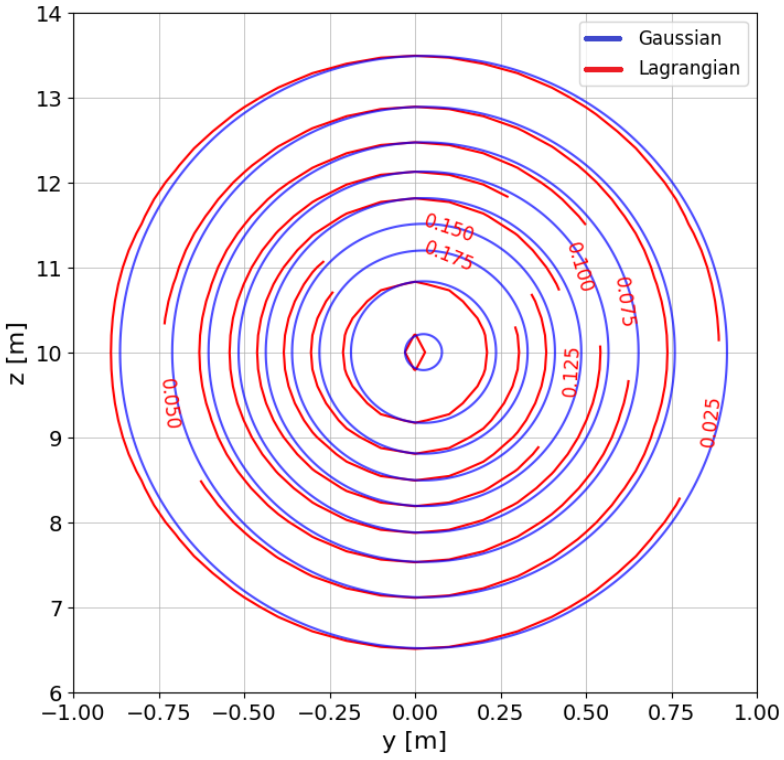
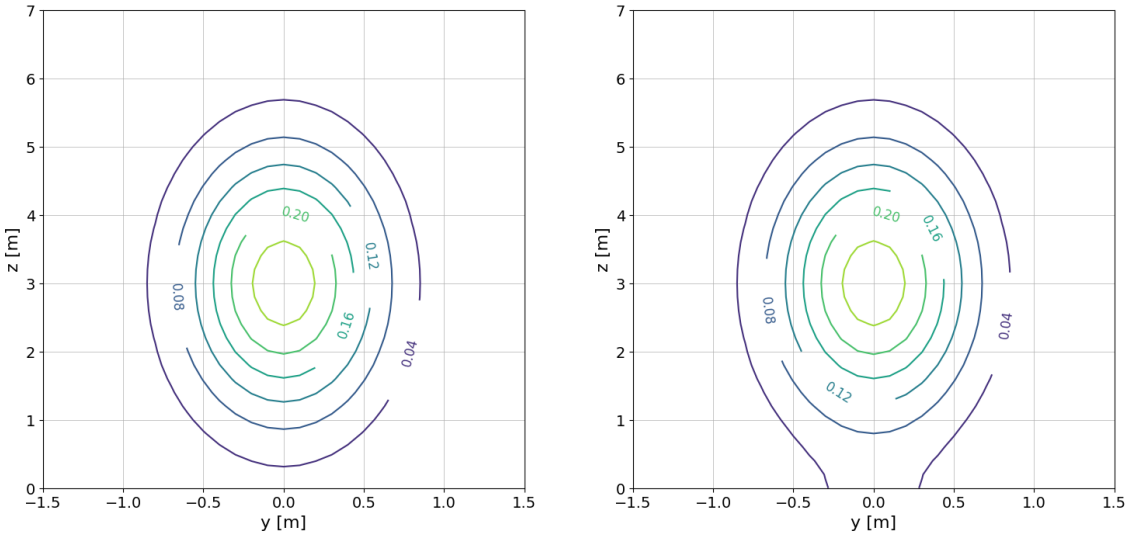


Figure 3.10: Comparison between Gaussian and Lagrangian concentration fields with N=200

In the plot the blue line represents the Gaussian concentration field while the red line represents the Lagrangian one, as in the previous section.

Now we can see a modest difference between the two fields.

It also be possible to change the height of the source at $he = 3m$ to see the difference between using the formula with infinite image sources 2.13 and with a single image source 2.12:



(a) Concentration field with image sources

(b) Concentration field with a single image source

Figure 3.11: Concentration field with $he = 3m$

We can see from the plots, that in 3.11b there is deposition on the ground while in figure 3.11a it does not.

It is particularly interesting to observe the impact that wind speed along x has on the standard deviations along y and z.

