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Urban Pollutant Dispersion on a Turbulent Fluid Model

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ABSTRACT. In 2019, more than 90% of the world's population was living in places where pollutant concentrations exceeded the air-quality guidelines. Anthropogenic activity has been the main cause of climate change in the last 20 years, especially in urban centres where industrial activities and motorized traffic mainly occur. This article presents a study of air pollutant dispersion by computational fluid dynamics modelling using OpenFOAM for urban street canyon simulations. The aim of this study was to investigate the influence of vegetation on natural ventilation, dispersion and CO_2 mitigation. The behavior of pollutants was modeled by the Reynolds-averaged Navier–Stokes equations (RANS) and the $k-\varepsilon$ fluid turbulence model. The results indicate that aerodynamic effects are more important at lower pollutant wind velocities, as they reduce turbulent dispersion and allow a higher reduction in the concentration of air pollutants. In addition, the direction of the wind, relative to the main axis of the street, had a significant impact on the results found. In general, in the presence of trees, perpendicular winds can lead to higher concentration of pollutants, while parallel winds allow improve air quality, considerably reducing those pollutant concentrations.

Keywords: air pollution, CFD, street canyon, urban centres.

1 INTRODUCTION

Air pollution is a big problem in the 21st century, causing harm to human health and the environment. The magnitude of the problem is reflected in the World Health Organization (WHO) estimation of around 4.2 million deaths worldwide due to air pollution in 2016 [25]. In 2019,

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according to Pan American Health Organization (PAHO) [20], more than 90% of the world's population were living in locations where pollutant concentrations exceeded the WHO guideline of 2005 for long exposure to $PM_{2,5}$. However, despite the new WHO guidelines [26] - which has more restrictive standards - the number of people in the world who breathe air above the recommended standards has not decreased.

Several countries have been adopting measures to improve air quality, these must be encouraged and expanded. Air pollutants can be of natural or anthropogenic origin. Natural sources, such as volcanoes, salt spray, dust storms, decomposition of organic matter and fires, cannot be controlled. Also, it is noteworthy that natural phenomena can release high concentrations of atmospheric pollutants.

Political actions, for the most part, do not include more sustainable strategies, as they are economically unfeasible at present, but in the long term, they would generate a reduction in health care costs [25]. A responsible analysis and preventive measures can be proposed for areas that have a great polluting potential, such as large urban centers.

One central issue is that in big cities can observe large pollutant concentrations [16], and people living in these cities are exposed to those concentrations [5]. As a consequence, they show a major probability of developing several diseases, related to heart and lungs, which contribute to the increase in morbidity and mortality rates. Since [23] about a quarter (24%) of all adult deaths due to heart disease, 25% stroke, 43% chronic obstructive pulmonary disease, and 29% lung cancer are caused by air pollution [2, 20].

Local-scale dispersion models can be used to predict the behavior of air pollutants in street canyons. Alternatives such as the use of vegetation - trees, green walls or barriers -, photocatalytic paints, among others, have been investigated by preliminary studies by Georgii [8] in Frankfurt, Germany; Dabberdt, Ludwig and Johnson [4] in San Jose and St. Louis, USA; and Oke [18] in Vancouver, Canada. Pollutant dispersion models are based on the mathematical description of the processes of atmospheric dynamics, as a function of the spatial and temporal evolution of the pollutants emitted by a referenced source.

The kind of pollutant constituents and the average distance followed by the fluid field must be also considered. Each pollutant composite has an specific mean-life, which can be short (minutes to hours), long (hours to days), and very long (days to weeks). As a consequence, the fluid dispersion model has to consider these features. The models can distinguish different spatial scales, and are usually classified according to global, regional and local scope. These models are used in several types of studies, such as air quality assessment, urban planning, interpretation of monitoring data, traffic management, pollution prediction and impact studies of population exposure to pollutants. There are several types of dispersion models in the literature, which can be classified according to physical or mathematical principles, e.g., reduced scale, Eulerian and Lagrange box, Gaussian, computational fluid dynamics [11, 23].

Various softwares simulate the dispersion of atmospheric pollutants by means of computational fluid dynamics (CFD), e.g., ANSYS CFX, FLUENT, NUMECA, OpenFOAM. In this study, the OpenFOAM software, which consists of over 80 solvers and 170 utility applications that solve complex fluid flows involving chemical reactions, turbulence and heat transfer for solid and electromagnetic dynamics [9].

Focusing on the problem of pollutants for large urban centers, mentioned above, it was developed here a study on the influence of natural ventilation, trees and dispersion of CO_2 pollutants, testing different numerical settings.

2 METHODOLOGY

To simulate the pollutant concentration for a hypothetical street it was opted to use the CFD modelling. Here, for instance, it is possible to evaluate the physical processes involved in complex geometries of urban canyons.

The computational simulations were done considering as basis the model proposed by Jeanjean et al., [13, 14], on which it is supposed an incompressible, isothermal and turbulent flow.

