



Modelling of pollutant dispersion in air

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NOMENCLATURE

Abbreviations:

AEMET	State Meteorological Agency
SO₂	Sulphur dioxide
SO₃	Sulphur trioxide
CO	Carbon monoxide
NO, NO₂, NO_x	Nitrogen oxides
O₃	Ozone
PM	Particulate matter
PM_{2.5}	Particulate matter with size less than 2,5 micrometer
PM₁₀	Particulate matter with size less than 10 micrometer
VOCs	Volatile Organic Compounds
EPA	Environmental Protection Agency
CFD	Computational Fluid Dynamics
WHO	World Health Organization
EPA	Environmental Protection Agency
WAS	Water, Air and Soil
R&D	Research and Development
FVM	Finite Volume Method
FEM	Finite Element Method
FDM	Finite Difference Method
ODE	Ordinary Differential Equations
PDE	Partial Differential Equations
RBF	Radial Basis Function
Python	Computational program for numerical simulation
Octave®	Computational program for numerical simulation

Mathematical Notations:

c	Concentration [kg/m ³]
t	Time [s]
D	Diffusion coefficient [m ² /s]
J	Diffusion flux [mol/(m ² · s)]
Δx, Δy, Δz	Step-size in direction x, y, z, respectively [m]
T	Temperature [K]
rad	Particle radius [m]
K	Boltzmann constant
η	Viscosity [Pa · s]
r	Reaction rate [mol/(L · s)]
S	Source focus [kg/(m ³ · s)]
R	Reaction source term [kg/(m ³ · s)]

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ABSTRACT

Air quality has become one of the main concerns of public administrations. This is due to the evidence that air quality is directly linked to health, as polluted environments have been shown to be the cause behind many health problems. According to public administrations, nitrogen oxides and particulate matter should be reduced in cities and ozone and volatile organic compounds in rural zones. In this regard, one of the focuses of public administrations is to properly model pollutant dispersion in order to have air quality maps and act consequently.

The work presented here aims at developing a computational tool which can quickly predict pollutant dispersion in air. Existing tools mostly calculate pollutant dispersion in two steps: first a meteorological module computes the air velocity field and then pollutant concentration is calculated. This results in a large computational cost due to the need to calculate the air velocity field. In order to reduce computational cost, the tool developed here replaces the computation of the air velocity field by retrieving data from weather stations. In addition to reducing the computational cost, it also allows the use of real time data in the model.

The open source programming language Python is used to develop the computational tool. There were two preliminary versions developed by Eurecat of a web scraping tool to download data from online databases and a computational tool to solve the convection-diffusion equation. The former was written in R language while the latter was developed in Octave. The starting point of this project was analysing those two codes to later rewrite them and extend their features.

The web scraping module connects and retrieves data from the meteorological stations of the Agencia Estatal de Meteorología (AEMET)^[1] to extract the wind velocity magnitude and direction for the last 24 hours. It also interpolates the data obtained to set the wind velocity in all the cells of the computational domain. This module also connects to a file in .csv format where information from the National Air Quality Index^[2] is entered to process the pollutant concentration data and interpolate its values in the computational mesh.

The second module consists in the two-dimensional simulation of one or multiple pollutants with one or more emission sources. The emission can also be continuous or instantaneous. The convection-diffusion equation for a scalar transport is solved in two dimensions for all the computational domain, since the data acquired from weather stations does not include the vertical component of the wind velocity. This wind velocity is updated at the frequency provided by the meteorological database. Pollutants can be passive or reactive, with the chemical reaction and its parameters being previously defined.

The tool has been validated using data from the eruption of the Cumbre Vieja volcano in La Palma. This case has been chosen because it has been a very important continuous emission of sulphur dioxide (SO₂) and the kinetics of formation of its secondary pollutant, sulphur trioxide (SO₃), is known. The results show good agreement with the observed data except for two points located at different sides of a mountain ridge. This shows that the tool developed during this project, at its current stage, can quickly predict with accuracy pollutant dispersion as long as the topography of the domain is not too complex.

1. INTRODUCTION

Currently, there are many pollutants present in the air, although the main ones^[3] are carbon monoxide (CO), nitrogen oxides (NO, NO₂, NO_x), sulphur dioxide (SO₂), ozone (O₃), particulate matter (PM) and volatile organic compounds (VOCs). The main sources^[4] of these pollutants are from transport emissions, from the burning of fuels in industry, from combustion for the generation of mechanical and electrical energy, from forest fires and from volcanic activity. In addition, some sources of pollutants come from the decomposition of organic matter.

According to data from medical-scientific societies and the World Health Organization (WHO), air pollution causes 7 million premature deaths^{[5] [6]} worldwide and more than 10,000 in Spain. Furthermore, a study published in the Environment International journal^[7] carried out in recent years has concluded that an increase of 5µg/m³ in the concentration of PM10 particles reduces life span by almost one year, while an increase of 5µg/m³ of PM2.5 particles has repercussions with a reduction of approximately 7 months of life.

Today there are many problems^[8] due to pollution that cause serious damage to our health and planetary balance. Some effects produced in the environment are sudden changes in the climate, the appearance of severe meteorological phenomena, holes in the ozone layer that allow the entry of ultraviolet rays, the disappearance of animal and plant species, the drought of rivers and the disappearance of water sources.

But that is not all, there are also effects on human health that cause respiratory problems, cardiovascular diseases, problems in cognitive development, fertility problems or cancers, producing an increase in premature deaths. There are several reasons why these deaths^[9] occur due to pollutants present in the air, which in 34% of cases due to a stroke or cerebrovascular accident, 26% due to a myocardial infarction, 22% due to pulmonary obstruction, 12% for pneumonia and 6% for lung cancer.

In recent years, Law 34/2007^[10] has been approved, which enables the Spanish government to approve plans and programs to prevent and reduce atmospheric pollution. In addition, Article 24 of Royal Decree 10/2011 was established where the autonomous communities will approve air quality plans for certain areas or agglomerations where the levels of pollutants in the air exceed the established limit values. In this way, each autonomous community has one or several plans to improve air quality. In the community of Catalonia, the Generalitat has proposed measures defined by 14 environmental objectives^[11], which are shown below:

- Objective 1: Strengthen, encourage and promote public, urban and interurban transport.
- Objective 2: Promote modal exchange, energy diversification and the rational use of private vehicles.
- Objective 3: Environmentalization of the vehicle fleet.
- Objective 4: Adaptation of authorizations to the new environmental regulations.
- Objective 5: Encourage energy improvements.
- Objective 6: Electricity generation with air quality criteria.
- Objective 7: Reduce emissions associated with the traffic of people and goods to access the airport.
- Objective 8: Follow-up of the implementation of the measures to be carried out by AENA to reduce emissions associated with airport activity.
- Objective 9: Promote rail freight transport.
- Objective 10: Management of ship controls and inspections.

- Objective 11: Use of alternative fuels in port activities and in their surroundings.
- Objective 12: Improve energy efficiency or savings and encourage the use of fuels that emit fewer particles.
- Objective 13: Dissemination of the Action Plan and its measures, as well as making the population aware of air quality levels and giving the general public the tools to assess this situation.
- Objective 14: Creation and enabling of financing mechanisms for the improvement of air quality.

In this way, the community of Catalonia achieves the air quality objectives set by the European Union, which has been working to improve air quality since the 1970s by controlling emissions of harmful substances. In 2013, the European Commission adopted a series of clean air policies^{[12] [13]}, which established goals for 2020 and 2030, and on November 11, 2019, the European Green Deal was approved, which fights against climate change produced by various pollutants. It should be noted that the European Union during this 2021 has revised the air quality standards of the European Green Agreement to comply with the recommendations of the World Health Organization; it has held the Third Clean Air Forum where it focused on the challenge of zero pollution, on the commitment of cities and citizens with pollution, on how clean air affects economically, on air pollution and the climate change it generates, on the human right to have clean air and on the review of air quality regulations; and, in addition, it has presented an analysis of the perspectives of air pollution until 2030.

Pollutant dispersion modelling^[14] is used to predict how pollutants are dispersed in the atmosphere through a mathematical simulation, being one of the most important scientific problems. In this way, computer programs are made to solve the mathematical equations of diffusion-convection. Being these important tools for government agencies in charge of protecting and managing air quality. Currently, there are several commercial and open source tools that simulate the dispersion of pollutants in the environment, but these are either very expensive or with very limited features. The United States Environmental Protection Agency (EPA)^[15] recommends the CALPUFF and AERMOD dispersion models. The CALPUFF^[16] tool was developed by scientists at Exponent, Inc. and performs unsteady-state air quality and meteorological modeling, consisting of a set of pre-processing and post-processing programs. In addition, it has a free license but limited use due to several restrictions. The AERMOD^[17] tool is a steady-state dispersion model based on planetary boundary layer turbulence and a terrain data preprocessor, but it can only do short-range designs. Another available contaminant dispersion tool is HYSPLIT^{[18] [19]} developed by NOAA Air Resources Laboratory and the University of Huelva, which is free and online. It uses archived meteorological data from the National Centers for Environmental Prediction (NCEP) to calculate the trajectory of a single particle using the Lagrange method by running simple air sector trajectories, but it has many limitations because information is only available in a few cities.

This project aims to develop a computational tool that allows the prediction of the pollutants dispersion at a given time of day and during a given period of time. This integrates the wind information in real time through the meteorological databases. In this way, it saves calculation time, since the dynamic field of the air is not calculated because updated real information is obtained. For this reason, the tool is a two-dimensional model, since in the meteorological stations only the velocity and direction of the wind are available. This implies that in places where the orography is very complex, it can affect the accuracy of the result, since the vertical dimension is not included.

