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Numerical simulation of atmospheric pollutants dispersion in an urban environment

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Abstract: The results of different CFD simulations looking to diagnose and predict the concentration of pollutants in an urbanized area are presented in this paper. Two simulation engines were used to cover the considered domain, being the main one an incompressible flow solver called caffa3d.MBRi, providing a more precise and detailed concentration field in the considered subdomain. As a secondary solver, a Gauss Plume Dispersion program was used to take into account the pollution of the sources outside the small (caffa) domain. Moreover, in-situ air quality measurements where taken in order to compare against the simulated results when considering the current emission rates. Furthermore, predictions on the level of pollution when changes in technlogies are applied were also computed, reaching interesting results.

Keywords: Computational Fluid Dynamics, Air Quality, Finite Volume, Scalar Transport.

1 Introduction

In highly populated urban areas, the exposure to air pollutants may increase significantly due to the generation of poor air dispersion conditions, given by the characteristic microclimate and the reduction of natural ventilation caused by the urban topography. There are many different studies concerning the dispersion of pollutants in urban landscapes, which include a wide variety of emissions, such as the ones produced by industrial plants [1], the use of wood for domestic heating [2], traffic in highly urbanized areas, also known as street canyons [3, 4], etc. In cities with a considerable amount of traffic, despite the different sources of emissions, the pollution is dominated by vehicular emissions according to [5], moreover, for some pollutants this may not necessarily be the case. Despite many improvements in fuels and technologies, atmospheric pollution is still responsible for many negative effects on human health [3, 6], therefore, many pollutants have strict regulations concerning different exposure time. Moreover, different energetic politics are being proposed all over the world in order not only to diversify the energetic matrix and reduce expenses, but also to control the environmental impact of traditional sources and technologies, thus making the study of the possible consequences of said politics relevant when planning them.
The aim of this paper is to present the results of CFD simulations in which different pollutants as well as sources are considered at the same time, including residential, vehicular and industrial emissions, in an urbanized area of the city of Montevideo. Furthermore, different pollution rates were simulated to recreate changes in the technologies involved in the emissions in order to study the effect of such improvements on the air quality.
Sections 2 presents the simulations done, describing the different tools used as well as the selection of the domain and the sources considered on it, and the representation of them in the simulation engines. Section 3 explains the in-situ measurements done in order to compare with the simulation results, while in Section 4 different results are depicted, leading to the final conclusions drawn in Section 5.

2 Simulation Setup

2.1 Solvers

Two solvers were used to recreate the pollutant concentration in an specific domain, being the main reason for doing this the existing computational limitations to simulate big domains with high levels of precisions. So a CFD solver using the finite volume method was used to simulate the main small domain while a Gaussian dispersion code was used to account for the pollution inside the small domain caused by the sources existing outside it.

The CFD solver used is caffa3d.MBRi [7, 8], an open source, finite volume code, with second order accuracy in space and time, used to simulate three-dimensional incompressible flows in block structured curvilinear grids. The program counts with MPI parallelization, a key feature in the study case, different turbulence models, being LES the one used for the simulations, and an immersed boundary method module allowing to represent complex geometries without using an intricate grid. Last but not least, the program has the capacity to compute the scalar transport of passive tracers, method used to compute the concentration of the different pollutants.

On the other hand, the pollution caused by the emissions outside the small domain was estimated by a program that uses a Gaussian Dispersion method [9, 10], using statistical data in order to get a mean concentration field over a certain period of time. The results reached through this solver were taken into account as a background concentration caused by the outer emissions in the main domain.

2.2 Simulation Domain

The selected simulation area is a residential and industrialized neighbourhood of Montevideo city, Uruguay. In that area two main state industries are included and also many smaller ones, making it an interesting area to study air quality. What is more, one of the main entrances to the city goes right through it accounting for important vehicular emissions. Also, a residential neighbourhood is located inside said area, thus including residential emissions to the simulations.

The domains for each solver were chosen accordingly to their capabilities, and the possibilities to evaluate the results in the domains. Therefore, a small box domain of 1km x 1km x 0.2km was selected for caffa3d.MBRi, because of its computational limitations. The box location was chosen upon the inclusion of different sources and most important the existence of an air quality station in the area, in order to compare some results and validate the model.

On the other hand, a bigger domain of 4.4km times 5km, which includes the previous one was used when computing the background concentration with Gauss. Even though, the small domain is included in the big one, the emissions of it are not considered when computing the background concentration as it is explicitly computed with caffa3d.MBRi.

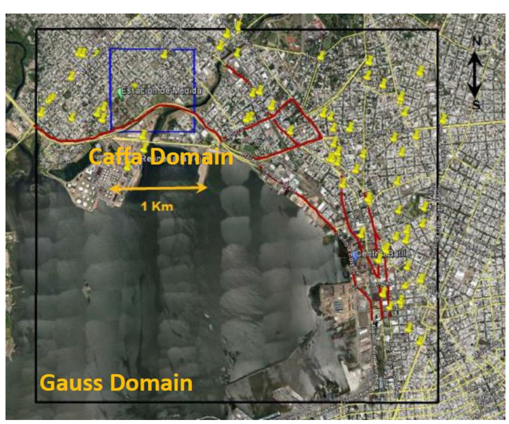

Figure 1: Selected domains with the sources considered. Yellow markers are punctual sources, red lines are linear sources considered. The blue square is the caffa domain, while the one in black is the Gauss domain.

Once the domains were selected, the different sources had to be considered, listing the particular emissions in the domains, and choosing the streets with the biggest amount of traffic to include those sources, resulting in a map with different emissions to be included in each solver (see Figure 1).
When creating the domain for the CFD solver (caffa3d.MBRi), the selected area was divided in 64 regions, in order to assign one core to each one of them. Every region consists on one block divided in 98x98x98 cells having close to one million cells per region. The cells are distributed in an orthogonal coordinate system, having the same horizontal dimensions, while having a height depending on how close to the ground they are, an exponential increasing height is used in order to have better resolution close to the ground so as to accurately represent the boundary layer. Moreover, the topography of the terrain is considered, giving the domain an starting height different to zero, and an upper height of 200 meters.
While the topography of the terrain is considered when constructing the grid the roughness is not, mainly because of the difficulty this may result in. The roughness in this case, consisting of the urban environment, is represented with Immersed Boundary Conditions [11]. This method loads a patch that describes the roughness explicitly and imposes a given speed inside said patch, giving a great flexibility in terms of preparing the domain as there is no need for heavy regridding when changing the domain. Consequently, the topography and the patch had to be developed in the study area giving the possibility to change the domain easily, (see Figure 2 and 3).