2.1 Hypothetical street geometry

Computational details of this analysis include the correct implementation of dynamical equations on the correspondent domain (mesh). This mesh consists on the division of the geometry in little cells. A basic ingredient for the whole procedure, the mesh must contain the maximum number of cells as possible, without affecting the computational time. Working with the CFD in OpenFOAM, the mesh can be divided in different zones, the walls contributions are represented in the majority of cases as boundary conditions.

In order to simulate an hypothetical street of an urban region (Fig. 1) the strategy adopted was similar to the one adopted by Gromke and Ruck [10], this meaning two buildings of 100 m in length (L) 10 m in height (H) and width (W), with a mutual distance of 10 m. This implies into the relation H/W = 1, and according to Vardoulakis et al., [23] this canyon is then classified as regular.

The geometry consisted of two big regions of cells, one for the group of trees and the other to the remaining of the computational domain, thatis, the buildings and the street. In the street sector it was considered a central boulevard, 5 m distant from the building walls. This boulevard includes 7 trees, with their domes being represented by rectangular blocks of 5 x 5 x 5 m^3, distant from each other by 10 m. The central region of this model was considered as a source of pollutant emissions.

The geometry implemented was discretized using the Salome-Meca software [19]. It was adopted a group of 708.000 cells, in order to minimize the computational time and maintain the precision. The Salome-Meca subroutine was chosen mainly because it furnishes a generic platform of pre and post data processing with an open architecture.

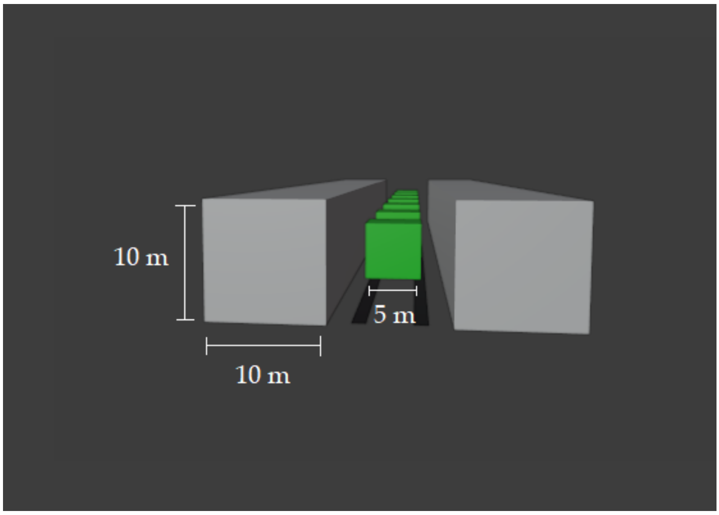

Figure 1: Urban canyon geometry used on simulations.

2.2 Modelling

To describe the pollutant behavior it was considered: (i) the continuity equation; (ii) the Navier-Stokes equation considering the Newtonian model for viscosity and (iii) the pollutant concentration equation. The state equations were constructed considering the thermodynamical equilibrium. For a better characterization of the pollutant dispersion the atmospheric turbulence has to be considered too [11, 14, 15, 23, 24].

The inclusion of turbulence is important for considering flexible structures; the aerodynamical behavior of those structures can only be correctly estimated when atmospheric turbulence is considered [16].

According to Vardoulakis et al., [23] the most useful turbulence models can be classified in two categories: (1) the models based in Reynolds Averaged Navier Stokes (RANS), e.g., the $k-\varepsilon$ model, which includes turbulent kinetic energy and the rate of dissipation and (2) the big scale models (LES). The LES models, in general, do a better prediction of the turbulence behavior than the RANS models. On the other hand, due to boundary conditions issues RANS and $k-\varepsilon$ models are more usually applied in simulations that include vegetation [7, 10, 13, 14, 15].

In these study the RANS and $k-\varepsilon$ model has been adopted, using equation 2.1 for the wind flux.

Based on these ideas the RANS and $k-\varepsilon$ model has been adopted here, using equation (2.1) for wind flux:

$$\frac{\partial U_i}{\partial x_i} = 0, \tag{2.1}$$

where is U_i the wind velocity, and can be decomposed in two terms:

$$U_i = \bar{U_i} + U_i^{'}, \tag{2.2}$$

where $\bar{U_i}$ is the average value of the wind velocity, and Ui' its fluctuation.

The $k-\varepsilon$ model considers the equation 2.3 to calculate the turbulent kinetic energy (k) and its dissipation rate (ε):

$$k = \frac{1}{2}\bar{U_i'}\bar{U_i'}, \tag{2.3}$$

$$\varepsilon = \frac{C_U^{0.75}k^{1.5}}{l}, \tag{2.4}$$

where C_U is a model constant and l the turbulent longitudinal scale.

Because equation (2.4) depends directly on the systems geometry, Greenshields [9] considered it as a tubular structure, with rectangular section.