2. SCOPE OF THE PROJECT AND SPECIFIC OBJECTIVES

The goal of the project is to develop a computational tool to predict pollutant dispersion in air. As it has been mentioned in the previous chapter, this tool will implement wind data from weather stations in real time by using web scraping techniques. That makes the code execution faster as it avoids the need to compute the air velocity field and uses current and validated data for the wind.

There are currently two domestic codes developed by Eurecat which tackle those two features. There is one code, written in R programming language, which retrieves information for a small set of weather stations located in the area of Tarragona. The second code, written in Octave, solves the convection-diffusion equation for a passive scalar. In this project the integration of those two codes have been performed by rewriting both of them in Python and then their features have been extended.

The web scraping module is improved by adding a greater number of AEMET meteorological stations, which are chosen depending on the area studied, and by updating the wind velocity and direction data every simulation hour to use the data from the corresponding real hour.

In the case of the dispersion module, its new features include greater code stability, due to the fact that the variables are created based on previous inputs, and the addition of a chemical reaction, which simulates the reactivity of pollutants with the atmosphere or with another compound present in the air.

To carry out this project, the following specific objectives have been established:

- Familiarization with Python: A preliminary study of the nomenclature of the open source program offered by Python is carried out in order to later be able to write the code for the pollutant dispersion in air and the web scraping tool.
- Familiarization of computational fluid dynamics: Knowledge of Computational Fluid Dynamics must be obtained to carry out the project, learning the convection-diffusion equations and evaluating the different numerical methods used to solve this equation numerically.
- Rewrite the current version of the dispersion code in Python: Previously, there was an early version of the computational code for contaminant dispersion written in the open source offered by Octave, but in this project Python is used because offers greater freedom when communicating with other languages.
- Rewrite the web scraping code: Previously, there was a version of the web scraping code written in the R programming language, but it is being rewritten in the open source language of Python.
- Create a common core for the web scraping and dispersion codes: It consists of creating a code capable of communicating the web scraping module with the pollutant dispersion module. In this way, the dispersion code is linked with the meteorological data extracted from the AEMET.
- Add more weather stations to the code: More weather stations should be added to the web scraping module in order to have more precise results or a larger study area, since the coordinates of the stations are used.
- Study of the different meshes: Different distances between the points in the mesh are studied and how they influence the results of the dispersion of pollutants.
- Study of validation cases: A real case is studied to carry out a validation of the computational code of the dispersion of pollutants.
- Evaluate the influence of chemical reactions: Code is extended for the addition of chemical reactions which generates secondary pollutants.

Figure 2.1 shows a schedule with the dedicated time on each task performed.

Week	Dates	Task
1	7-10 SEP	Read project documentation, understand goals
2	13-17 SEP	Get familiar with Python
3	20-24 SEP	Get familiar with Computational Fluid Dynamics
4	27 SEP - 1 OCT	Rewrite current version of the dispersion code in Python
5	4-8 OCT	Rewrite current version of the dispersion code in Python
6	11-15 OCT	Rewrite current version of the dispersion code in Python
7	8-22 OCT	Rewrite the web scraping code
8	25-29 OCT	Create a common core for the websrapping and dispersion codes
9	1-5 NOV	Add more meteorological stations into the code
10	8-12 NOV	Study of the different meshes
11	15-19 NOV	Study of the different meshes
12	22-26 NOV	Study of validation cases
13	29 NOV - 3 DEC	Study of validation cases
14	6-10 DEC	Evaluate the influence of chemical reactions
15	13-17 DEC	Evaluate the influence of chemical reactions
16	20-24 DEC	Study of validation cases
17	27-31 DEC	Additional simulations / writing

Figure 2.1. Schedule used to carry out this project.

3. STUDENT'S ROLE IN COMPANY

I did my internships and master's thesis at the Eurecat company at the Tarragona headquarters in the Water, Air and Soil Technology Unit (WAS). During this period of time, the tool that simulates the dispersion of pollutants was carried out, which was from September 10 to December 31, 2021.

Due to the COVID-19 situation, it was agreed that they would mainly work from home and go to the Eurecat offices once a week, instead of going daily.

3.1. About Eurecat

Eurecat was founded on May 1, 2015 from the merger of advanced technological centers, which were Ascamm, Barcelona Digital (BDigital), Barcelona Media and Cetemmsa. In addition, over time more technological centers have been incorporated. Currently Eurecat has sites at Barcelona, Tarragona, Lleida, Girona, Manresa, Cerdanyola, Reus, Vilaseca, Amposta, Mataró and Canet.

Eurecat has more than 650 professionals who provide differential technology and advanced experience to offer solutions to the needs of innovation in the industrial and business sector. In this way, it enhances its competitiveness.

This company offers more than 200 R&D projects to its more than 1.700 client companies. These projects are focused on applications and market needs, on the acquisition of new knowledge, on the transfer of knowledge for the creation of new products, processes or services and on the improvement of products and services that currently exist.

All R&D projects can be of a private nature (direct contracts with private companies), of a public nature (competitive calls from public administrations) and of an internal nature (funding projects to broaden the company offering).

Eurecat has an international presence with 88 patents and 7 spin-offs.

Eurecat is divided in four different areas: Biotechnology, Digital, Industrial and Sustainability. The Water, Air and Soil (WAS) Technological Unit forms part of the Sustainability Area, and its personnel is split between the sites of Manresa and Tarragona. It has three different research lines and four different technological fields, given place to a 12-cell research and technological matrix. The three lines are Water, Air and Soil while the four technological fields are Separation Processes, Advanced Oxidation Processes, Risk Assessment and Modelling and Simulation.

3.2. aiRECAT project

This Final Master Project (FMP) is carried out within the framework of the aiRECAT project, which is an internal project at Eurecat where the goal is to position Eurecat as a reference center in the air vector. In order to accomplish that goal, it is needed to detect the problem affecting air quality, to predict how that can evolve and to provide solutions. Aligned with that strategy, the aiRECAT project is structured in three work packages: the first one deals with monitoring and analysing different pollutants in air; the second one consists in developing a computational tool to predict pollutant dispersion; and the third one aims at developing treatment technologies to remove these pollutants. This FMP is therefore included in the second work package of the project.

As it has already been described in the first chapter of this document, some dispersion modelling tools already exist but they either are expensive in terms of licensing or cannot be used for commercial purposes. In addition, they do not have the ability to dynamically incorporate data from weather stations. For this reason, the aiRECAT project aims to develop a computational tool that communicates with meteorological data to dynamically

incorporate wind velocity and direction information. This data will be two-dimensional, as the velocity field from data extracted from meteorological stations does not provide the vertical dimension.

3.3. My work in Eurecat

In order to reach the goals proposed in the aiRECAT project, some steps previously explained in Chapter 2 have been established, which have been achieved during the internship period.

At the beginning of the project I had to familiarize myself with the project and with the objectives that it had to fulfil. In this regard, as the scope of the project was to develop a computational tool that predicts the dispersion of pollutants in air using the open source programming language Python, I had to learn the basic notions. In addition, I followed several tutorials to acquire a good understanding of the language.

Once I had learnt Python I proceeded with learning Computational Fluid Dynamics (CFD). To do this, I reviewed the convection-diffusion equation and documented myself on the various numerical methods to be able to solve the equation analytically. Actually, I did not know many numerical methods or forms of discretization for the convection-diffusion equation, but my supervisor guided me a lot when looking for information, which was very helpful.

When I already had some knowledge about CFD, I continued with the transcription of the code available previously written in Octave into the Python language. That was not easy because I had first to become familiar with another language, Octave, in order to understand what the code actually did and once I fully understood that, I had to look for its equivalent form in Python. Also, once I had the translation of the code, I realized that some parts of the existing code contained errors. That way, I went through the code thoroughly so that I could catch some bugs and correct them.

The reason why the code was required to be written in Python was to make all communications between the different modules easier and also the external communications, for example, to retrieve data from the AEMET weather stations. To do this, I had to import into the code a file in .csv format containing the web addresses of the different AEMET stations. However, when the data was imported and the velocity interpolation on the computational mesh was performed, some errors occurred, since there was some blank data from the information downloaded from the AEMET website. I had to look for ways to eliminate this blank data automatically and thus avoid the problems linked to partial data missing.

Later on, I added more stations to the .csv file, but I didn't want to write code that was limited by the previously designed inputs. That is why I had to do an exhaustive search to create variables automatically depending on the number of rows in the file. When I found this information, I proceeded to fix the code to be more flexible when introducing variables.

Once I had the code ready, I carried out the mesh independency test to make sure that the results were not affected by the mesh resolution. Then I realized that as the distance between the grid points decreased, the concentration decreased exponentially and that was due to not taking into account the area of the emitting focus. This step took us longer than we expected since it was not easy to find the error.

When I had already established the distance between the grid points for the calculation of diffusion, it was decided that we could study the eruption of La Palma, since it at the moment it was a focus of public interest. The current version of the code, by that time, had the georeferenced map of Catalonia as the background for plotting results, since that

was the area of interest initially. So I had to change that feature to include the La Palma map.

After running the code for La Palma's case and comparing it with the real data from the available stations, I had a few more weeks left to invest in the project. For that reason it was decided to invest this time in adding chemical reactions into the code to predict the formation of secondary pollutants. Once I had that, I continued to simulate the case of La Palma on the same day to assess how the chemical reaction generated those secondary pollutants.

4. THEORETICAL FRAMEWORK

This section provides the theory behind the physical and chemical phenomena that will be solved with the computational tool developed in this project. The convection-diffusion equation is shown in Equation 4.1, which describes the physical and chemical phenomena which lead to pollutant dispersion in air due to the following processes.

$$\frac{\partial c}{\partial t} = \nabla(D \cdot \nabla c) - \nabla(v \cdot c) + S + R \quad (4.1)$$

where c is the concentration, t is the time, D is the diffusion coefficient, v is the wind speed, S is the source of the contaminant, and R is the chemical reaction term.