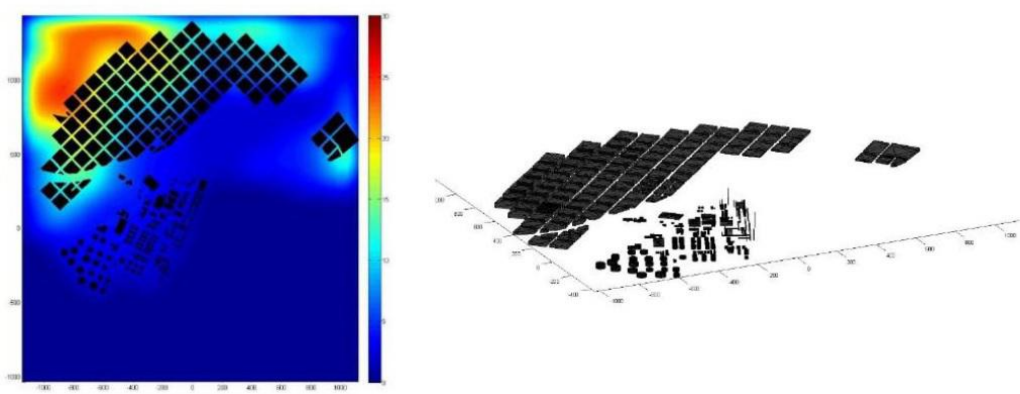

Figure 2: Ground level height colormap with the patch used to describe the urban environment seen from above (left), and panoramic view of the patch (right). The origin of coordinates is located at Lat: $34^o52'32.50"S$ and Long: $56^o13'38.04"O$.

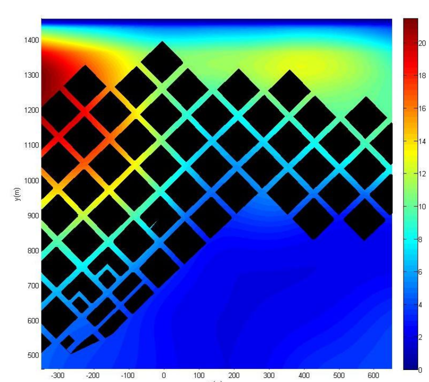

Figure 3: Domain used for the simulation, with ground height (m) colormap and patch seen from above.

The Figure above shows that the patch that defines the Immersed boundary Conditions has a certain distance from the North boundary condition, this was done in order not to disrupt the incoming flow, even though there are buildings in that area. However, the emissions of those houses is taken into account.

On the other hand, the domain simulated with the Gauss Dispersion solver, is divided by the program itself, using a Quadtree method, refining the mesh when needed, in order to get better precision when computing the concentration fields.

2.3 Flow Conditions

After defining the domain, one has to impose the boundary conditions in order to get the desired flow. In the study case the conditions were determined based on historic data of the considered period. Given that the simulation is supposed to describe the pollutant dispersion of August of 2016, the most common wind condition of that month was chosen. So a Northern wind with a mean speed of 1.7 m/s was simulated, value taken from in-situ measurements done.
In order to reach a proper Atmospheric Boundary Layer (ABL), auxiliary blocks were used, this technique consist on using an extra domain with periodic boundary conditions and a force in order to reach the desired speed (see Figure 4). This outer domain runs for a warm-up period of time in order to get an appropriate ABL. Afterwards, both domains run together using the profile of the auxiliary blocks as the inlet profile in the main domain. This Boundary Condition is implemented on every timestep, using CrossBlock Boundary Conditions.
Once both domains start running together they must run with no emissions for some timesteps so as to get the accurate flow conditions.

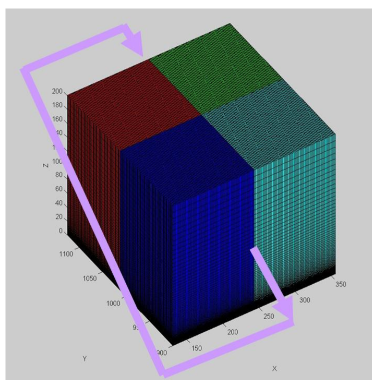

Figure 4: Auxiliary blocks with periodic conditions to generate the wanted inlet conditions.

As far as the Gauss solver is concerned, the flow conditions are loaded from serial measurements from the study period, meaning every wind velocity is considered, thus giving an average concentration field that works as the background pollution.

2.4 Tracer Dispersion Computation

In order to compute the pollutant dispersion a passive scalar transport module was used, which, according to its name, treats the pollutants as passive tracers, meaning they are only influenced by diffusion and advection. The aforementioned module was modified in several ways in order to have the capabilities to achieve two main goals, having the possibility to work with different pollutants at the same time and including all kind of sources, punctual, linear and superficial ones.
As far as the amount of tracers to compute is concerned, some modifications were done, adding the possibility to select the amount of tracers to compute as input data of the simulation meaning no recompilation is needed if the number of tracers needs to be changed. Moreover, as each tracer is independent of the next one, one could simulate the same tracer under different emission conditions on the same run.
Regarding the types of sources to consider, various approaches were taken, mainly concerning the linear emissions that correspond to vehicles. First of all, punctual emissions are due to industrial or services chimneys with a known emission rate and location, this sources are computed as spheres around the chimney, computing the sources in the cells which fall into said sphere, in this case the emission per cell is distributed proportional to the volume of each cell. Secondly, the linear emissions were once computed as the punctual

ones, that is behaving as many punctual emissions in a row, but were then upgraded so as to represent a prism of a certain height and width around a straight line segment, this sources are also distributed between the cells inside that prism proportional to the volume of each cell, and having a total emission proportional to the length of the segment (the street). Additionally, the emissions corresponding to domestic heating have to be taken into account, and they are by adding a superficial emission. This emission is computed above the houses in the domain by selecting points to define a convex polygon, adding a source term to every cell inside said polygon at a certain height with an emission rate proportional to the top area of the cell.
All the information needed to assign an emission to each cell was compacted in an input file containing the number of sources, the geometrical parameters and the emission rates of each source for every tracer. As the emission rates had to be known, data had to be collected. For the punctual ones, each business was consulted, for the linear emissions the amount of cars going through a certain spot were counted so as to relate that to the emission data of the street. And in order to get the superficial emission rates statistical data about the number of chimneys per squared meter was used to get an emission rate proportional to the area.
Furthermore, apart from the scalar transport module, a module to compute statistical values was included so as to get the mean concentration over a period of time. This was added mainly because most of the regulations existing to control the pollution levels are averages over a certain period of time. So once this modules are implemented, the instant and mean concentration of each pollutant are available on every cell of the domain providing the user with a great amount of information.