According to Jeanjean et al., [14] the presence of vegetation affects turbulence and also the momentum sink, that is, dissipation (S) and the pressure loss coefficient (λ). Therefore, the presence of vegetation can be modeled as a porous zone, with the dissipation being determined by the equation (2.5), that obeys a power law solution:

$$S = -\lambda(\rho|U_i|U_i), \tag{2.5}$$

where λ is the pressure loss coefficient, induced by the presence of trees; ρ is the fluid density.

In addition to the equations mentioned previously, the scalar transport equation for a scalar C (2.6) was considered to be:

$$\frac{\partial U_i}{\partial t} + \nabla(U_iC) - \nabla^2(DC) = 0, \tag{2.6}$$

where C is the pollutant concentration and D its diffusion coefficient.

In these study was chose CO_2 as pollutant. Those reactions in atmosphere are very fast, and therefore this constituent can be considered as being inert for this scale [23].

2.3 Model implementation using OpenFOAM

For the implementation of this model on OpenFOAM, it was considered the k-ε model, through the porousSimpleFoam solver. This platform was chosen for doing this analysis because it permits a phenomenological approach to the various scenarios found when one considers pollutant dispersion in urban centres, and the results emerge, in general, with clarity and good accuracy. In order to calculate the dissipation (S) the power law related to (2.5) was included only for porous zones, that is, in the trees. For CFD simulations the adopted boundary conditions that are listed on Table 1.

The porousSimpleFoam solver was used for incompressible simulations of steady state with turbulence; in this study was not considered temporal evolution of the physical variables. The models were added for the simulation in the OpenFOAM was: powerLaw, for the porous regions; scalarTransportFoam, for the C scalar, with RANS model and $k-\varepsilon$. For the numerical solution used was finite volume method what permited for discretization of the equations.

Table 1: Boundary conditions adopted.

Variable	Parameters OpenFOAM
U_i - wind velocity	$fixedValue$
	$noSlip$
	$zeroGradient$
p - kinematic pressure	$fixedValue$
	zeroGradient
C - pollutant concentration	$fixedValue$
	$advective$
v - turbulent viscosity	$nutkWallFunction$
k - turbulent kinetic energy	$kqRWallFunction$
e - dissipation rate	$epsilonWallFunction$

2.4 Numerical simulations

Looking for a better understanding of the velocities fields and the dispersion in the presence and absence of trees, it were considered different values for the initial wind velocities (U_i): 1 m/s, 2 m/s and 10 m/s in parallel and perpendicular directions. These values were chosen based on the Curitiba (Brazil), [22].

The values for velocities varied between 1 and 2 m/s with wind gusts near 10 m/s. The initial conditions adopted in this study are listed on Table 2, where, with the exception of the wind velocity field, the other parameters remained constant.

Table 2: Initial values used on OpenFOAM software.

Variable	Value	Unities	Source
C	1	kg/m³	estimated
U_i	(X, Y, Z)	m/s	estimated
e	0,029	m²/s³	[9]
v	$1{,}5\text{x}10^{-5}$	m²/s	[5]
k	0,25	m²/s²	[9]
C_0	0,6	-	[14]
p	0,1	m²/s²	estimated
D	$1{,}6\text{x}10^{-5}$	m²/s	[6]

2.5 Data processing

With the results of simulations it was done a post-processing using [7], with which it was possible to visualize the average wind velocity field (U_i) and the average concentration of CO_2 (C). Be-

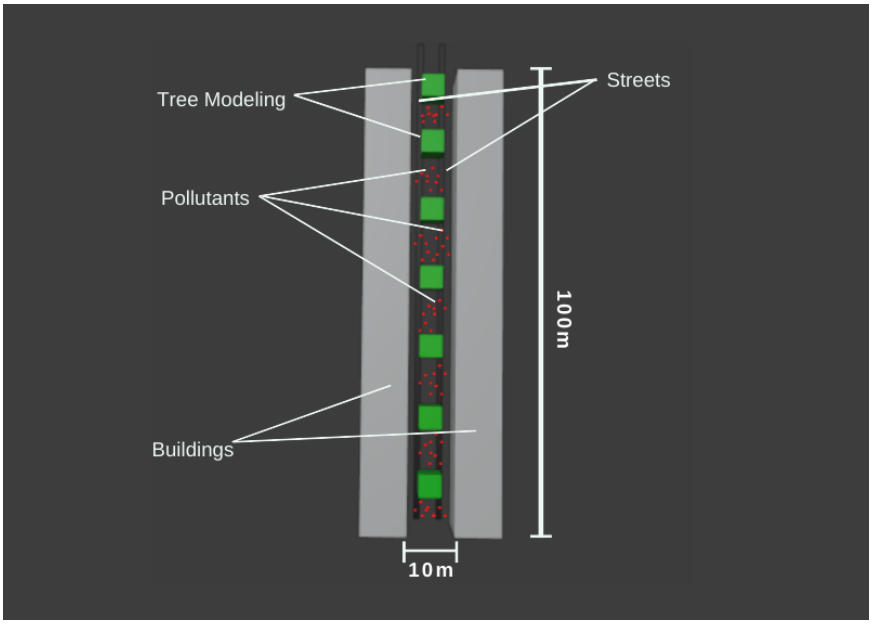

Figure 2: Simulation model - Hypothetical street.

sides, it was investigated a longitudinal cut in the central region of the canyon (Fig. 2), with 10 m in height and 100 m in length. The generation of images was done with Paraview software [21].