This equation shows the variation in the concentration of the different pollutants over time. This is influenced by diffusion (blue coloured part), convection (green coloured part), the pollutant emission source (purple coloured part) and chemical reaction (red coloured part), both when it is consumed and when it is produced. Each part of this equation is detailed below.

4.1. Diffusion^[20]

Diffusion is a transport process found in nature. It consists of the flow of particles from a higher concentration region to a lower concentration one, but the particles continue to move when the concentrations are equal due to the self-diffusion process.

There are three different types of diffusion^[21]: molecular diffusion, Brownian diffusion, and turbulent diffusion. However, the computational tool developed in this project only takes into account molecular diffusion at its current stage of development.

4.1.1. Molecular diffusion

Molecular diffusion is produced by the thermal movement of molecules. It occurs at a higher rate in gases, at a lower rate in liquids and even less in solids. The differences of the different states are explained by the nature of their thermal movement.

The flow of molecular diffusion at constant temperature and pressure is described by Fick's law, shown in Equation 4.1.1.

$$J_A = -D_A \frac{dC_A}{dz} \quad (4.1.1)$$

In this equation, it can be seen that the diffusion flux, J_A , is proportional to the molar concentration gradient in one direction, dC_A / dz . This proportion is called the diffusion coefficient, D_A .

In the case of a binary system, the flow of the components has to balance between them. If a component is moved to one side, the other has to occupy that space, as it can be seen in Equation 4.1.2.

$$\frac{dC_A}{dz} = \frac{dC_B}{dz} \quad (4.1.2)$$

In that way, the diffusion of the two components has to be the same, as shown in Equation 4.1.3.

$$D_A = D_B = D_{AB} \quad (4.1.3)$$

4.1.2. Brownian diffusion^[22]

Brownian diffusion consists of the random movement of small particles (smaller than a few microns) suspended in stationary gas or liquid at rest and is independent of the chemical properties of the medium.

The projection of the displacement of a particle on an arbitrarily chosen axis is proportional to the observation time, as it can be seen in Equation 4.2.1.

$$\Delta z^2 = 2 D_A t \quad (4.2.1)$$

The diffusion coefficient for spherical particles of a given radius, *rad*, is determined by the Stokes-Einstein equation, shown in Equation 4.2.2.

$$D_A = \frac{K T}{6 \pi \eta \text{ rad}} \quad (4.2.2)$$

Here the coefficient is defined as *Da*, the Boltzmann constant as *K*, the temperature as *T* in Kelvins and the viscosity of the medium as *η*.

If a gas or liquid contains a large number of particles in its volume, they appear to be uniformly distributed throughout the volume.

4.1.3. Turbulent diffusion^[23]

Turbulent diffusion occurs at the macroscopic level in gas or liquid flow. This estimates the concentration field in a turbulent flow or in artificially agitated media that includes the statistics of the average concentration fields and the associated flows. Currently, the understanding of this diffusion is covered by semi-empirical models.

In addition, the total mass transfer has to take into account molecular diffusion such as that produced by eddies.

4.2. Convection^[24]

Convection is the process by which particles or heat are transferred through the velocity of a fluid. There are two types of convection:

- Natural convection is produced by the expansion of fluids when heated. In this way, a circulation is produced due to the effect of the increase in buoyancy, due to the decrease in the density of the fluid.
- Forced convection involves the transport of the fluid through movement produced by an external force.

4.3. Pollutant source

Most of the air pollutants come from artificial sources called pollutant source, among which we can distinguish between mobile sources or stationary sources. Only stationary sources are taken into account in this project.

There are two types of stationary sources, those called Major Point Sources that emit more than 10 tons of a single pollutant or more than 25 tons of various pollutants in a year, and those called Area Point Sources, which are the rest of the emissions.

4.4. Chemical reaction

The pollutants emitted by the source are called primary pollutants and then secondary pollutants are created in the lower atmosphere by means of chemical reactions. To determine the reaction rate of each species, in the first place it would be convenient to have an independent form of the reactants and products. In this way, a generic equation such as the one shown in Equation 4.2 is defined.



where a , b , c and d are the stoichiometry of the species defined as A, B, C and D.
That way, the reaction rate is defined in Equation 4.3.

$$-r_A = k c_A^m c_B^n \quad (4.3)$$

In this equation, r_A is considered as the reaction rate, k as the kinetic constant, c_A and c_B as the different concentrations of the reactants, and m and n as the different reaction orders for each compound.

Once the reaction rate of a certain reagent is obtained, the value for each of the species can be calculated as it can be seen in Equation 4.4.

$$r = -\frac{r_A}{a} = -\frac{r_B}{b} = \frac{r_C}{c} = \frac{r_D}{d} \quad (4.4)$$

5. THE NUMERICAL METHOD

The convection-diffusion equation, shown in Equation 4.1 in Chapter 4, cannot be solved analytically for most actual cases. Typically, powerful computers are used to approximate the solution of differential equations. Some of the methods used to solve differential equations numerically are the following:

- The finite volume method (FVM)^[25] evaluates and represents partial differential equations in the form of algebraic equations. This method consists of converting the volume integrals in a differential equation into surface integrals using the divergence theorem and is called "finite volume" because each node in a mesh is surrounded by a small volume.
- The finite element method (FEM)^[26] numerically solves differential equations that arise in engineering and mathematical modelling. This method consists of dividing a large system into smaller and simpler parts, using intermediate interpolations.
- The finite difference method (FDM)^[27] consists of the approximation of derivatives with finite differences, converting ordinary differential equations (ODE) or partial differential equations (PDE) into linear equations that can be solved using matrix algebra.

In this work, to solve the convection-diffusion equation, the finite volume method and the finite difference method will be used, since it is a conservative system. Below are more details to solve the equation.

5.1. The mesh generation

A computational mesh divides the space into cells, which are a representation of a large geometric domain using smaller discrete cells. This allows to discretize the partial differential equations into algebraic equations, which can then be solved.

To create a specific mesh to solve the convection-diffusion equation, it is necessary to choose the structure of the mesh, the cell shape and the grid layout. The options and the one chosen to solve the equations are detailed below.

The convection-diffusion equation can be solved for two or three dimensions. In this case, it will only be established for two dimensions to simplify the calculation and to be consistent with the information retrieved from meteorological databases, which do not provide data from the vertical component of the wind velocity.

5.1.1. Structure of the mesh

There are three types of mesh structures, which are the following:

- Structured grids have regular connectivity and are very efficient in terms of space, producing better convergence and high resolution.
- Unstructured grids have an irregular connectivity that makes it difficult to express it as a matrix, producing a very inefficient model in terms of space.
- Hybrid grids have a mix of structured and unstructured grids efficiently. In this way, the structural grid is used in the regions where the geometry is regular and the unstructured grid is used for the complex regions.

Figure 5.1.1 shows various representations of the different types of grids.

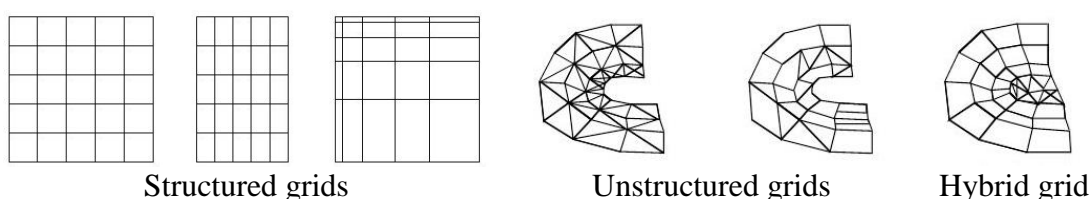


Figure 5.1.1. Types of grids.

To solve the convection-diffusion equation, a structured mesh will be used, since it is the most efficient and has the highest convergence.

5.1.2. Cell shapes

For two-dimensional cells there are only two shapes, which are the triangle and the quadrilateral. The triangle shape is quick and easy to create, although it is often used in unstructured meshes. In contrast, the quadrilateral shape is more basic and is more common in structured meshes. In this case, as a structured grid is going to be used, the best is to use the quadrilateral shape, specifically the square shape.

5.1.3. Grid layout^[28]

In order to solve the differential equations, there are two different ways to store the information in a mesh, which are the following:

- The collocated grid uses the same location on the grid to calculate all the variables. Mainly, it is used to solve in meshes with non-orthogonal shapes, but a special discretization has to be carried out to guarantee the non-singularity of the system.
- The staggered grid is so named because the components of the vectors (velocity in the current case) are staggered with respect to the scalars (concentration in this case), which is found at the centre of the cells. This method is the most common as it provides a non-singular discrete system.

Figure 5.1.2 shows a scheme of the two grid layouts in a square-shaped structured mesh.



Figure 5.1.2. Scheme of the grid layouts.

In this case, the staggered grid will be used to solve the convection-diffusion equation, since it is the most natural way since it is a convection-dominated dispersion.

5.2. Discretization method

In order to discretize the diffusion-convection equation, the finite difference method (FDM) is used, as mentioned above. Therefore, the derivatives with finite differences are approximated, converting the partial differential equation (PDE) into an algebraic equation. The general mathematical expression of the first derivative is shown in Equation 5.2.1, defined by the limit.

$$f' = \lim_{z \rightarrow 0} \frac{f(x+z) - f(x)}{z} \quad (5.2.1)$$

If in the previous equation there is a fixed value, different from zero, of the variable z then it can be described as Equation 5.2.2.

$$f'(x) \approx \frac{f(x+z) - f(x)}{z} \quad (5.2.2)$$

For higher order equations, approximations can be obtained. Using the central difference for a second-order derivative, Equation 5.2.3 is obtained.

$$f''(x) \approx \frac{\frac{f(x+z) - f(x)}{z} - \frac{f(x) - f(x-z)}{z}}{z} = \frac{f(x+z) - 2f(x) + f(x-z)}{z^2} \quad (5.2.3)$$

As detailed in section 5.1.3, a staggered grid is used, since the wind velocity is stored on the sides of the mesh squares while the concentration is in the centre, as shown in Figure 5.2.1. For that reason, the upwind differencing scheme is used. This is the most used method in CFD for convection-diffusion problems, especially for strong convective flows such as in this case^[29].