3 Air Quality Measurements

In order to get the pollution levels in the domain, a measurement station was installed above a public high school at an approximate height of 5 meters above ground. The location was chosen based on availability and then it was used to determine the already mentioned domain so as to allow comparison between simulation results and field data.

Figure 5: Station location in the map (left), station installed on the roof of the building (right). The coordinates of the station are Lat: $34^o 52' 06.38''$ and Long: $56^o 13' 47.09$.

As seen in figure 5, south to the station ANCAP's refinery can be found and in between them the national route $N^o 1$ goes through.
During the time measurements were taken, two different equipment were used. The first two month the station used was capable of measuring the temporal evolution of the concentration levels of total suspended particles (TSP), PM_{10}, $PM_{2.5}$, O_3 and NO_2, beside weather parameters such as wind speed and direction, temperature and humidity. This station determines the concentration of pollutants using photometry, and

stores the values with a pre-established frequency.
The rest of the time a different equipment was used, a nephelometer that automatically measures and registers the environment concentration of (TSP), PM_{10}, $PM_{2.5}$ or PM_1, in the air, being able to register only one pollutant at a time. Given that one of the most important emissions to consider, mainly due to domestic heating, is PM_{10}, it was the one measured with this equipment. Furthermore, this station can collect particulate matter in a filter, allowing to calibrate the measurements taken with the nephelometer, which was done at the measurement site, prior to the monitoring campaign.
Given that the simulation represents the emissions and meteorological conditions on August 2016, the data from the first station was used, considering in this project only the weather data and the PM_{10} concentration. Having measuring all the values with the same instrument, correlation between the different parameters could be reached. Figures 6, 7 and 8 show some of the collected data.

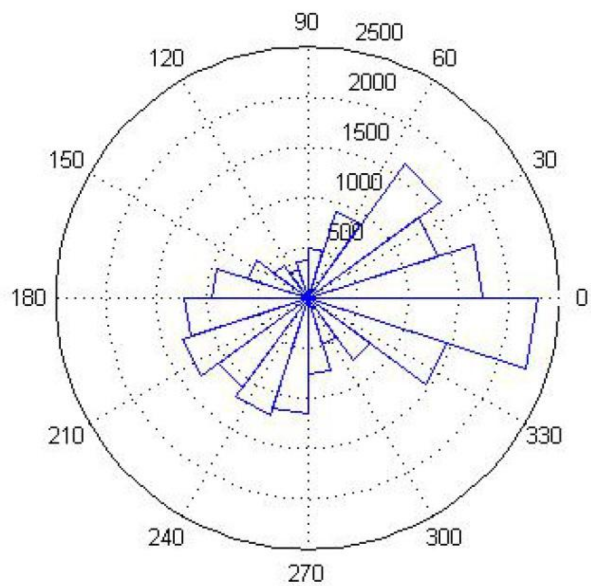

Figure 6: Windrose for August 2016, 0^o being North direction.

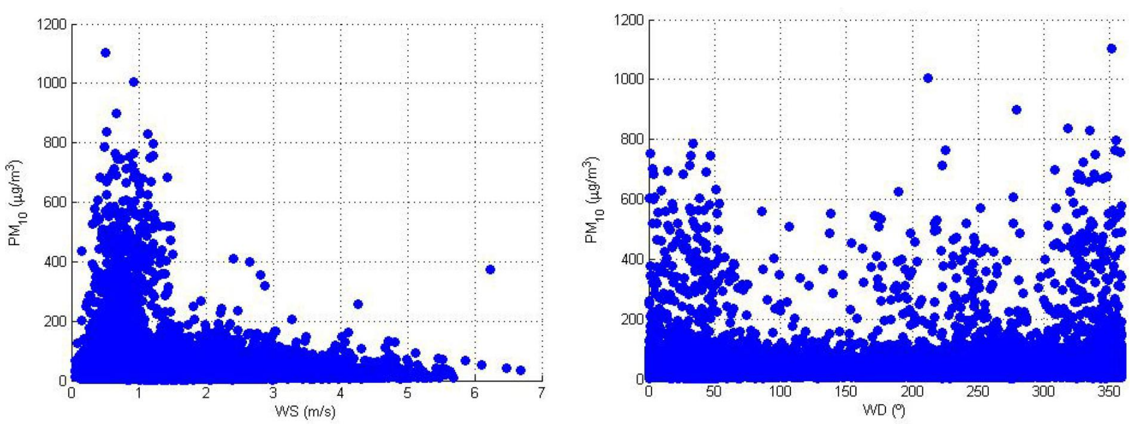

Figure 7: PM_{10} concentration against wind speed (left), and PM_{10} concentration against wind direction, 0^o being North direction (right).

As can be seen in Figure 6, the main wind direction is the Northern one, having also the greatest amount of high PM_{10} concentrations as Figure 7 shows, this can be explained due to the fact that North from the station there is an important residential neighbourhood, which emits PM_{10} when using heaters. Moreover,

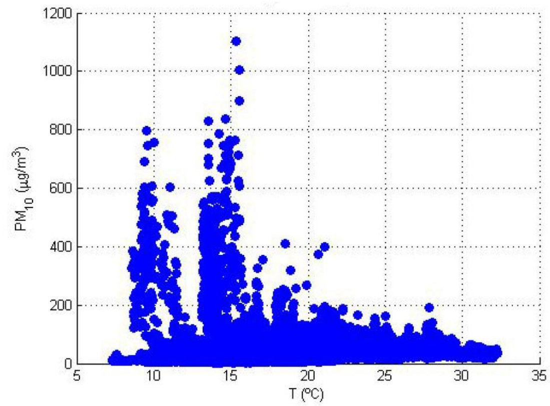

Figure 8: PM_{10} concentration against temperature.

there is a rise in concentration when low temperatures are reached (Figure 8), also explained by the fact that domestic heaters are the main sources of PM_{10}.
From the measurements taken some statistical data was determined, having a mean concentration of PM_{10} of $40.5\mu g/m^3$, and an standard deviation of $61.5\mu g/m^3$, for the whole month data. However, given that the simulations done consider only Northern wind, a sub-population was considered. Using only the data with a wind direction of $0^o \pm 10^o$ and a wind speed between 1.6 m/s and 2.0 m/s, a mean concentration of PM_{10} of $31.8\mu g/m^3$, a median of $26.1\mu g/m^3$, and a standard deviation of $26.2\mu g/m^3$ were reached. The speed interval was taken from the values gotten from the simulation.