We can then plot standard deviations for different winds speeds along x:

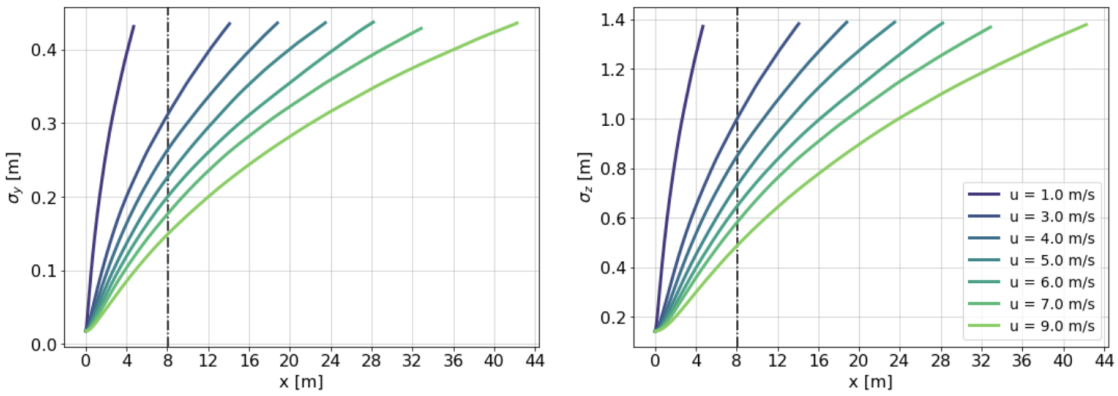


Figure 3.12: Standard deviations for different wind speeds along x

It can be seen from 3.12 that as the wind increases the standard deviation rises faster as a function of x. We can graph the standard deviations for a fixed value of $x = 8m$ and see the trend:

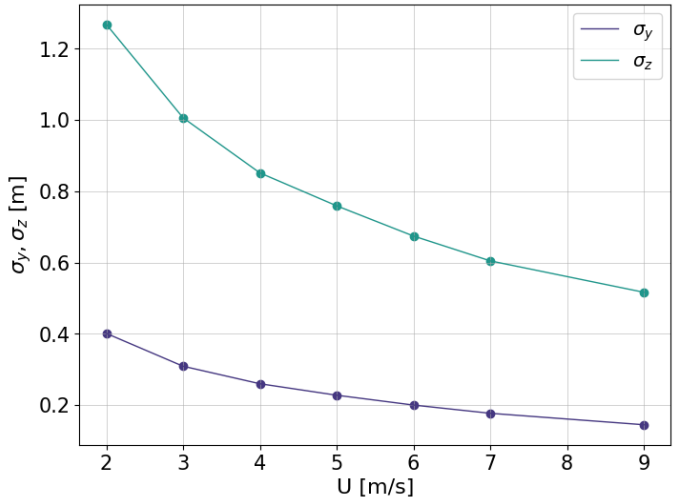


Figure 3.13: Standard deviations for a fixed value of $x = 8m$.

The shape of the curve that can be qualitatively deduced is exponential: for the wind speed which tends to infinity the standard deviation tends to zero. That is, the wind stabilizes the motion of the particles.

Various types of sources can be also hypothesized which can emit pollutants with various initial velocities. To simulate these and study the shapes of standard deviation, we can initialize various values of the starting standard deviations for velocities: σ_v and σ_w keeping the other parameters fixed.

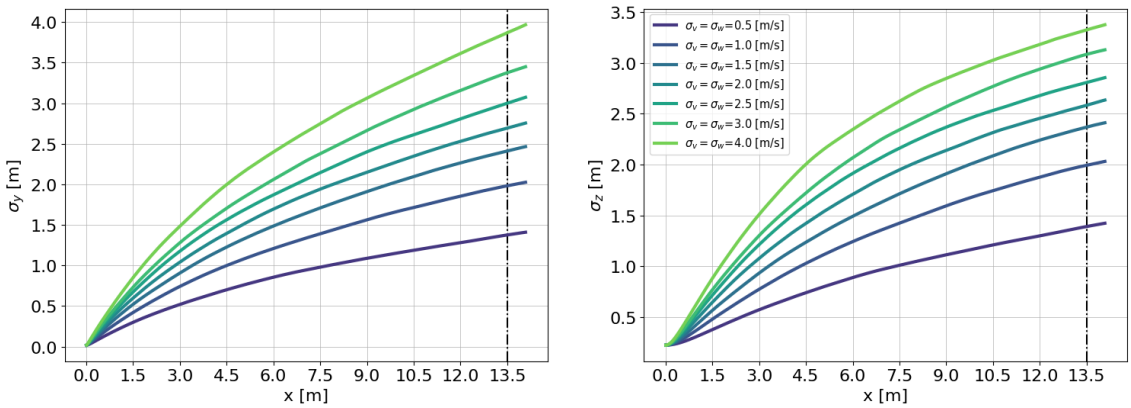


Figure 3.14: Standard deviations for different values of σ_v and σ_w

We can see from the plot that the more σ_v and σ_w increase the faster the standard deviations increase as function of x.