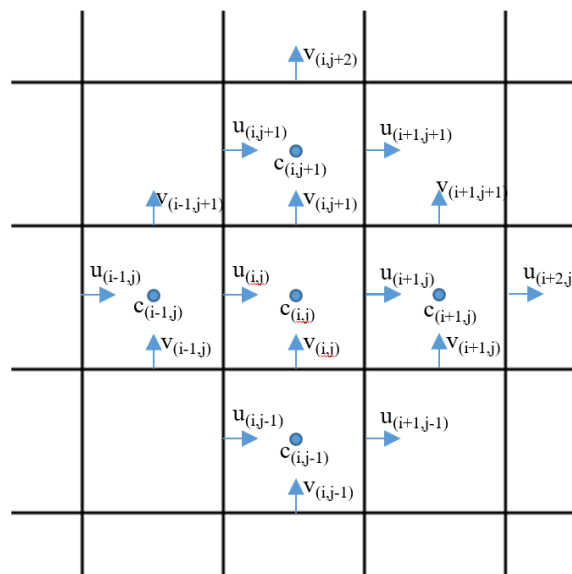


Figure 5.2.1. Scheme of how variables are stored in a staggered grid.

To solve the convection-diffusion equation, the upwind differencing scheme takes into account the direction of the flow. As it is solved for two dimensions, four possible scenarios are presented and each has a different discretized equation.

- When the velocity is positive for both axes, Equation 5.2.4 is used.

$$\begin{aligned} \frac{c_{new}(i,j) - c_{old}(i,j)}{\Delta t} = & D \left(\frac{c_{old}(i+1,j) + c_{old}(i-1,j) - 2c_{old}(i,j)}{\Delta x^2} + \right. \\ & \left. \frac{c_{old}(i,j+1) + c_{old}(i,j-1) - 2c_{old}(i,j)}{\Delta y^2} \right) - \left(\frac{u_{(i+1,j)} c_{old}(i,j) - u_{(i,j)} c_{old}(i-1,j)}{\Delta x} + \right. \\ & \left. \frac{v_{(i,j+1)} c_{old}(i,j) - v_{(i,j)} c_{old}(i,j-1)}{\Delta y} \right) + S + R \end{aligned} \quad (5.2.4)$$

- When the velocity of the x-axis is negative while that of the y-axis is positive, Equation 5.2.5 is used.

$$\begin{aligned} \frac{c_{new}(i,j) - c_{old}(i,j)}{\Delta t} = & D \left(\frac{c_{old}(i+1,j) + c_{old}(i-1,j) - 2c_{old}(i,j)}{\Delta x^2} + \right. \\ & \left. \frac{c_{old}(i,j+1) + c_{old}(i,j-1) - 2c_{old}(i,j)}{\Delta y^2} \right) - \left(\frac{u_{(i+1,j)} c_{old}(i+1,j) - u_{(i,j)} c_{old}(i,j)}{\Delta x} + \right. \\ & \left. \frac{v_{(i,j+1)} c_{old}(i,j) - v_{(i,j)} c_{old}(i,j-1)}{\Delta y} \right) + S + R \end{aligned} \quad (5.2.5)$$

- When the velocity of the x-axis is positive while the velocity of the y-axis is negative, Equation 5.2.6 is used.

$$\begin{aligned} \frac{c_{new}(i,j) - c_{old}(i,j)}{\Delta t} = & D \left(\frac{c_{old}(i+1,j) + c_{old}(i-1,j) - 2c_{old}(i,j)}{\Delta x^2} + \right. \\ & \left. \frac{c_{old}(i,j+1) + c_{old}(i,j-1) - 2c_{old}(i,j)}{\Delta y^2} \right) - \left(\frac{u_{(i+1,j)} c_{old}(i,j) - u_{(i,j)} c_{old}(i-1,j)}{\Delta x} + \right. \\ & \left. \frac{v_{(i,j+1)} c_{old}(i,j+1) - v_{(i,j)} c_{old}(i,j)}{\Delta y} \right) + S + R \end{aligned} \quad (5.2.6)$$

- When the velocity is negative for the two axes, Equation 5.2.7 is used.

$$\begin{aligned} \frac{c_{new}(i,j) - c_{old}(i,j)}{\Delta t} = & D \left(\frac{c_{old}(i+1,j) + c_{old}(i-1,j) - 2c_{old}(i,j)}{\Delta x^2} + \right. \\ & \left. \frac{c_{old}(i,j+1) + c_{old}(i,j-1) - 2c_{old}(i,j)}{\Delta y^2} \right) - \left(\frac{u_{(i+1,j)} c_{old}(i+1,j) - u_{(i,j)} c_{old}(i,j)}{\Delta x} + \right. \\ & \left. \frac{v_{(i,j+1)} c_{old}(i,j+1) - v_{(i,j)} c_{old}(i,j)}{\Delta y} \right) + S + R \end{aligned} \quad (5.2.7)$$

These equations cited above are conservative and robust. This is due to the fact that transportivity is integrated in the formulation of the discretization through the flow direction and because the coefficients of the discretized equations are always positive, thus they do not produce instability in the solution.

5.3. Boundary conditions

Finally, to solve the convection-diffusion model, boundary conditions must be applied. In this case, the Neumann boundary conditions are used. These conditions specify that the normal derivative at the boundary is has a given value. This is true in the computational domain studied, since it is assumed that the flow is fully developed at the boundaries. For this reason, the concentrations at the boundaries of the domain are equal to the neighbouring cells within the domain, that is, a zero-gradient boundary condition.

5.4. Interpolation method

To extract values from the wind velocity for the entire mesh, an interpolation method must be used because there are values retrieved from weather stations only at some points on the mesh.

The two most common methods to perform an interpolation within the Python language with one of its most common modules, SciPy, for scientific computing are Griddata and RBF (Radial Basis Function).

These two methods are good at producing correct output from a sparse data input and support large dimensions, but what sets them apart is that Griddata is a linear interpolation that takes the surrounding values and RBF maintains the symmetry of the data from input causing less noise when the data is sparse. For that reason, RBF has been chosen as the interpolation method for the code.

RBF interpolation is an advanced method that interpolates using the weighted sum of radial basis functions, such as Gaussian distributions. Also, it does not need to be in a structured mesh and can interpolate high-dimensional spaces.

6. COMPUTATIONAL TOOL FEATURES

For the simulation of pollutant dispersion, which solves the convection-diffusion equation, two operation modes have been implemented in the code: the first one consists of a continuous emission of pollutant and the second one is an instantaneous emission. These are detailed in the following sections.

First, the code asks which model the user wants to use for the simulation of pollutant dispersion, in this way, it chooses the option desired by the user. Subsequently, it asks how many pollutants the user wants to study, since the code allows the simultaneous calculation of several pollutants.

For each species introduced in the code, the required information is extracted into a file in .csv format. This must include the focus of the source, which is where the pollutant will be emitted, with its coordinates in decimal degrees of longitude and latitude, the amount that is emitted, the diffusion coefficient and the area of emission of the pollutant, to normalize the emission using the relationship shown in Equation 6.1.

$$S_{normalized} \left[\frac{kg}{m^3 s} \right] = S \left[\frac{kg}{m^3 s} \right] \cdot \frac{A_{source} [m^2]}{A_{mesh\ cell} [m^2]} \quad (6.1)$$

where $S_{normalized}$ is the normalized source term, S is the source term, A_{source} is the focus area, and $A_{mesh\ cell}$ is the area of a mesh cell.

But before moving on to the simulation, a pre-treatment of data entered in the code is done. First, the longitude and latitude range to be studied in meters is entered. Subsequently, the step increment through the mesh is indicated, for the x and y axis, and then with that the number of steps available in the mesh is calculated. The refinement of the mesh is determined and discussed in the next chapter (Chapter 7).

The entered distances are transformed to decimal degrees using the approximation shown in Equation 6.2.

$$longitude_{[decimal\ degrees]} = longitude_{[km]} \frac{1[decimal\ degrees]}{111.1\ km} \quad (6.2)$$

where $longitude_{[decimal\ degrees]}$ is the domain distance in decimal degrees and $longitude_{[km]}$ is the domain distance in km.

6.1. Continuous pollutant source

One of the operation modes is the constant emission of one or more pollutants in the air. This, as its name suggests, consists of a continuous emission of pollutant into the air. For this reason, the part of the pollutant source, S , of Equation 4.1 of Chapter 4 is taken into account.

In the first place, in order to simulate the system, the user is asked if a pollutant is present in the air. In the event that no pollutant is found, the initial concentration is set to zero. On the other hand, if pollutants are present, the information from the National Air Quality Index must be collected and entered into a file in .csv format. This file must include the coordinates of the stations where the information has been collected and their concentrations. The code then proceeds to the location of the coordinates on the mesh and subsequently creates an interpolation to estimate the concentration throughout the mesh. Those interpolated values are used as the starting concentration.

Once this concentration is available, the quantity emitted from the source focus and the extracted data are used to introduce them in the corresponding positions in the mesh.

Then the simulation is carried out knowing how long it has been since the incident and how long the emission lasts, previously requested from the user.

Once the simulation is performed, the tool generates .csv format files with the concentrations of each pollutant in various simulation times, shows and stores a graph of the final concentrations in the form of contour maps and shows and stores a graph of the vectors wind velocity. These results are shown on a georeferenced map of the region of interest.