4 Results

4.1 Simulated Scenarios

Once the program was developed different simulations were done, changing the emission rates between one another. First of all, the current situation was simulated in order to determine the concentration of four different pollutants: CO, NO_x, $PM_{2.5}$ and PM_{10}. Those were chosen due to having the highest emission rates on different sources, either linear or superficial. However, not all of them emit on every source, having the following distribution:

Emission Source	CO	NO_x	$PM_{2.5}$	PM_10
Punctual	Yes	Yes	No	Yes
Linear	Yes	Yes	Yes	No
Superficial	Yes	Yes	No	Yes

Table 1: Emission sources considered depending on the pollutant.

After this initial simulation was completed, another one was done looking for the concentration of those pollutants when changes in technology are introduced. Two main improvements were taken into account, firstly, a change of half the heaters to high efficiency ones in residences, having an important reduction of the superficial emission rates of CO and PM_{10}, secondly, converting a 15% of cars to electric ones and a 5% of the public transport to electric as well. This last scenario has a direct impact on the linear emission rates of CO, NO_x and $PM_{2.5}$. So in order to simulate this, five tracers were considered, two of them to represent CO and PM_{10}, when changes in domestic heating are implemented, changing only the superficial emission rates, and the other three tracers account for CO, NO_x and $PM_{2.5}$, when some vehicles are converted to electric ones, changing only the linear emission rates of those pollutants.

4.2 Current Scenario

Using the assumed emissions for the current situation, a concentration field for each pollutant was reached, making possible a wide variety of analysis. One of the most important aspects to evaluate is the concentration at ground level given that it is the one assumed to affect pedestrians. In Figure 9 the instant concentration of the pollutants can be seen.

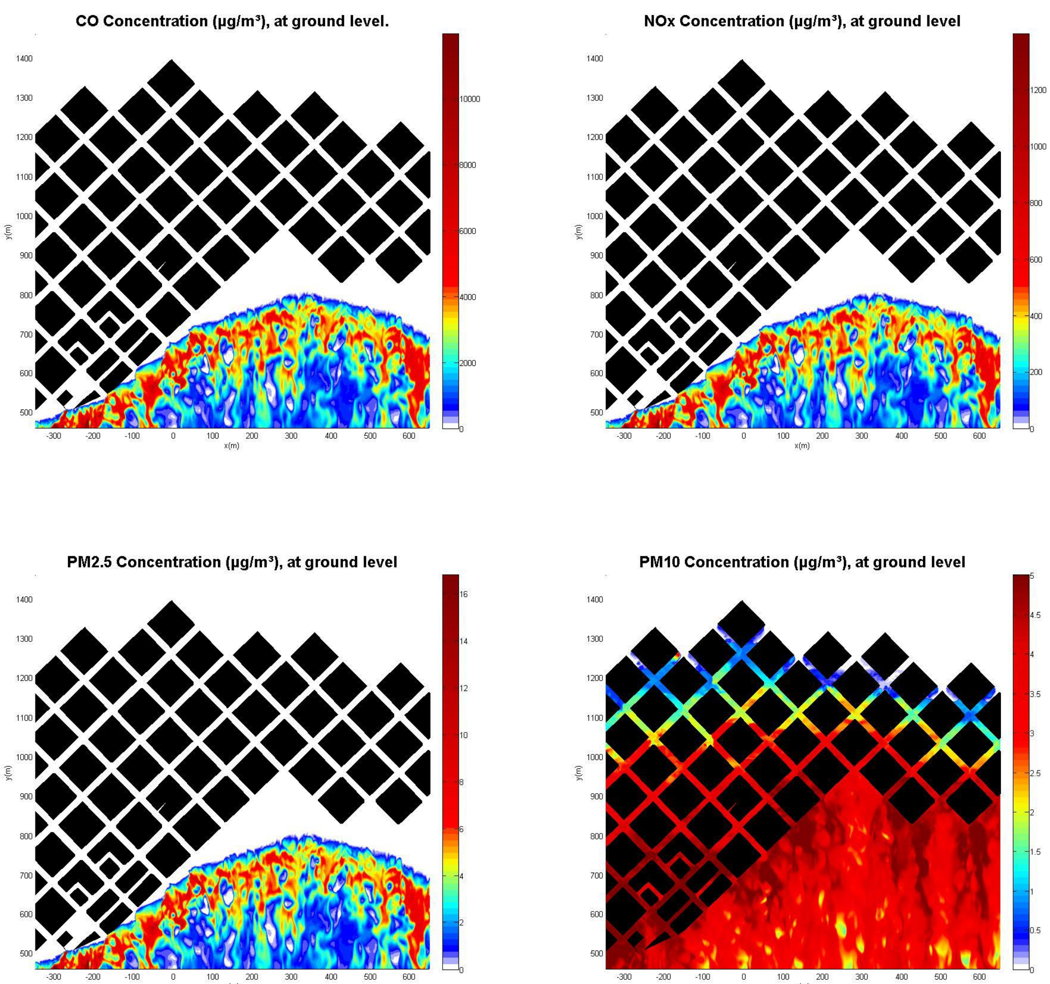

Figure 9: Pollutants instant concentration at ground level.

As the pictures above show, the first three tracers, ($CO, \quad NO_x, \quad PM_{2.5}$), have a very similar concentration field with a difference only in the scale, this is due to having vehicular emissions, which override the other sources. On the other hand, PM_{10} concentration has a totally different field, given that the main source is superficial, having a more uniform field with lower concentrations. Another aspect to point out is that the pollutants with vehicular emissions have a small area of impact, downstream from the source (the route). Also it can be seen the maximum concentrations reached at that moment for each field, $MAX(CO) = 12000\mu g/m^3$, $MAX(NO_x) = 1400\mu g/m^3$, $MAX(PM_{2.5}) = 17\mu g/m^3$ and $MAX(PM_{10}) = 5\mu g/m^3$. This values are reached in very few points, mainly in the first three tracers, and thus will be reduced when the mean concentration over time is computed, resulting on the field being smoothed.

The mean concentration was then computed during 1800 timesteps, representing 1800 seconds or half an hour. So the values reached are the mean concentration over said period of time, and can be seen in Figure 10.