The trees influence was evaluated making a comparison between the pollutant concentration with and without their presence:

$$var = 100\frac{C_t - C}{C} \tag{2.7}$$

where *var* is the variation of the pollutant concentration, with and without the presence of trees in the hypothetical street (C_t, C).

3 RESULTS AND DISCUSSION

It were verified here several properties of the system, related to the presence or absence of trees, on a hypothetical street. The results can be compared to the analysis of Gromke and Ruck [10] and Jeanjean et al., [13, 14].

The simulations carried out in this study were obtained using the OpenFOAM shown on Tables 3, 4 and 5. Those are the results for the mean values for: the pollutant concentration and average velocity field (Fig. 2).

These results have been obtained for different initial velocities and initial values of pollutant concentration and wind directions, considering also the effect caused by the presence of trees, on different scenarios.

Table 3: Average wind velocity and pollutant concentration for different initial values of the fundamental variables. Wind direction: perpendicular to the street main axis.

Initial velocity (m/s)	Pollutant concentration (kg/m³)	Average velocity (m/s)	Presence of trees
(1,0,0)	$5.813 \mathrm{x} 10^{-9}$	0.583	No
(1,0,0)	$5.792 \mathrm{x} 10^{-9}$	0.580	Yes
(2,0,0)	$1.095 \mathrm{x} 10^{-7}$	1.338	No
(2,0,0)	$1.086 \mathrm{x} 10^{-7}$	1.302	Yes
(10,0,0)	$5.005 \mathrm{x} 10^{-7}$	8.127	No
(10,0,0)	$5.729 \mathrm{x} 10^{-7}$	7.619	Yes

Table 4: Average wind velocity and pollutant concentration simulations for different initial values. Wind direction: parallel to the street main axis.

Initial velocity (m/s)	Pollutant concentration (kg/m³)	Average velocity (m/s)	Presence of trees
(0,1,0)	$1.895 \mathrm{x} 10^{-15}$	0.567	No
(0,1,0)	$1.095 \mathrm{x} 10^{-15}$	0.459	Yes
(0,2,0)	$5.423 \mathrm{x} 10^{-14}$	1.669	No
(0,2,0)	$2.244 \mathrm{x} 10^{-14}$	1.147	Yes
(0,10,0)	$3.433 \mathrm{x} 10^{-11}$	12.752	No
(0,10,0)	$3.909 \mathrm{x} 10^{-13}$	7.268	Yes

Table 5: Average velocity and pollutant concentration simulations for different initial values. Wind direction: parallel and perpendicular to the street main axis.

Initial velocity (m/s)	Pollutant concentration (kg/m³)	Average velocity (m/s)	Presence of trees
(1,1,0)	$1.202 \mathrm{x} 10^{-12}$	0.597	No
(1,1,0)	$7.963 \mathrm{x} 10^{-13}$	0.482	Yes
(2,2,0)	$2.967 \mathrm{x} 10^{-10}$	1.768	No
(2,2,0)	$8.879 \mathrm{x} 10^{-11}$	1.211	Yes
(10,10,0)	$1.698 \mathrm{x} 10^{-7}$	9.683	No
(10,10,0)	$9.915 \mathrm{x} 10^{-8}$	8.661	Yes

For a wind direction perpendicular to the street main axis,e.g. perpendicular to main axis Y, it was possible to verify that (Table 5) in the presence of trees there is a reduction of the wind average velocity, but this reduction is feeble for initial velocities between 1 m/s e 2 m/s. The Fig. 3 makes evident that the velocities field does not change when one includes trees.