6.2. Instantaneous source

Another model is that of an instant source. In this way, the pollutant source of the convection-diffusion equation is not taken into account since it is only a quantity of pollutant that is emitted instantaneously in one or more sources.

To perform the simulation in this operation mode, the source focus is interpreted as the instantaneous emission of pollutant, which can be greater than one. In addition, it is interpreted that initially there is no pollutant present in the air, only the instantaneous emission.

Then, the emission sources are placed in the corresponding positions within the mesh and the simulation is carried out knowing how long it has been since the incident and how long the emission lasts, previously requested from the user.

Once the simulation is performed, the tool generates .csv format files with the concentrations of each pollutant in various simulation times, shows and stores a graph of the final concentrations in the form of contour maps and shows and stores a graph of the vectors wind velocity. These results are shown on a georeferenced map of the region of interest.

6.3. Web scraping

Velocity is needed to calculate the convection term of Equation 4.1, shown in Chapter 4. In order to add it to the code, three different options have been used: one is a constant velocity for the entire domain, another one is an imported velocity for certain points and, finally, the last and most important one is the velocity extracted from the AEMET (Agència Estatal de Meteorologia) website.

The latter is the most important, because it uses the updated velocity of the AEMET website. The code uses this method by default and requires a file in .csv format from which it imports the number of weather stations and the web page addresses of each of them. Then it enters each of the stations and stores the wind information for each hour of the last 24 hours in files in .csv format, which do not have the name of the station but its identifier.

Once the information is in the files, the user is asked how many hours have passed since the emission. From this data, the velocity and direction of the wind in each of the stations along with their coordinates are extracted.

Then, the values are placed inside the mesh and an RBF (Radial Basis Function) interpolation is performed, previously explained in Section 5.4 of Chapter 5, to obtain the air velocity at each point of the computational mesh. With these values, the simulation is calculated during the period that is equivalent to one hour and once this has elapsed, the wind velocity and direction are obtained for the following hour and the interpolation process is repeated to obtain the new velocity at each point. This procedure is repeated continuously every hour until the end of the simulation.

In the event that the simulation time is longer than the entered hours that have elapsed since the emission, then the process of downloading the information given from the AEMET website is carried out again.

6.4. Reactivity of components in air

Sometimes one or more reactions in air occur sporadically. For this reason, the reaction part of Equation 4.1 of Chapter 4 is taken into account. The user is first asked if the environment is reactive. The calculation process is only changed if the answer is yes, which then takes into account the reaction term of the convection-diffusion equation. Then an editable file in .csv format is required, containing the stoichiometry, the order of reaction of each species, the molecular mass and the kinetic constant for this reaction. The molecular mass is required because the calculations are made in SI units, in kg/m^3 , and the rate constant is obtained so that the concentrations are in mol/m^3 . Then, all this data is entered into the code and the system is simulated in the same way.

7. MESH INDEPENDENCE TEST

This section shows the mesh independence test for the two operation modes mentioned above. Several distances between the cells of the mesh were taken into account for a computational domain of 100km in length by 100km in latitude.

7.1. Continuous source

First, the continuous emission mode was studied. It was concluded that in order to compare the meshes, the source should be normalized, since a certain amount must come out of the source cell and a concentration determined by an area higher or lower than the real one is not equivalent. In this way, the source is determined as Equation 4.1 of Chapter 4.

For the continuous emission, two significant studies were carried out: one at a certain constant velocity throughout the mesh and the other with a profile of air velocity.

The one of the constant velocity in the whole mesh was carried out twice changing the velocity in the axis of the x and the concentration was observed after 10000 s in a determined coordinate within the dispersion of pollutant. Figure 7.1.1 and 7.1.2 show the results obtained for each study.

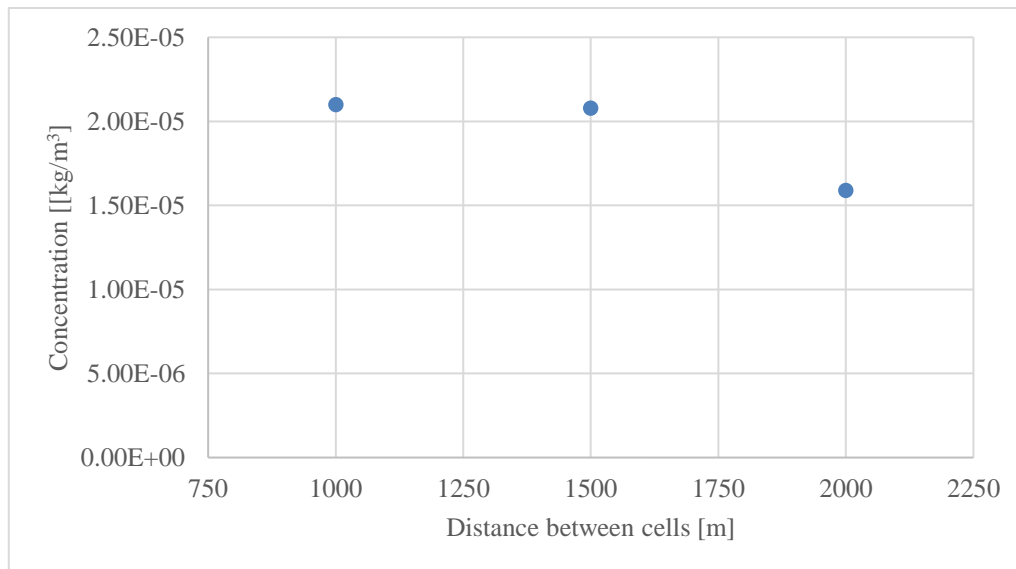


Figure 7.1.1. Concentrations obtained for the study carried out with constant x and y axis velocity of 10 m/s and 1.6 m/s, respectively.

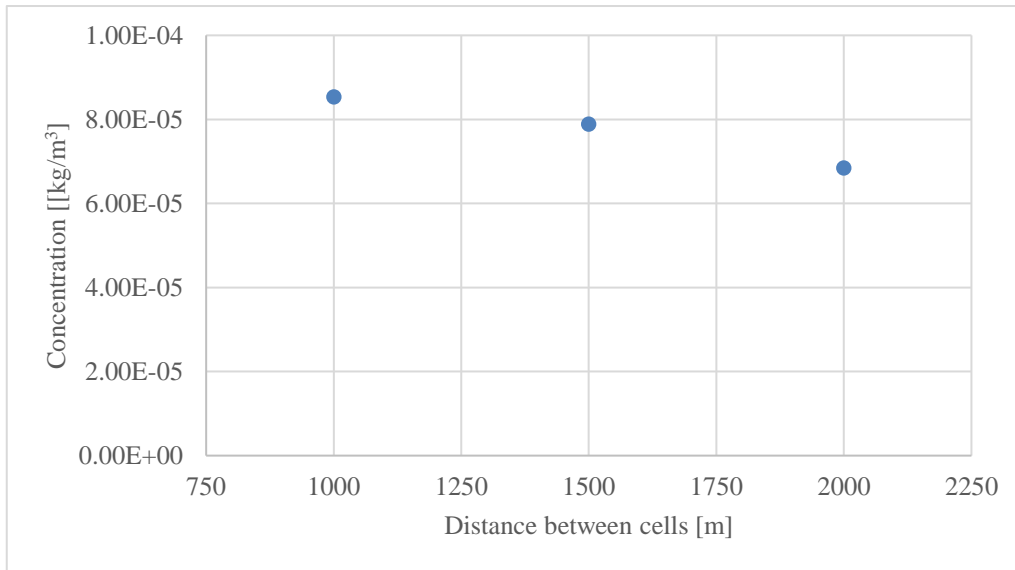


Figure 7.1.2. Concentrations obtained for the study carried out with constant x and y axis velocity of 1 m/s and 1.6 m/s, respectively.

In the previous graphs it can be seen that the concentrations follow the same trend, since the concentrations obtained from the distances between cells of 1 km and 1.5 km are similar values, while the one obtained for the distance of 2 km differs from the others.

To check whether the mesh can be considered independent, another study is carried out with a non-constant air velocity profile along the entire mesh. In addition, it has been considered opportune to use more values of distances between cells of the mesh and to observe a point close to the emission focus to check if the concentration values follow the same trend. For this study, a simulation of 11000 s is carried out and the results are shown in Figure 7.1.3.

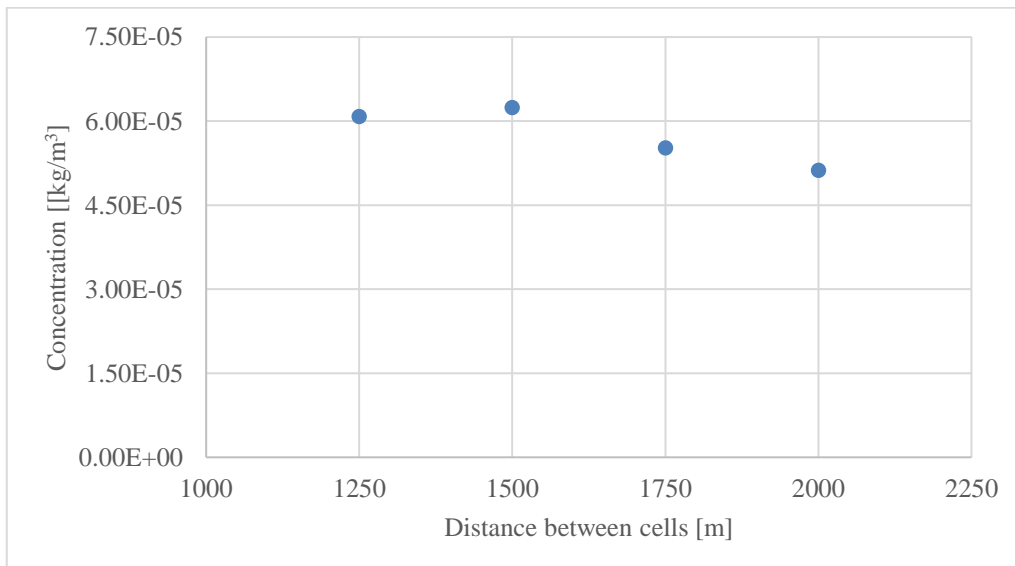


Figure 7.1.3. Concentrations obtained in the study carried out with a certain velocity profile.