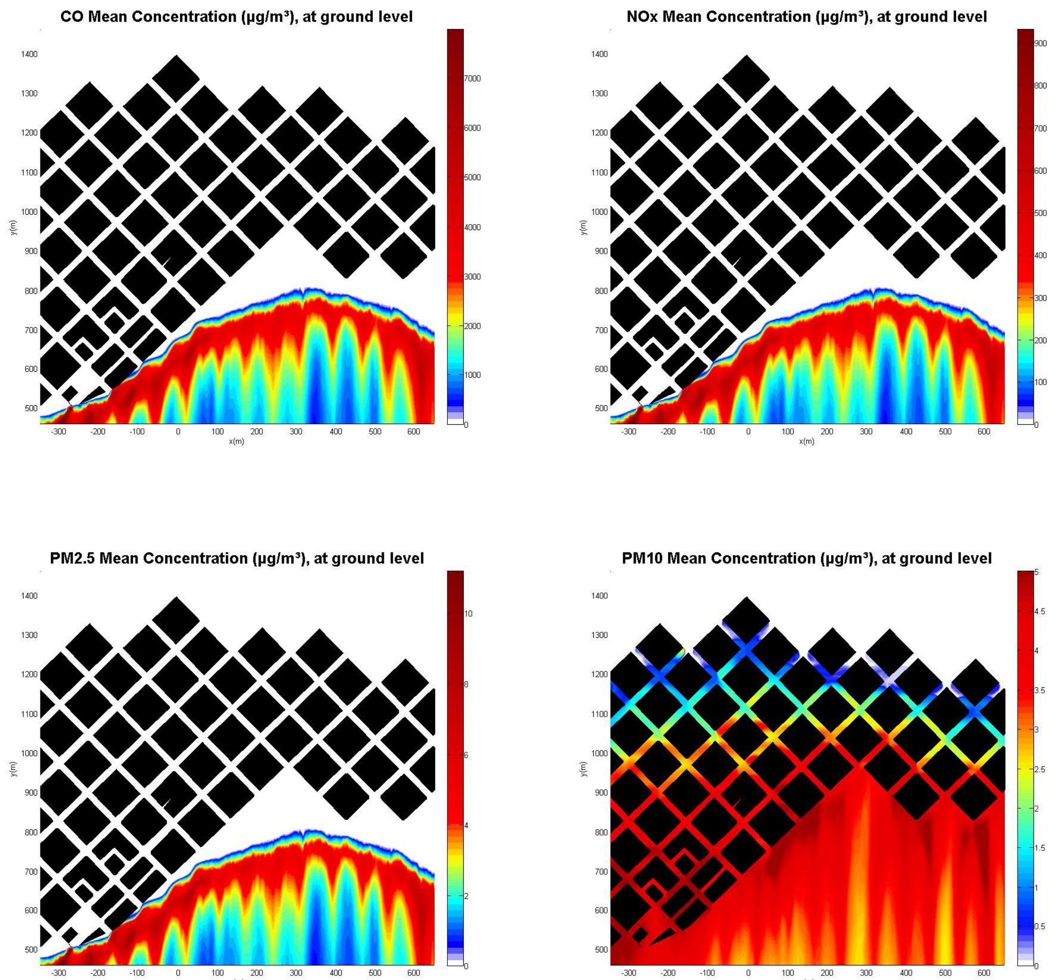

Figure 10: Pollutants mean concentration at ground level.

As predicted the mean concentration fields are smoother than the instant ones, and the highest concentration have decreased, reaching the following values $MAX(CO) = 8000\mu g/m^3$, $MAX(NO_x) = 910\mu g/m^3$, $MAX(PM_{2.5}) = 11\mu g/m^3$ and $MAX(PM_{10}) = 4.5\mu g/m^3$.
Also from this images it can be concluded that at ground level even when taking time averages the vehicular emissions are far more important than the residential emissions. Furthermore, it can be appreciated that for the first three tracers the amount of pollution decreases when one gets further from the source, while in the residential emissions the highest concentrations at ground level are reached downstream from the sources, which can be explained by the fact that those emissions are at around 6 meter from the ground, while the vehicles are much closer to it.

Another interesting behaviour to see is the concentration variation with height, Figure 11 shows the instant and mean concentration of CO at 3m and 6m.

