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SIMULATION OF AIR POLLUTANTS DISPERSION IN A MICRO REGION OF THE MUNICIPALITY OF RIO DE JANEIRO IN REAL SCALE

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Abstract. *In the city of Rio de Janeiro, for reasons of economic and administrative character, the number of measurement points of the air quality monitoring network is limited and especially the spatial arrangement of them may not have been adequate. Therefore, to support the concentration measurements and to know their evolution, in this study it was used models based on computational fluid dynamics. The area surrounding the Tijuca station was chosen as the study site and it was investigated the dispersion of pollutants emitted by vehicular sources: carbon monoxide, nitrogen dioxide and sulfur dioxide. This was performed in a neutral atmospheric condition, more common in the winter months. It was used the commercial package Fluent version 17.1 and the RANS transport equations were closed with the standard $k-\epsilon$ turbulence model. Among the most important tasks it can be mentioned: to support a developed atmospheric boundary layer over the computational domain, to develop the appropriate settings of boundary conditions, to define the model constants, the modification of the law of the wall constants and to perform the computational grid tests based on convergence criteria for an increase in the mesh density. The study allowed us to analyze the influence of the turbulent kinetic energy generated by the movement of vehicles on the tracks over the behavior of the plume, and to determine which is the turbulent Schmidt number for the model that best fits the real dispersion profiles. The results obtained in the simulations were compared between each other and with available experimental data from the Tijuca monitoring station, observing good agreement with the data.*

Keywords: Air quality, exhaust emission, numerical simulation, CFD, ANSYS Fluent.

1. INTRODUCTION

Currently, vehicular emissions into urban cities represent almost all carbon monoxide emissions and most of the nitrogen oxides (Moreira; Tirabassi, 2000 and CETESB, 2010). Thus, it is necessary to evaluate the releases of pollutants and their dispersion into the atmosphere in different scenarios, aiming to plan programs to minimize environmental impacts.

Among the mathematical models used for these purposes, the CFD (Computational Fluid Dynamics) based models nowadays studied by research groups such as Blocken et al. and Kim et al. deserve special attention because they are able to combine the practicality and robustness of theoretical methods with possibility of provide information about the wind flow and the dispersion of pollutants on real and complex geometries in the same way as in laboratory experiments, but with much lower cost. CFD simulations can also assist in planning the experimental work by providing initial ideas of what properties should be measured and their probable magnitude.

Several researches were conducted related to the dispersion of atmospheric pollution on urban landscapes since it became an evident issue in the last decades. For instance, Kim (2004) used the RNG $k-\epsilon$ model to simulate the dispersion of pollutants in urban canyons. Then used a wind tunnel experiment to validate the model, getting good results in predicting the velocity field, recirculation of fluid over the canyon and dispersion of the pollutants themselves. In 2007, Blocken et al. discussed some problems and negative consequences using wall functions when simulating the horizontally homogeneous ABL (Atmospheric Boundary Layer) over a uniformly rough terrain, given later some suggestions to improve the CFD simulations. Two years later Yang et al. (2009) introduced new boundary conditions at the entrance of the domain in order to produce a homogeneous neutral stratified atmospheric boundary layer in an empty domain, this was accomplished using the standard $k-\epsilon$ turbulence model with modified constants. Richards and Norris (2011) addressed issues about the excessive generation of turbulence near the ground and the excess of stagnation pressure, proposing possible solutions.

In recent works, Akhatova et al. (2015) simulated the dispersion of contaminants taking into account vehicle emission rates and meteorological conditions, at the intersection of Bogenbay Batyr and Zhenis avenues in Astana, Kazakhstan. Otherwise Kim et al. (2016) simulated the vehicle induced turbulence on the tracks, focusing on the impact

of vehicle interactions, traffic density and vehicle composition, by developing equations to estimate the mean turbulent kinetic energy as a function of number and type of vehicles.

The objective of this article is to show a first approximation of the flow and dispersion of pollutants from vehicular sources in a micro-region with obstacles (buildings), in order to develop in a next work an approach that can provide in a real-time an improved estimation of gas dispersion and health risk information to the public by the integration of gas detectors, neural network and CFD based models.