As we have done before, we can fix a value of the distance from the source: $x = 13.5m$ and graph values of standard deviations along y and z as function of σ_v and σ_w:

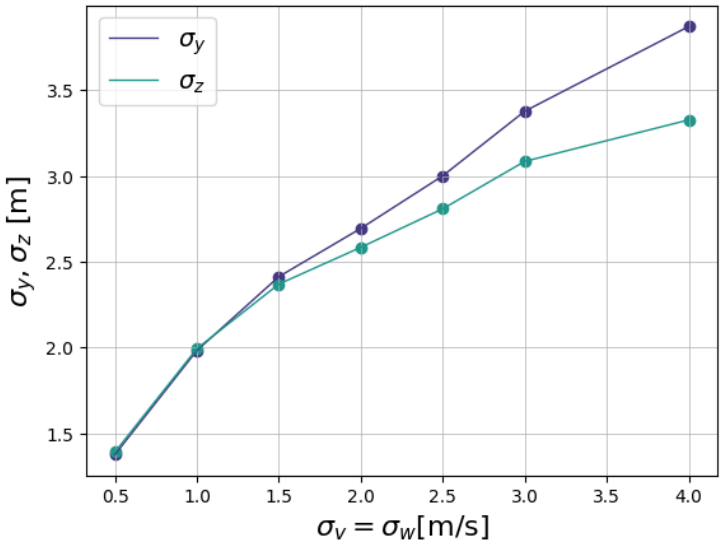


Figure 3.15: Standard deviations for a fixed value of $x = 13.5m$.

It can be seen from the plot that the shape is qualitatively logarithmic indeed σ_y and σ_z increase fast for the first values of σ_v and σ_w while the speed of the curve decreases for the last values of σ_v and σ_w. To have a confirmation about the shape of the curve we can plot in logarithmic scale the previous graph 3.15:

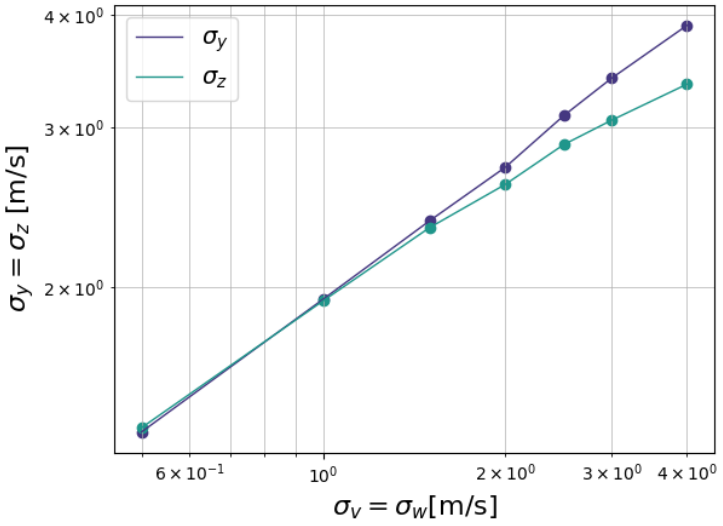


Figure 3.16: logarithmic scale of standard deviations for a fixed value of $x = 13.5m$

We can see the linear trend of the standard deviations along y and z as function of σ_v and σ_w in the logarithmic plot as expected.

Chapter 4

Conclusions

In this thesis, a numerical simulation of the diffusion process in the atmosphere using a particle Lagrangian model was conducted.

The study aimed to explore different approaches to simulate the dispersion of a tracer, with also a mathematical descriptions, and validate the Lagrangian approach through comparison with the Gaussian one.

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.

Additionally, a sensitivity analysis of the dispersion of the plume was performed to identify the main factors influencing the dispersion of the tracer. The 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.

This is consistent with what we might expect, indeed if we increase the wind speed along a single direction the particles will tend to be more stable dragged by the wind and therefore the mean value of the ensemble will fluctuate less.

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. The findings can contribute to the knowledge of the diffusion of pollutants in the atmosphere and can be used to develop effective mitigation strategies.

Overall, Lagrangian model provides a powerful tool for understanding the behavior of pollutants in the atmosphere. The results of this research can aid in the development of

effective pollution control strategies and policies to improve air quality and protect public health.

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