As in the two previous cases, the stability of the mesh can be considered from a distance of 1.5 km between cells of the mesh, since the difference in concentrations obtained at this distance and a smaller one is not significant.

For this reason, it is considered that the appropriate distance between cells is 1500m, since from this distance it can be considered that the mesh is independent. But in the same way, a study was carried out when an emission was instantaneous to see if the same thing happened.

7.2. Instantaneous source

To validate that an independent mesh is obtained, a study was carried out for an instant source. For this, a simulation of 200 s with an emission of 1 kg/m^3 was carried out and the concentrations of a point close to the emitting focus were studied. Figure 7.2.1 shows the concentrations obtained at the focus for three different distances.

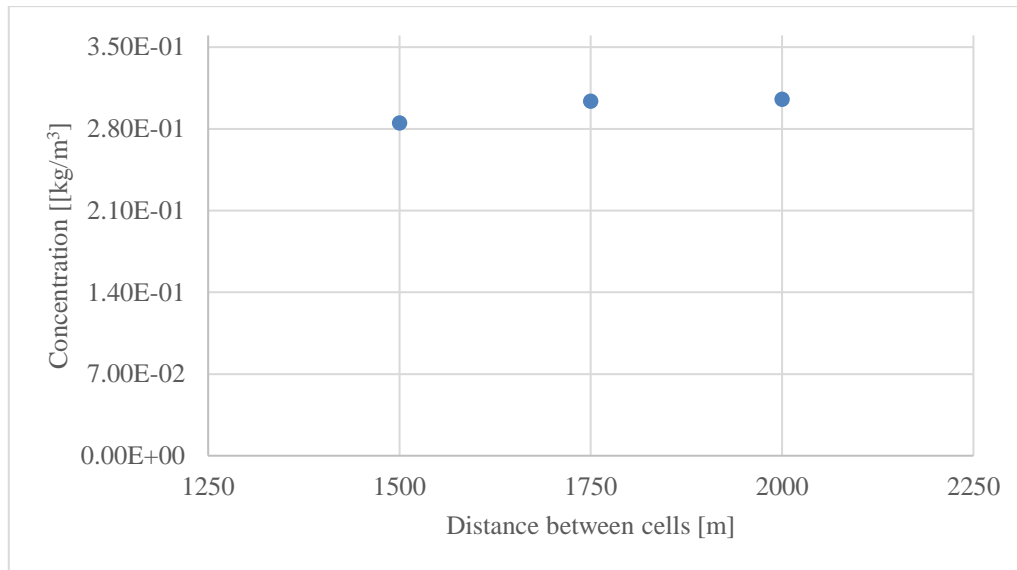


Figure 7.2.1. Concentrations obtained at the focus in various mesh steps.

As can be seen in the figure above, the study concentrations at 1750 m and 2000 m are practically the same, although they do not differ from that obtained for 1500 m.

For this reason, it can be concluded that the distance between cells of the 1.5 km mesh is sufficiently precise for simulations of contaminant dispersion.

8. RESULTS

To validate the code results, two simulations have been carried out, one without chemical reaction and another one with chemical reaction, and they have been compared with the data available for the La Palma eruption.

It has been decided to compare it with this case because it has been a very important event during 2021. The Cumbre Vieja volcano has broken the record^[30] of the island of La Palma in the Canary Islands because it has been the longest eruption in the last 500 years, which has been of 85 days. This has caused the devastation of many houses due to the lava and the eviction or prevention of many people due to the gases and ashes emitted by the volcano.

This volcano has a crater area^[31] of 30.778 m² and has emitted approximately 50.000 T of sulphur dioxide^[32] (SO₂) per day. In addition, it is estimated that there were 2 million m³ of magmatic chamber^[33]. Then, with these values, the constant emission was estimated and entered in the .csv file for subsequent treatment of data.

The two simulation studies are carried out on December 3 from 8:00 a.m. to 11:00 a.m. In this case, as several days had passed since the start of the eruption, an initial concentration of SO₂ was found throughout the island of La Palma. The specific concentrations throughout the island are not available, but there are data from fixed and mobile stations, installed during the eruption of the volcano, and their specific coordinates. These data are extracted from the National Air Quality Index of Spain and entered into a file created by default, which will be treated with the code to perform an interpolation to obtain the concentrations throughout the entire mesh.

On December 3, the wind data was extracted from the AEMET website using the code and stored to later study how the chemical reaction interfered. With these values, the interpolated velocity field shown in Figure 8.1 was obtained.

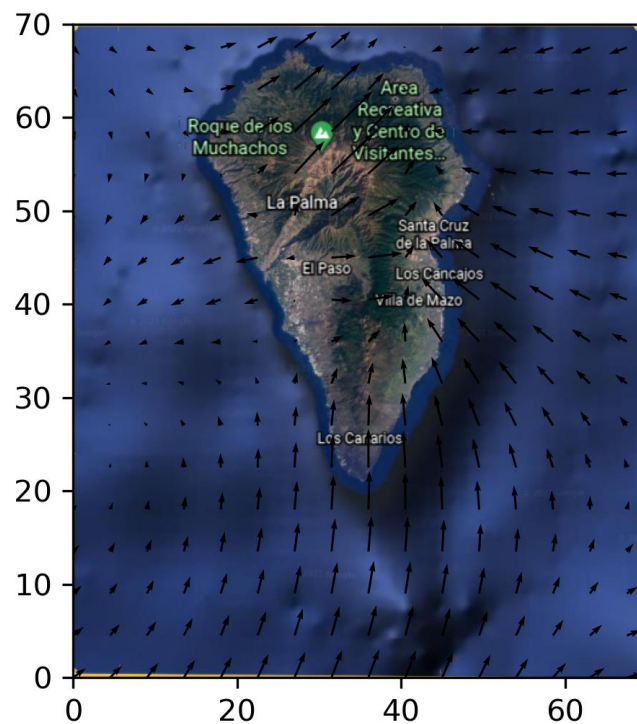


Figure 8.1. Interpolated velocity field for the simulation of La Palma.

The figure above shows a topographical map of the island of La Palma with the velocity field, which has two dimensions for the entire domain. This is because the data acquired from weather stations does not include the vertical component of wind velocity.

8.1. Case study: La Palma without reaction

The first case study carried out was the simulation of SO₂ dispersion without chemical reaction. Taking into account the information mentioned above and that no reaction occurs, the simulation of 10800 s has been continued for only one pollutant. The results obtained are shown in Figure 8.1.1, where the concentration contours for SO₂ are shown at 11 a.m.

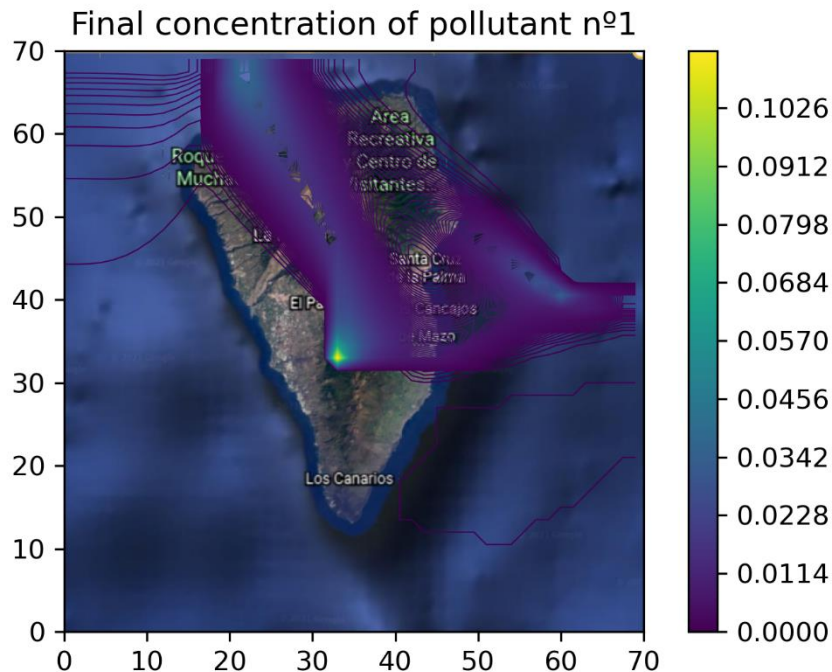


Figure 8.1.1. Contours of sulphur dioxide concentrations in ppm obtained in the simulation of La Palma.

As can be seen in the previous figure, the point of highest concentration is located at the source, since the volcano emits more SO₂ than can be dissipated with the wind. In addition, it can be seen that the contaminant is dispersing to the north-west and to the east due to the fact that it follows the wind trend, as can be verified by comparing it with the speed profile shown in Figure 8.1.

The pollutant dissipated towards the north-west, firstly disperses towards the north due to the high speed with a vertical direction and then slowly dissipates towards the north-west because the speed is reduced and there is a change in the direction of the wind. . Instead, the contaminant dissipated to the east is due to convection produced by the wind speed to the east from the south of the volcano's crater.

All this is because convection has a greater influence than diffusion for contaminant simulation. It must be noted, however, that turbulent diffusion is not included in the current version of the model.