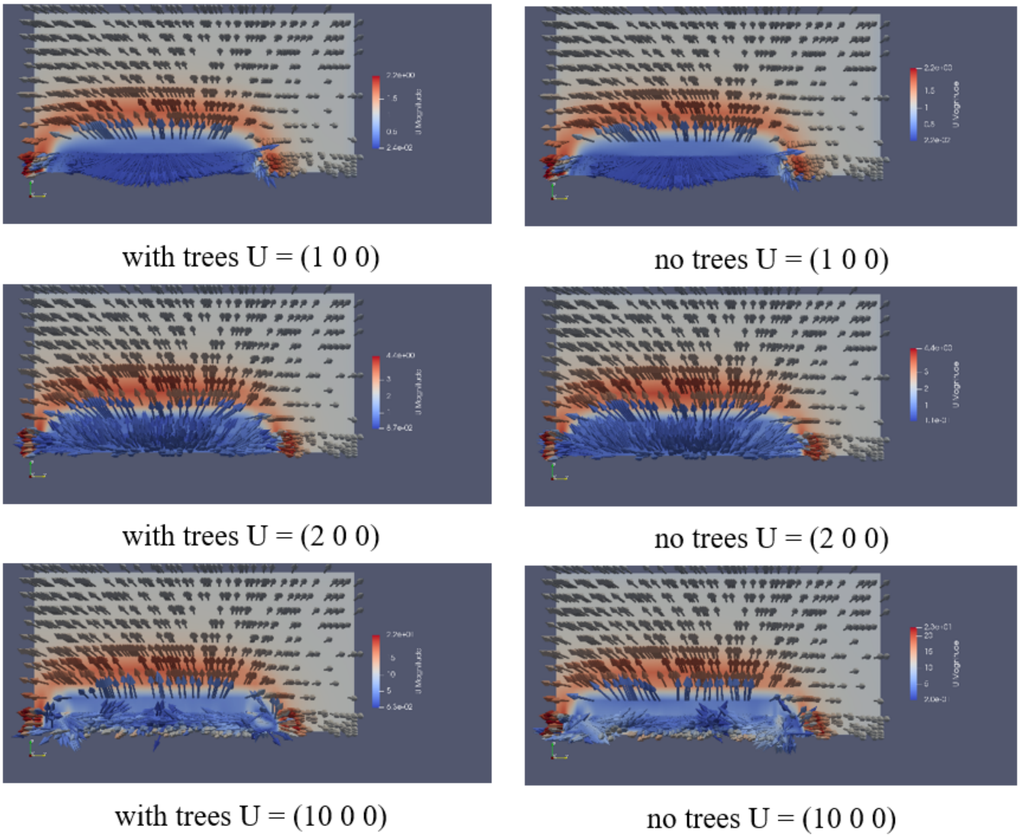

Figure 3: Velocity profiles for perpendicular wind incidence, with and without trees.

On the other hand, when the considered velocities were about 10 m/s (parallel and perpendicular cases), the presence of trees reduced the natural ventilation (average) from 9.68 m/s to 8.66 m/s (Table 5). Besides, as the velocity field profile shows, the trees reduce the wind flow, and at the same time, associated to the geometry of the system, promote higher values of pollutant concentration, this is showed in Fig. 4.

On simulations that include an initial wind velocity field of $U = (10,0,0)$ the pollutant concentration is reduced without trees. This can be understood by contrast, seeing that in the presence of trees the average wind velocity diminishes (Fig. 3), making the concentration higher in regions where the trees are present (Fig. 4).

It is worth mentioning that the vortex generated by the presence of buildings enhance the concentration in the street surface and in the building's walls [1,4,8,23]. However, in another work, it was shown that presence of trees reduces that pollutant concentration for $U = (0,10,0)$ m/s [3].

In Fig. 4 it is possible to see that the pollutant concentration is higher at the end of the street, but the presence of trees reduces that concentration. The results are in tune with those of Jean-

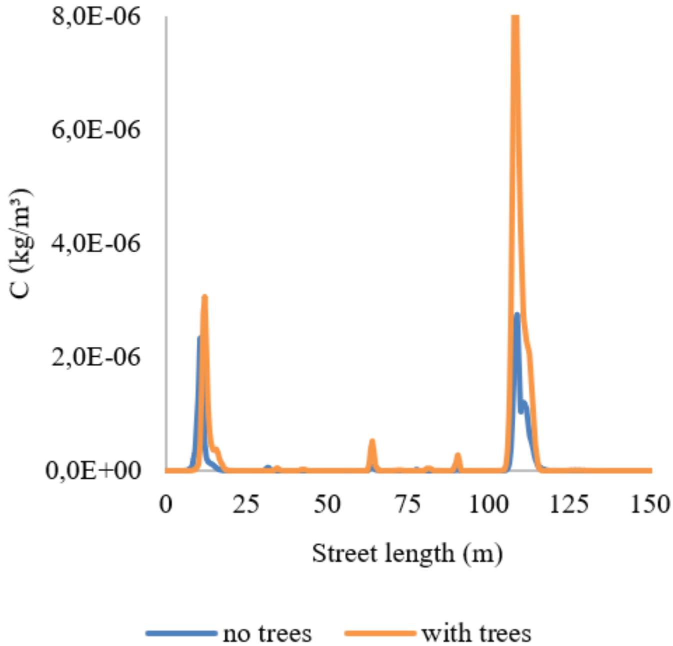

Figure 4: Pollutant concentration for initial wind velocity 10 m/s, perpendicular to the street main axis, U = (0,10,0).

jean et al., [13, 14], where they observed that perpendicular wind can diminish concentration in street canyons. In order to evaluate the incidence of perpendicular wind flows, was did several simulations, whose results are condensed in Table 5.

For parallel wind fields it was possible to verify that the presence of trees reduces the natural ventilation in the central boulevard, and when the average wind velocity is 10 m/s the reduction approaches a 43%. Fig. 5 shows that the presence of trees changes the velocity field when the initial velocity is 10 m/s. On the other hand, it is possible to verify a reduction of CO_2 concentration for all scenarios. Specially for wind velocity modulus around 10 m/s it was verified that the velocity field modulus is of high value, together with a reduction of pollutant concentration.