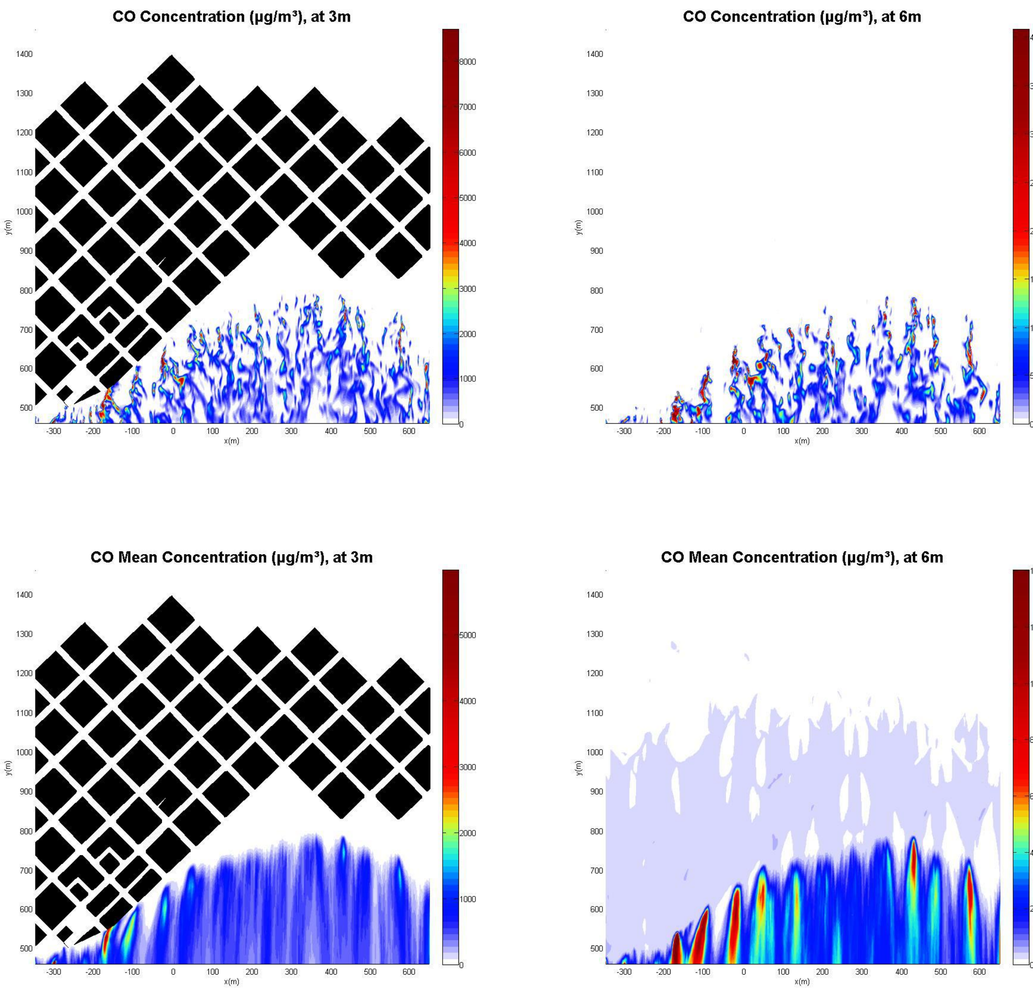

Figure 11: CO Concentration (instant and mean), at different heights (3m and 6m).

It can be appreciated that the instant CO concentrations at those heights does not resembles the one at ground level having a more random distribution on the impact area with lower maximums. Moreover, at 6 meters height, the field seems to be at a souther location than the one at 3 meters, being coherent with the flow conditions (Northern wind). On the other hand, when the mean concentrations are studied, a higher concentration can be seen above the route, meaning that overall the concentration is higher right above the emission. In addition to this, it can be seen that at 6 meters the residential emissions become important when computing the mean concentration as a shadow can be seen upstream from the source. This happens probably because of the decrease in the concentration due to vehicles emissions and the closeness to the residential ones. However, this phenomenon can not be appreciated with NO_x, probably because of having a higher ratio between the linear emission rates and the residential ones.

Given that the PM_{10} has a concentration field that covers most of the domain, some other analysis can result appealing, such as a concentration field on a longitudinal cut of the domain (Figure 12).

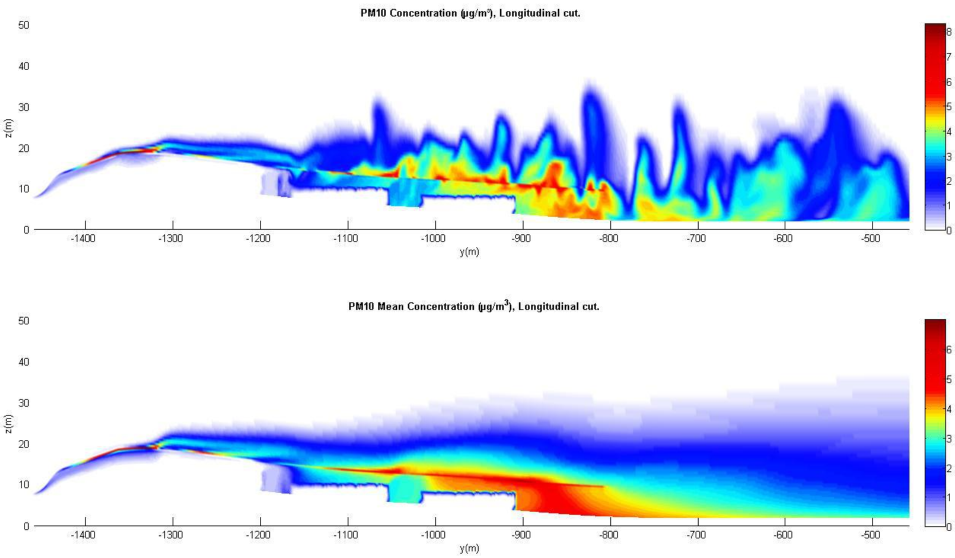

Figure 12: PM_{10} Concentration (instant and mean), longitudinal cut.

This pictures show the affected zone in terms of height, allowing to determine the maximum affected height, around 40 m above ground. Moreover, it can be seen the effect of averaging over time as many of the peaks present in the instant concentration are smoothed and the long term affected region can be identified, being the area downstream from the buildings close to the ground. Furthermore, the line with strong concentration that can be seen in both images corresponds to where the emissions take place.
Apart from the two dimensional cuts a tridimensional view can be obtained for a certain concentration, revealing a dispersion plume (Figure 13).

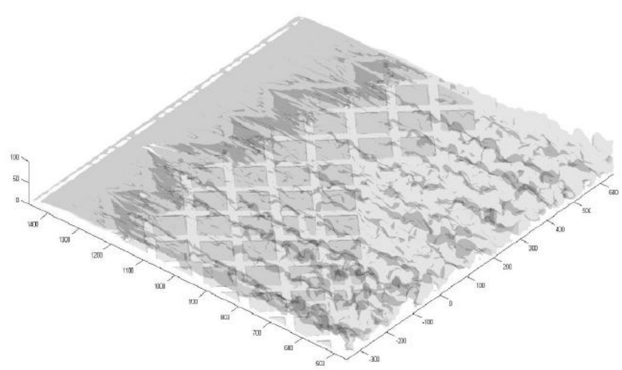

Figure 13: PM_{10} dispersion plume with a concentration of $1 \mu g/m^3$.

In this last figure the role of turbulence can be appreciated, as the plume develops along the flow direction.

Last but not least, the comparison between the simulation and the measured values can be made. In order to do so, the concentration of PM_{10} was calculated at a height similar to the one from the station. The concentration fields of PM_{10} at 6 meters can be seen in Figure 14.

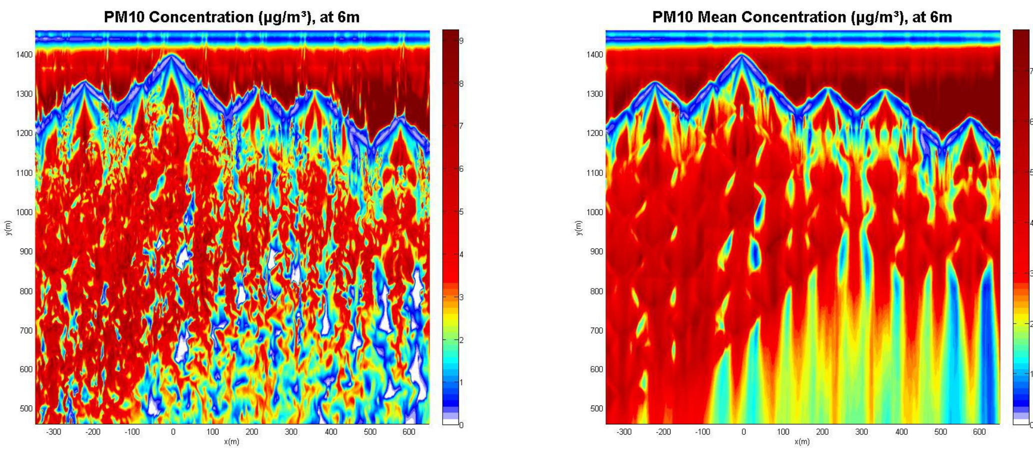

Figure 14: PM_{10} Concentration (instant and mean), at 6m above ground.