In addition, to validate the results, it must be compared with the concentrations throughout La Palma. Figure 8.1.2 shows the National Air Quality Index of La Palma for December 3 at 11 a.m. and Figure 8.1.3 shows its legend (blue means good quality, green means reasonably good air quality, yellow means fair air quality, red means poor quality,

burgundy means there is a very unfavorable air quality and the violet means an extremely unfavorable quality).



Figure 8.1.2. Palma air quality index.

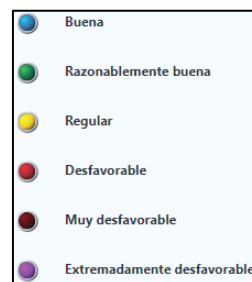


Figure 8.1.3. Legend of the National Air Quality Index

Comparing the concentrations obtained in the simulation, shown in Figure 8.1.1, and the air quality, shown in Figure 8.1.2, it can be seen that they are similar. The results obtained are in good agreement with the data available from La Fajana and Los Canarios, since practically no concentration of SO_2 is observed at those points. In addition, if the study is focused on the east coast, where three meteorological stations are located, it can be seen that the results from the simulation in the two points that would correspond to those in green there is practically no SO_2 and there is a higher concentration in Santa Cruz de la Palma. On the west coast, it can be seen that there is a high concentration of SO_2 , both in the simulation and in the National Air Quality Index.

However, the two central points near El Paso do not agree with observations so much. This may be due to the fact that the topography of the island is not taken into account during the simulation, as the retrieved wind data is two-dimensional. The different observed air quality in those two points which are so close may be explained by them being located at the different sides of a mountain ridge. Therefore, the code is not able to reproduce that behavior at his current stage of development as the third dimension will be needed.

8.2. Case study: La Palma with reaction

The second case study carried out was the simulation of SO_2 dispersion with chemical reaction. Taking into account the information mentioned above and that the reaction shown in Equation 8.2.1 occurs, the simulation of 10800 s has been carried out for two

pollutants, since the third is oxygen and it is considered that the concentration remains constant.



Once the stoichiometry of the reaction is obtained, the kinetic rate is needed, which is shown in Equation 8.2.2.

$$-r_A = k c_{SO_2} c_{O_2} \quad (8.2.2)$$

This reaction rate is determined by k , which as mentioned in Chapter 4.4 is the rate constant, and the concentrations of the two reactants. The reaction rate is of first order with respect to each reactant. The kinetic constant^[34] for this reaction has a value $1,30 \cdot 10^2$ L/(mol · s).

Once the simulation has been carried out, the concentration contours of SO_2 and SO_3 are obtained, which are shown in Figures 8.2.1 and 8.2.2, respectively.

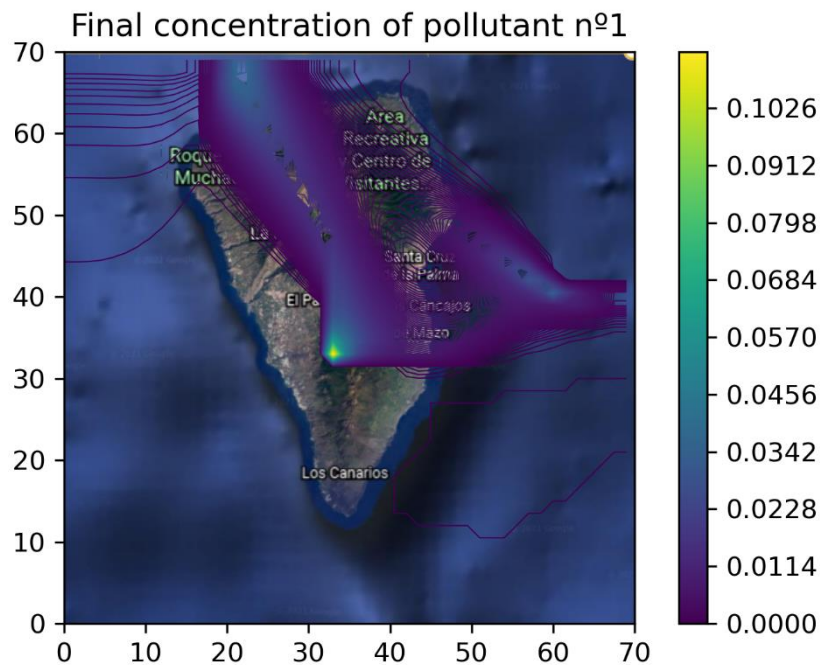


Figure 8.2.1. Contours for sulphur dioxide concentrations in ppm obtained in the simulation of La Palma.

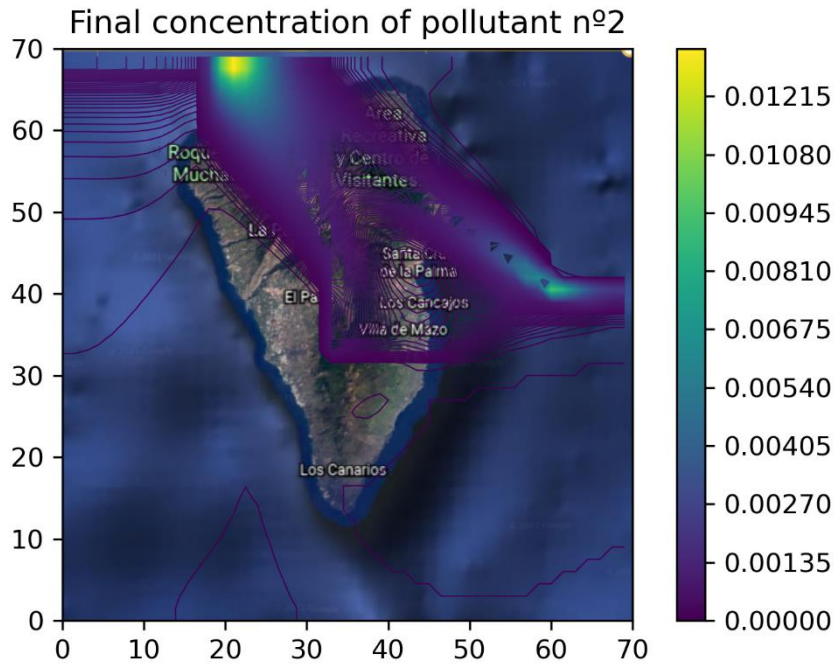


Figure 8.2.2. Contours for sulphur trioxide concentrations in ppm obtained in the simulation of La Palma.

If the two figures of sulphur dioxide obtained through the simulations with and without reaction are compared, Figures 8.1.1 and 8.2.1, it can be seen that they present very similar concentrations throughout the entire domain studied. In addition, looking at Figure 8.2.2, where the final concentration of sulphur trioxide is shown, it is seen that it has very small concentrations because the units of the colorbar are in ppm. The maximum concentration is one order of magnitude smaller than that of sulphur dioxide. This is due to the fact that the reaction in the atmosphere is quite slow, since the kinetic constant is not very high and there are not large amounts of SO_2 present in the air. On the other hand, if the concentration contour of SO_3 is observed, it is seen that it reacts over time and moves driven by convective forces. That is why the maximum concentration is at the northwest of the island.

9. CONCLUSIONS

A computation tool that predicts pollutant dispersion in air has been developed using the open source programming language Python3.8.8. It uses real time wind data from weather stations and incorporates that into the computation module which solves the convection-diffusion equation for a scalar transport. That makes the tool quick when compared to existing software for pollutant dispersion.

The tool uses web scraping techniques to download and extract meteorological data for the past 24 hours from the AEMET web page. This is used to set the wind velocity magnitude and direction in all the cells of the computational domain by using RBF interpolation. This same procedure is used to connect to a .csv file where the information from the National Air Quality Index is entered to process the pollutant concentration data and interpolate its values and use these as the initial field for the simulation.

The second module solves a two-dimensional convection-diffusion equation for a scalar transport. It is solved in two-dimensions because the data retrieved from weather stations does not include the vertical component of the wind velocity. The tool has several different operation modes: one or multiple pollutants, one or multiple emission sources, continuous or instantaneous emissions, with or without chemical reaction. The wind velocity is updated at the frequency provided by the weather stations.

Once the simulation is performed, the tool also generates and shows the results in a graphical form, with concentration contours maps for the pollutants and velocity vectors for the wind. These results are shown on a georeferenced map of the region of interest.

The eruption of the Cumbre Vieja volcano in La Palma has been used to validate the results provided by the code. This case was chosen because it has been a very important continuous emission of sulphur dioxide (SO_2) and the kinetics of formation of sulphur trioxide (SO_3), its secondary pollutant, is known. There is good agreement between the prediction and the reported data except for two points located at different sides of a mountain ridge. The fact that the code is in two dimensions prevents to take into account the effect of complex topography in pollutant dispersion. As a consequence, the code at its current stage is useful to quickly obtain pollutant concentration maps which are accurate in regions where topography is not too complex.

The code currently has no limits with the number of variables, since they are created based on the variables entered through data in the file in .csv format or by answering the questions that the user is asked via terminal. This way, it avoids future conflicts for the addition of a greater number of pollutants or more meteorological stations. The drawback is that many more loops are required to perform all the calculations and if the number of pollutants or the domain studied is increased, the calculation time increases significantly. One of the proposed future improvements would be to be able to communicate the language with C or Fortran to make it more efficient.

The tool is still a work in progress, as it needs some upgrades to be more complete and reliable. Mobile sources of pollutants could be added providing another interesting future. This way it would be possible to model the pollution of the different types of transport and study how these emissions interfere with air quality.

Another improvement that could be made is the implementation of a graphical interface where the insertion of the necessary initial data would be more intuitive and user friendly, since currently there are two forms of information input available. One is from files in .csv format and the other one is from questions asked via Python console. This could be a bit confusing for users who are not familiar with computational codes.