Focusing on pollutant concentration Fig. 6 shows that, for parallel winds, the maximum concentration occurs at the beginning of the street. As the pollutant concentration behavior is not show in Fig. 6 completely, Fig 7 is also shown, verifying that the concentration peaks occur mainly at the 10 m to 30 m interval, as a consequence of the geometry chosen in this case.

Considering wind direction being parallel and perpendicular to the main axis Y, it was possible to verify that the presence of trees reduces the natural ventilation for every scenario. When the wind velocity was 2 m/s the reduction was maximum, and when 10 m/s the minimum 12%.

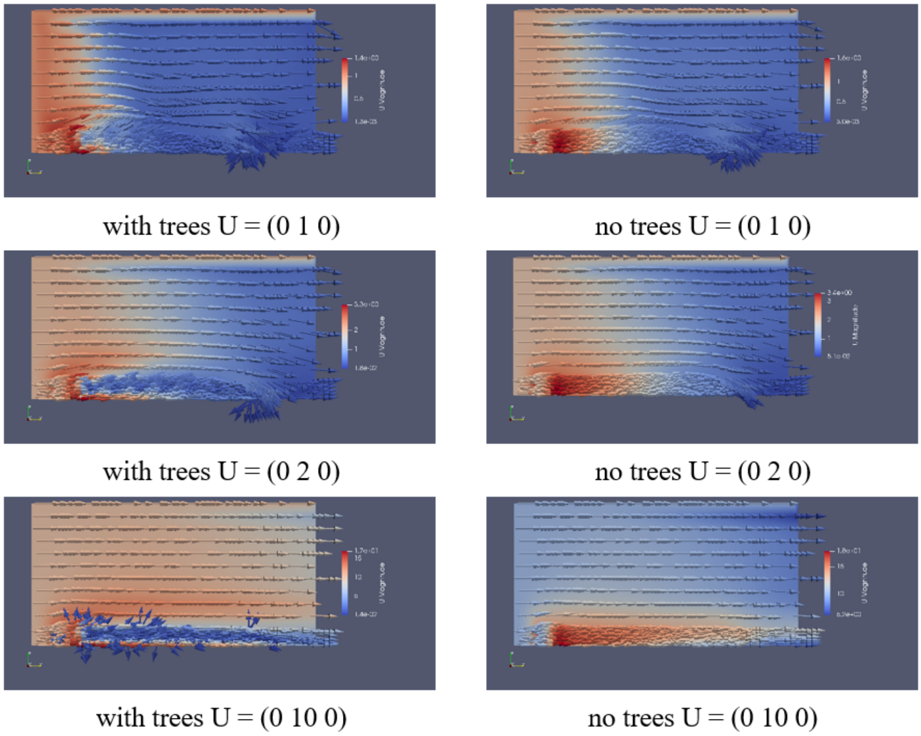

Figure 5: Velocity profile, with wind field parallel to the street axis, with and without trees.

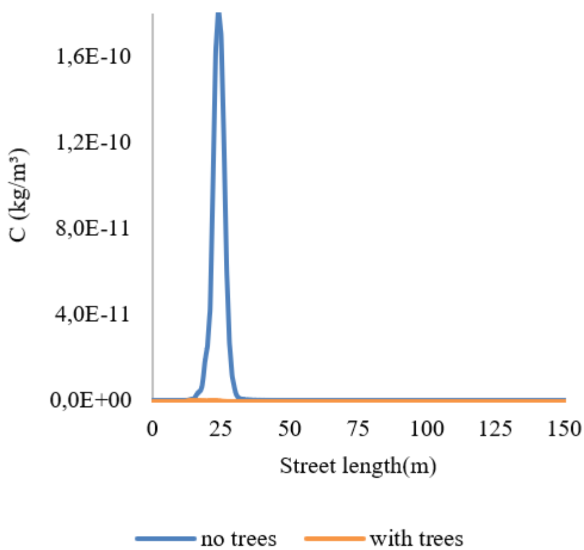

Figure 6: Pollutant concentration, for wind initial velocity 10 m/s, perpendicular to the street main axis - U = (0,10,0).

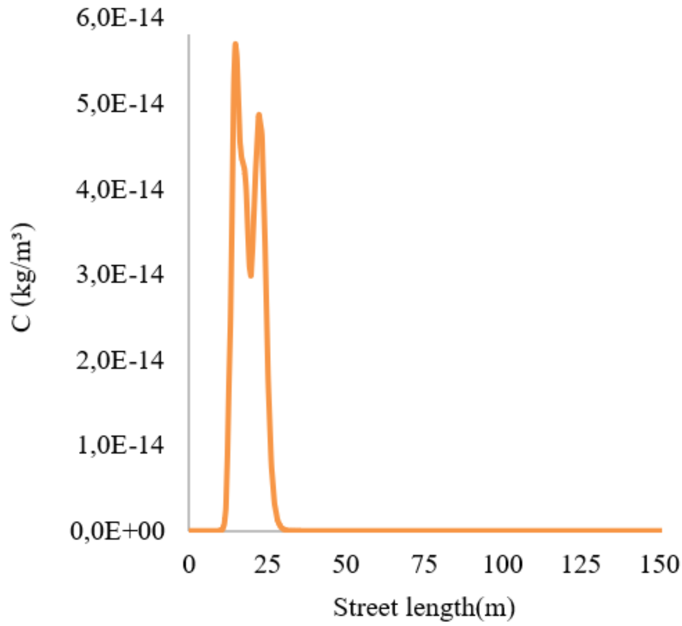

Figure 7: Pollutant concentration, with initial wind velocity 10 m/s with trees, perpendicular to the street axis - U = (0,10,0).