Once again the effect of time averaging can be seen, allowing the user to get a more representative value of the concentration at a certain point. A decrease in the concentration can also be appreciated at the start of the domain given that the emissions are instantly dragged by the incoming wind. Using the averaged field a value was reached for the PM_{10} concentration in the zone around the air quality station, $3.83\mu g/m^3$. In order to get the concentration from the whole tool, the background concentration has to be included, this one corresponds to the one computed with Gauss and has a value of $0.3\mu g/m^3$ for that location, having a total concentration of $PM_{10} = 4.13\mu g/m^3$ at the station.
As mentioned before, the values measured at the station for the weather conditions simulated were a mean concentration of PM_{10} of $31.8 \pm 26.2\mu g/m^3$ (standard deviation of $26.2\mu g/m^3$), and a median of $26.1\mu g/m^3$. Even though, this values are bigger than the one obtained from the simulation, they are still close in terms of order, and the computations are done based on bibliography emission rates that could differ from the real ones. Furthermore, when simulating, the neighbourhood up North from the domain is not taken into account by any of the solvers, meaning the amount of pollution due to that area is not considered. With this in mind, the values reached are satisfactory, and point that a bigger area should be considered for future simulations.

4.3 Future Scenarios

4.3.1 Domestic Heating Improvement

As far as the residential emissions are concerned, the main change implied by the improvement in the domestic heating situation is in the emission rates of CO and PM10, having a reduction of 19.1% and 18.3% respectively, when half the heaters are changed to high efficiency ones. So, in order to be able to evaluate the environmental impact of said improvement, a simulation was done using the reduced rates. Due to the time it takes to run the simulations, only the PM_{10} mean concentration was reached and the comparison between those results and the current situation can be seen in Figure 15.
When comparing the concentration fields one can clearly appreciate the impact of the change in technology, as the high concentration areas in the current scenario, have a lower concentration (around 20% less) in the new scenario.

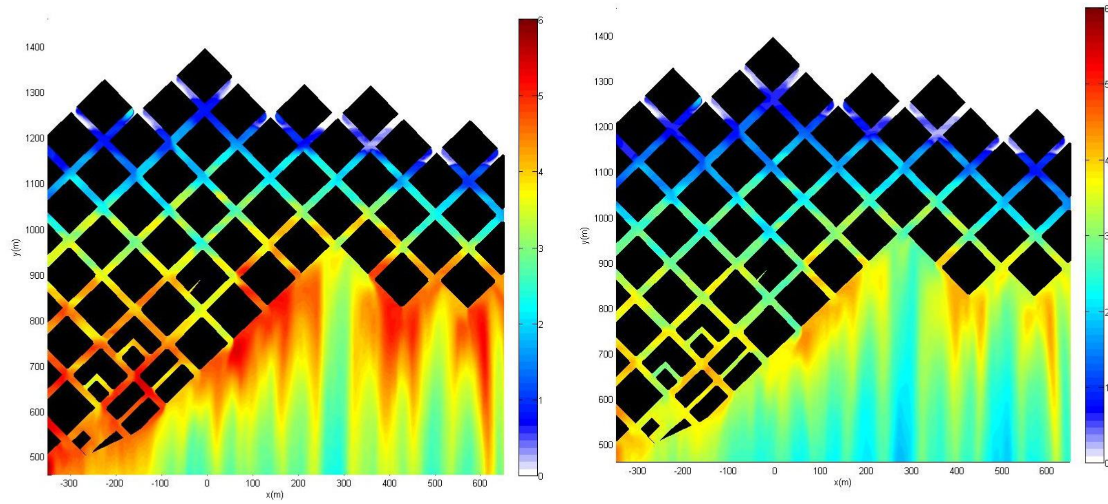

Figure 15: PM_{10} mean concentration ($\mu g/m^3$) at the current situation (left) and with the improvement of domestic heating (right), at ground level.

4.3.2 Electric Vehicles Conversion

Similarly to the changes done in the previous scenario, to take into account the effect of converting 15% of the cars to electric ones, and 5% of the buses to electric ones as well, the emission rates were reduced. In this cases the reduction was of 12.1% for CO, 6.7% for NO_x and of 3.5% for $PM_{2.5}$. Having changed those emissions rates the simulation was run, but the final results have not been reached yet, having only the instant concentration after 2000s of emissions. So in Figures 16, 17 and 18 the comparison with the current scenario and the vehicular one at the same time can be seen.

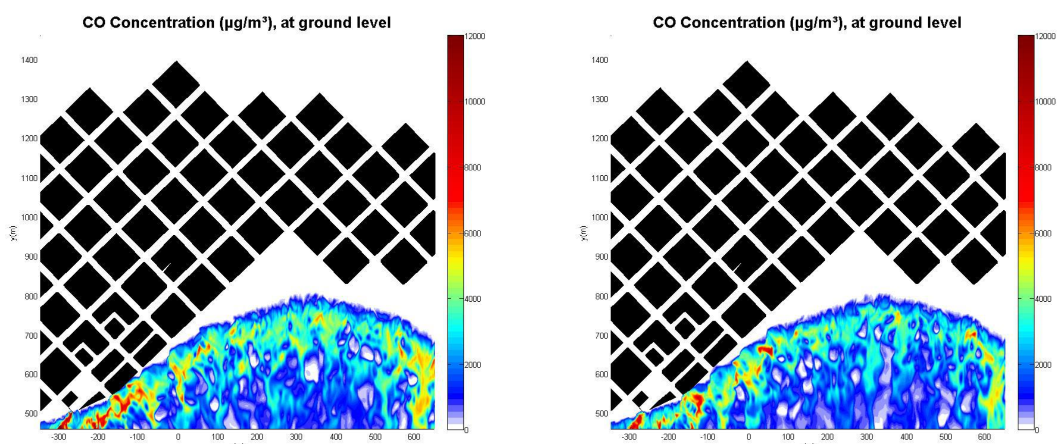

Figure 16: CO instant concentration ($\mu g/m^3$) at the current situation (left) and with the convertion of vehicles (right), at ground level.