In order to reproduce the results visually, a graphic representation of the area studied is added behind the contour lines of the concentrations. Currently, this image of the area

is added manually so that if the coordinates are changed, it is not modified. Although it has been studied, an efficient way has not been found for adding this image depending on the coordinates automatically. Being able to upgrade that feature would be an important improvement for the next version of the tool, as that will make the tool useful for any region.

As the case study of the Cumbre Vieja volcano in La Palma has shown, an area of improvement in terms of accuracy is the inclusion of the three-dimensional effect, as the results are not as good when the complexity of the topography increases. Different ways to deal with this are being considered, but the premise is that the code will still need to be fast enough when running.

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Appendices

APPENDICE 1. SELF-EVALUATION QUESTIONNAIRE (TO BE COMPLETED BY THE STUDENT)

a) Evaluate the acquired **competences** according to the **tasks** you have carried out.

Degree Competences		Task in which you have observed the competence	Self evaluation [Rank 1 to 10]	Aspects to be improved
SPECIFIC COMPETENCES				
A1.1	Effectively apply knowledge of basic, scientific and technological materials pertaining to engineering.	In the design of the contaminant dispersion tool because knowledge of computational fluid mechanics is used.	8.5	
A1.2	Design, execute and analyze experiments related to engineering	In developing the tool, designing it to improve its effectiveness and testing it to determine its validity.	9.0	
A1.3	Be able to analyze and synthesize the continuous progress of products, processes, systems and services, whilst applying criteria of safety, economic viability, quality and environmental management. (G6)	The tool is used to predict the dispersion of pollutants and, for this reason, it is capable of analyzing the evolution of pollutants in the air for environmental management. In addition, it allows it to be marketed, since there is no application that automatically interacts with meteorological data to reduce computation time.	9.0	
A1.4	Know how to establish and develop mathematical models by using the appropriate software in order to provide the scientific and technological basis for the design of new products, processes, systems and services and for the optimization of existing ones. (G5)	To obtain the simulation tool for the dispersion of contaminants in air, discretization models have been developed for the convection-diffusion equation. In addition, Python has been used as software to solve the equations.	8.5	
A2.1	Be able to apply the scientific method and the principles of engineering and economics to formulate and solve	The designed tool calculates the dispersion of contaminants in the environment, therefore it calculates how the	8.5	

	<p>complex problems that arise in processes, equipment, installations and services, in which the material undergoes changes to its composition, state or energy content, these changes being characteristic of industrial chemistry and other related sectors such as pharmacology, biotechnology, materials sciences, energy, food and the environment. (G1)</p>	<p>contaminant spreads in the air. In addition, it has been added to be able to simulate chemical reactions that occur in the atmosphere and in this way the concentrations of the various pollutants in the air are obtained and shown.</p>		
A2.2	<p>Conceive, project, calculate and design processes, equipment, industrial installations and services in the field of chemical engineering and related industrial sectors in terms of quality, safety, economics, the rational and efficient use of natural resources and the conservation of the environment. (G2)</p>	<p>In order to conserve the environment, it is possible to predict how a contaminant is dispersed in a leak or an emission and thus apply corrective systems, if necessary. In addition, as the time is reduced because the dynamic field is not calculated, but rather meteorological data is extracted from the web.</p>	8.5	
A2.3	<p>Lead and technically and economically manage projects, installations, plants, companies and technological centres in the ambit of chemical engineering and related industrial sectors. (G3)</p>	<p>Not part of my project</p>	-	
A3.1	<p>Apply knowledge of mathematics, physics, chemistry, biology and other natural sciences by means of study, experience, practice and critical reasoning in order to establish economically viable solutions for technical problems (I1).</p>	<p>The mathematical development to discretize the convection-diffusion equations through the upwind method to obtain a conservative resolution, the application of the chemical reaction and the use of a velocity field created from web scraping to obtain an economically viable tool,</p>	9.0	

		since the cost computational is very low.		
A3.2	Design and optimize products, processes, systems and services for the chemical industry on the basis of various areas of chemical engineering, including processes, transport, separation operations, and chemical, nuclear, electrochemical and biochemical reactions engineering (I2).	The tool has been improved to include weather data automatically from the web and no error occurs if no data is available for a particular weather station. In this way, it reduces the computational cost and the data pre-treatment cost.	9.0	
A3.3	Conceptualize engineering models and apply innovative problems solving methods and appropriate IT applications to the design, simulation, optimization and control of processes and systems (I3).	In order not to create a dependency on the previously defined input variables, it has been established that the number of variables is created automatically from the user's responses.	9.5	
A3.4	Be able to solve unfamiliar and ill-defined problems by taking into account all possible solutions and selecting the most innovative. (I4)	I adapted to working remotely and was able to develop the contaminant dispersion tool using code.	10	
A3.5	Lead and supervise all types of installation, process, system and service in the different industrial areas related to chemical engineering (I5).	Not part of my project	-	
A3.6	Design, construct and implement methods, processes and installations for the integrated management of waste, solids, liquids and gases, whilst also taking into account the impacts and risks of these products (I6).	Not part of my project	-	
A4.1	Lead and organize companies and	Not part of my project	-	

	production and service systems by applying knowledge and abilities regarding industrial organization, commercial strategy, planning and logistics, mercantile and labour legislation, and financial and costs accounting (P1).			
A4.2	Lead and manage the organization of work and human resources by applying criteria regarding industrial safety, quality management, occupation risk prevention, sustainability and environmental management (P2).	Not part of my project	-	
A4.3	Manage research, development and technological innovation whilst ensuring the transfer of technology and taking into account property and patent rights (P3).	Making a document explaining the instructions of the tool and checking that all the libraries used were freely accessible, in addition to checking if they could be marketed.	8.0	
A4.4	Adapt to structural changes in society caused by economic, energy or natural factors so as to be able to solve any resulting problems and to contribute technological solutions with a high commitment to sustainability (P4).	The tool monitors the concentration emitted by one or more sources instantly or continuously over time. In this way, the quality of the air in the continuous areas of the emitting focus can be predicted.	9.5	A mobile emission focus could be added.
A4.5	Lead and monitor the control of installations, processes, products, certification, auditing, verification, testing and reports (P5).	In the validation of the tool taking into account the volcanic eruption of La Palma.	9.0	
A5.1	Carry out, present and defend (once all the curriculum credits have been obtained) an original individually	I have not yet presented or defended the project before the university tribunal.	-	

	produced piece of work before a university panel. The work will consist of a professional integrated Chemical Engineering project that synthesizes (TFM1)			
TRANSVERSAL COMPETENCES				
B1.1	Communicate and discuss proposals and conclusions in a clear and unambiguous manner in specialized and non-specialized multilingual forums (G9).	Holding weekly meetings with my supervisor to discuss the status of the project and ideas to implement. Also in an internal meeting of Eurecat to comment on the evolution of the project before its closure.	9.5	
B1.2	Adapt to changes and be able to apply new and advanced technologies and other important developments with initiative and entrepreneurial spirit. (G10)	Troubleshooting is caused by some Python functions or some mistakes made by me without realizing it.	9.0	
B2.1	Lead and define multidisciplinary teams that are able to make technical changes and address management needs in national and international contexts. (G8)	Not part of my project	-	
B3.1	Work in a team with responsibilities shared among multidisciplinary, multilingual and multicultural teams	I presented the tool obtained to the aiRECAT team, which is part of a larger project.	8.5	
B4.1	Be able to learn autonomously in order to maintain and improve the competences pertaining to chemical engineering that enable continuous professional development. (G11)	I learned the languages used by Python and by Octave, although not much of it, on my own.	9.0	
B5.1	Carry out and lead the appropriate research, design and development of engineering solutions	Not part of my project	-	

	in new or little understood areas, whilst applying criteria of creativity, originality, innovation and technology transfer. (G4)			
B5.2	Bring together knowledge, make judgements and take decisions on the basis of incomplete or limited knowledge whilst taking into account the social and ethical responsibilities of professional practice. (G7)	Not part of my project	-	
NUCLEAR COMPETENCES				
C1.1	Have an intermediate mastery of a foreign language, preferably English	English	7.0	
C1.2	Be advanced users of the information and communication technologies	Using it in online meetings by Teams and in written communications, either by Teams or by email	10	
C1.3	Be able to manage information and knowledge	The direct application of all the obtained information and knowledge for the creation of the simulation tool.	9.5	
C1.4	Be able to express themselves correctly both orally and in writing in one of the two official languages of the URV	Weekly meetings with my supervisor and a presentation to the aiRECAT project team.	9.5	
C2.1	Be committed to ethics and social responsibility as citizens and professionals	I have practically worked online and when I went to work I used FPP-2 masks due to the current COVID situation.	10	
C2.2	Be able to define and develop their academic and professional project	The simulation tool has been carried out and at the end the improvement of the chemical reaction has been applied.	9.5	

b) Evaluate the final master project and suggest improvements.

Key steps	Evaluation [Mark 1 to 10]	Improvement proposed
Selection/assignment of the project (dissemination, communication, assignment requirements...)	9.5	The truth is that the requirements were well defined in the document uploaded in Moodle and they resolved some doubts during the interview that they asked me, having very fluid communication at all times.
Stay (welcome, length, relationship, follow-up made by the company...)	10	I have had a very pleasant stay and a very good relationship with my supervisor. In addition, I consider that the follow-up of my work has been very good, since I had weekly meetings and in case I had any questions or problems, they always tried to help me.
Follow-up made by URV tutor	9	The URV tutor guided me in the use of CPython and some libraries, although in the end they could not be applied due to lack of time.
Other aspects to be considered (which ones...)		I have no other aspect to consider.