Fig. 8 shows the effect produced by the presence of trees. In these simulations it was also possible to observe that the aerodynamical effects are more important when the wind velocities are smaller, because they diminish the turbulent dispersion, and therefore permit a higher reduction of pollutant concentrations. The Fig. 9 illustrates the pollutant concentration, when the wind velocity is of 10 m/s, and is possible to verify that the maximum of concentration of CO_2 occurs at end of the street, for the proposed geometry, and showing the effect produced by the wind velocity field.

With these results it was possible to estimate the pollutant concentration reduction CO_2 depending on the wind initial velocity. These results are shown in Table 6. It is possible to infer that the wind direction has an important effect into the reduction of pollutant concentration. The exception occurs for perpendicular winds and high velocity, in this case there was an increase in the concentration of pollutants of approximately 14.5%.

Table 6 shows that the reduction of pollutant concentration is smaller when the wind field incidence occurs perpendicularly to the street main axis, with $U = (1,0,0)$, $U = (2,0,0)$ e $U = (10,0,0)$. The simulations with initial velocities $U = (1,1,0)$, $U = (2,2,0)$ e $U = (10,10,0)$ also shows the importance of the perpendicular incidence of the wind field. This is globally in tune with the results presented by Gromke e Ruck [10].

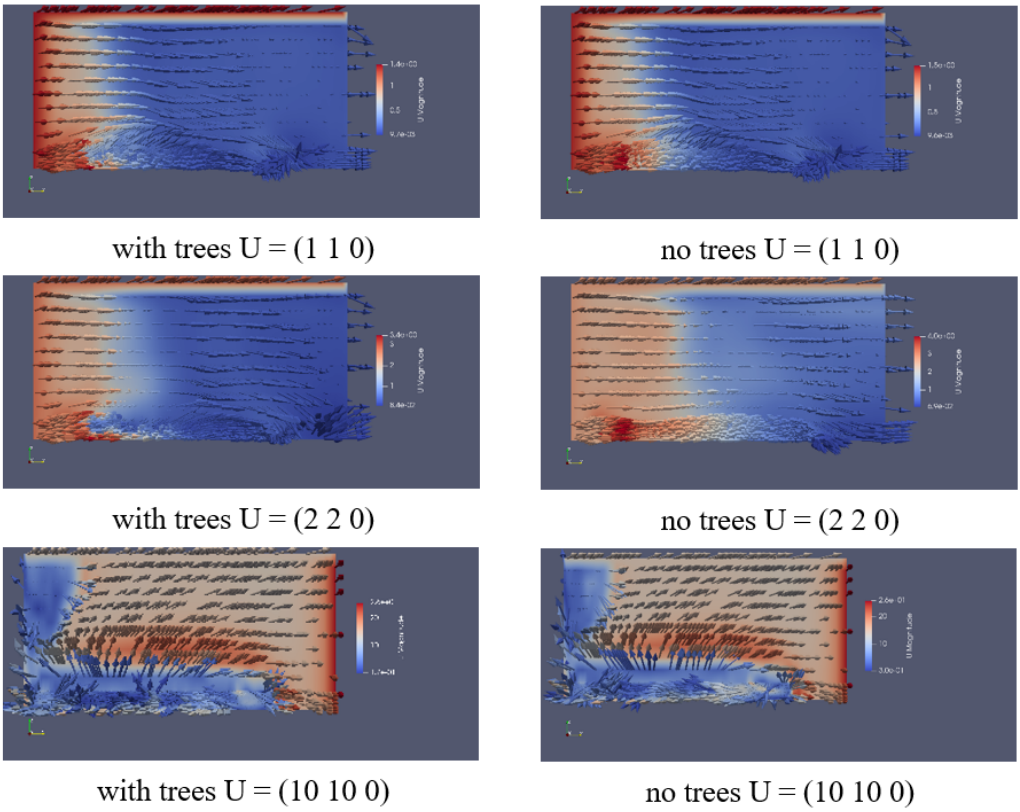

Figure 8: Pollutant concentration, with initial wind velocity 10 m/s with trees, perpendicular to the street axis - U = (0,10,0).

Table 6: Percentage variation of pollutant concentration with trees on the streets.