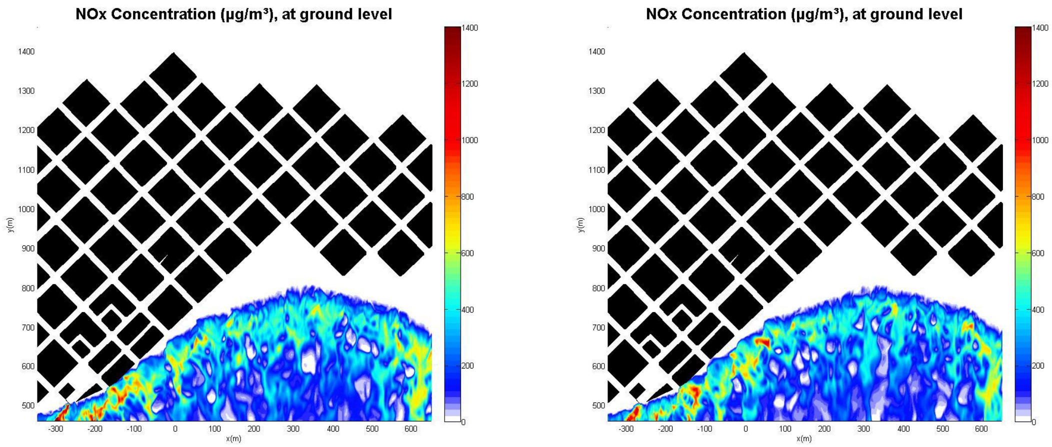

Figure 17: NO_x instant concentration ($\mu g/m^3$) at the current situation (left) and with the convertion of vehicles (right), at ground level.

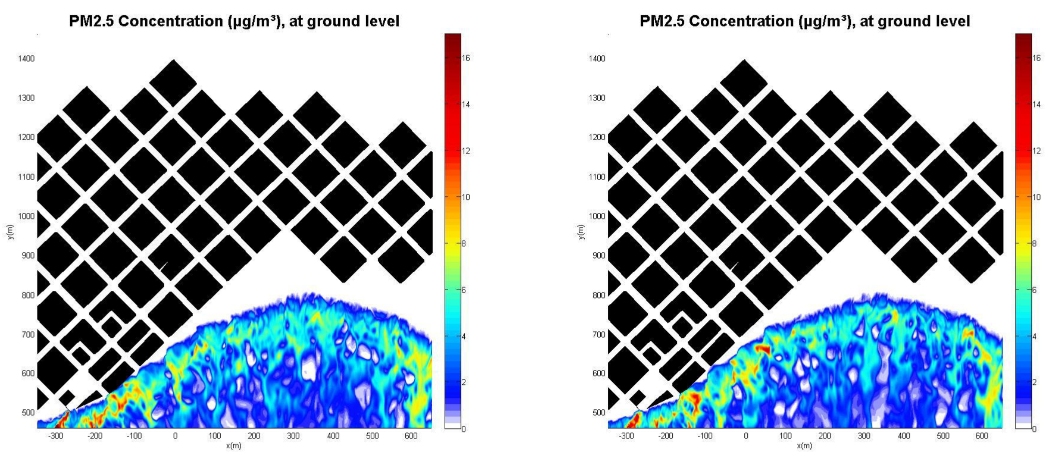

Figure 18: $PM_{2.5}$ instant concentration ($\mu g/m^3$) at the current situation (left) and with the convertion of vehicles (right), at ground level.

It can be seen that all the figures are practically identical except for the pollution levels involved, but the distribution is basically the same one in every case. Looking at this fields one can see that there is not an important difference between them but, at the current situation there is a high concentration band (yellow-light blue) that is wider than the one at the future scenario. Moreover, downstream from the route one can se more low concentration areas (white) in the future scenario as well, this would indicate that once the time averages are done a visible change in the pollution levels should be appreciated.
Nonetheless, this instant concentration fields could be deceiving, given that they are strongly dependant on the flow instant conditions that will be different from one simulation to the other due to the turbulence aleatory nature. So, if one looks for significant results, time averaged concentrations should be computed.

5 Conclusion and Future Work

From the different analysis made with results obtained from the simulations, it can be concluded that the developed tool can be very useful when evaluating the environmental impact of different emission sources. Despite its limitations, the tool has great flexibilities in terms of the domain selection, mainly because of the use of Immersed Boundary Conditions. Moreover, it gives the user the possibility of simulating different sources, and including multiple pollutants.

As far as the obtained concentration fields are concerned, the results seem to be coherent with the flow conditions and the emission rates simulated. Furthermore, the impact of the different sources, particularly the vehicular ones overriding the others, can be seen clearly on the results, which agrees with the bibliography. Also, the comparison between in-situ measurements and simulated data is satisfactory as both results are of the same order and some particular measurements surround the simulated value, meaning that, as expected, the computational method represents a particular situation.

As mentioned in the results some simulations have not yet been finished, and are currently being run, leading to two main roads of work. First of all, once the simulations are done an analysis similar to the one described should be done, allowing to quantify the impact of the technology changes assumed as future scenarios. This road of work is mainly in short term as the simulations should not take too much time and would close the analysis done.

On the other hand, an important issue to address is how long the simulations take, given that to get results of a certain run can take up to three months depending on the availability of computation cores. As a solution, one of the possibilities being studied is the passage of the CFD solver to heterogeneous computing, which means using both CPU and GPU in order to be more efficient in terms of time and energy consumed when running the simulations.

If this improvements are accomplished, this could mean that simulating bigger domains with good resolution would be possible, allowing a better analysis of the current situation and possible future scenarios. Moreover, different weather conditions could be explored so as to have more information about the effects of the emission sources. In addition, having more meteorological conditions simulated could give the possibility of better validation of the tool. This last point is complemented with the realization of more measurements campaigns, either at many locations in the domain or at different heights, having more data to compare against the simulations.

Overall, the model results are consistent with the measurements taken, nonetheless, the calibration of the parameters involved exceeds the reach of this work, being of the utmost importance having more in-situ measurements to compare against the simulations. Despite this we strongly believe this tool provides a solid starting point for future work.

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