Initial velocity (m/s)	Pollutant concentration variation (%)
(1,0,0)	-0.36
(2,0,0)	-0.85
(10,0,0)	14.46
(0,1,0)	-42.20
(0,2,0)	-58.62
(0,10,0)	-98.86
(1,1,0)	-33.75
(2,2,0)	-70.08
(10,10,0)	-41.63

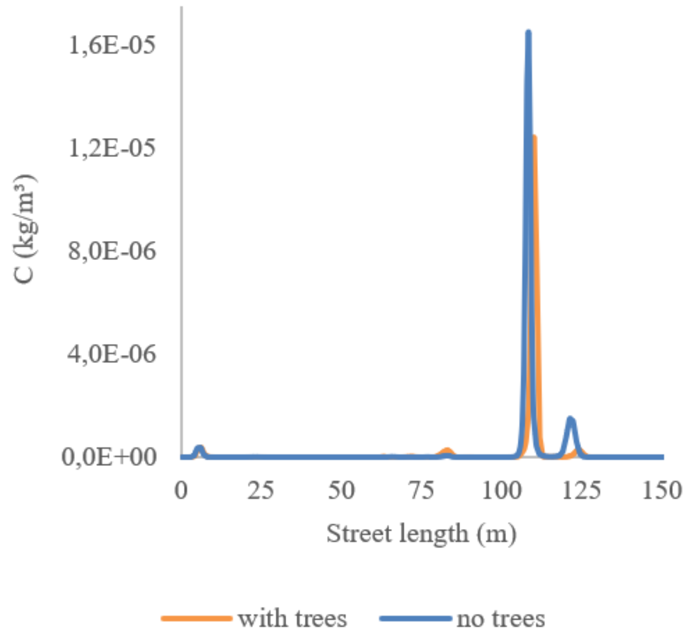

Figure 9: Pollutant concentration, with initial wind velocity 10 m/s with trees, perpendicular to the street axis - U = (0,10,0).

The high velocities evaluated are related to the wind gusts [22] are not predominant in urban centres, meaning that the presence of trees is a positive factor for the pollutants diminishing. Besides, other strategies can be adopted, e.g., green walls or barriers, but these alternatives also will depend on the urban geometry and local conditions, and will permit pollutant reduction when low wind velocities.

It is important to stress that this model did not consider the deposition of pollutants on the trees. According to Jeanjean et al. [14] the deposition could reduce in high percentages as 50%. On the other hand, Lorenz et al. [17] showed that areas with high tree density can even promote the increasing of pollutants presence on those areas. Table 5 confirms that tendency, showing that ventilation is also an important factor to promote the dispersion. These adjustments should be phenomenological. The simplified geometry simulations made here permitted to arrive to some basic conclusions about the pollutant behavior for an urban centre street. The presence of trees, according to these results, is a valid path to follow when one tries to mitigate the presence of pollutants. On these areas the increase of anthropogenic pollution is verified, and happens, in general, without a previous study about the negative impact that air pollution causes on the health of the population.

These effects were verified in computer simulations presented during the last IPCC meeting [12], where it was observed that the influence of natural and anthropogenic sources are main actors on the general behavior for global climate and its changes, observed in the last 40 years. Taking into account topographic and local climate peculiarities is also an important issue to extend the comprehension of these phenomena.

In this work it was considered a simplified geometry for the street configurations, compatible boundary conditions and fluid equations. The turbulent effect made possible the assertion that the average pollutant concentration diminishes in the presence of trees, besides being dependent on the wind velocity field modulus and direction. The use of an open user software permits that this kind of analysis can be done for any urban centre, proposing simple alternatives and with low costs to minimize the pollutant dispersion problem, but this requires professional qualification for the realize the simulations. On the other hand, the effect of mitigation using vegetable species is a field of work that needs new approaches and detailed investigation. Other types of trees, foliar density, geometrical configuration, combination with other types of pollutants, are factors that deserve new analysis. Besides, the local weather conditions, building construction details, variations in temperature and pressure are other parameters to be taken into account. These are relevant points for the future investigation related to the mitigation of pollutants in big urban centres.

4 CONCLUSIONS

With the model adopted in this work, using simulations done in OpenFOAM, it was possible to do an evaluation of atmospheric pollutant dispersion into a hypothetical street. It was verified that for perpendicular wind flows the presence of trees diminishes to a small amount the concentration of CO_2. For parallel flows, on the other hand, the results are beneficial. These results showed that for initial wind velocities as 1 m/s and 2 m/s, what occurs is a reduction of CO_2 concentration, on the presence of trees, 42,2% and 58,62%, respectively. In particular, the pollutant concentration reduction is higher when the initial wind velocity is increased, except when the initial velocity is 10 m/s in the perpendicular case. Besides that, when it was consider simultaneous wind fields (parallel and perpendicular cases) the pollutant concentration reduction is of 41.63%. A maximum value of 98,86% is obtained when one considers the parallel case, again with a wind modulus of about 10 m/s.

These results show that it is possible to reduce the pollutant concentration if one considers the presence of trees, which combined with geometrical considerations and wind field properties permit a significant better general health scenario.

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