2. METHODOLOGY

2.1 Physical Model

The RANS (Reynolds-Averaged Navier–Stokes) equations were used to model the mean turbulent flow. For closure of the RANS equations by modelling the Reynolds stress term as a function of the mean flow, was used the standard k - ε model. Therefore, we have four equations (conservation of mass, linear momentum, energy, turbulent kinetic energy and dissipation rate) and the respective boundary conditions to determine the mean velocity and pressure fields.

The main premises to solve the problem were: steady state, Newtonian fluid, incompressible and turbulent flow.

In modeling the conservation of chemical species, the local mass fraction for each specie, m_i , is calculated by the solution of the species conservation equation. Assuming permanent regime, the transport equation for the species in turbulent flow is:

$$\frac{\partial(\rho \overline{u_i m_i})}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t} \right) \frac{\partial m_i}{\partial x_i} \right] + S \quad (1)$$

An equation of this form is solved for N-1 species where N is the total number of chemical species present in the system. As the sum of the mass fractions of all species has to be equal to 1, the mass fraction of the nth specie is calculated from the known values of the other N-1 species.

The simulation of the horizontally homogeneous ABL over uniformly rough ground is often required in the upstream and downstream regions of the computational domain. This type of flow occurs when the vertical velocity and wind turbulence vertical profiles are in equilibrium with the roughness characteristics of the surface, which must be expressed by the appropriate z_0 value. Therefore, it is necessary to develop a special code capable of dynamically generate a vertical air intake profile from the meteorological data (speed and direction of wind). In Fluent all of this is possible by means of a user-defined function (UDF).

For the k - ε turbulence model, Richards (1989) proposed vertical profiles for the mean wind velocity u , TKE and the turbulent dissipation rate in the ABL.

$$U(z) = \frac{u_{ABL}^*}{\kappa} \ln \left(\frac{z+z_0}{z_0} \right) \quad (2)$$

Where u_{ABL}^* is the friction velocity in the ABL. According to Richards & Hoxey (1993), the constants of the k - ε turbulence model should be chosen in such a way that equation 3 is satisfied:

$$\kappa^2 = \sigma_\varepsilon (C_{\varepsilon 2} - C_{\varepsilon 1}) \sqrt{C_\mu} \quad (3)$$

Yang et al. (2009), with the intention of maintaining an adequate turbulence profile in the input domain, suggest to use the profiles for the TKE and the turbulence dissipation rate in the following way:

$$k = \frac{u_{ABL}^2}{\sqrt{C_\mu}} \sqrt{C_1 \ln \left(\frac{z+z_0}{z_0} \right) + C_2} \quad (4)$$

$$\varepsilon = \frac{u_{ABL}^3}{\kappa(z+z_0)} \sqrt{C_1 \ln \left(\frac{z+z_0}{z_0} \right) + C_2} \quad (5)$$

Where C_1 and C_2 are two independent model constants of u^* and z_0 . Normally, they can be determined by nonlinear adjustment of the TKE experimental data. Yang et al. (2009), determined the values of these parameters as $C_1 = -0.17$ $C_2 = 1.62$.

The work of Kim (2016) allows us to estimate the turbulence induced by the movements of vehicles for different vehicle compositions in the domain, varying from 3 $\text{m}^2 \text{s}^{-2}$ to 5.5 $\text{m}^2 \text{s}^{-2}$ for the average TKE value.

As in this work the mobile sources are represented as lines of pollutant release, representing a continuous vehicular flow, the turbulence generated by the movement of cars and buses on the highway must be implicitly reproduced, in order to evaluate the model response in function of TKE variation.

Considering that the vehicular flow is very variable throughout the day, and looking at the results of the cases studied by Kim et al., we took their TKE results as reference in the present simulation.

2.2 Computational Domain

The study area is located around the Tijuca Monitoring Station, and covers the Saens Pena Square, Conde de Bonfim Street and the buildings around this place. Land survey data and building geometries were provided by the Pereira Passos Institute (Figure 1). This area was considered as flat terrain, since the slopes varies in 1m only. The air quality in this microregion basically is affected by mobile sources.



Figure 1: Cadastral map of the study area (Pereira Passos Institute, 2015).

The buildings geometry at the study area was imported from the buildings digital layer map of Rio de Janeiro, provided by the Pereira Passos Institute, and was processed using SolidWorks Software, in order to obtain usable CAD files for CFD simulations.

The domain involving the geometry represents the fluid region (i.e., the atmospheric air). Figure 2 schematically represents the domain of study, as it is addressed in the present work.

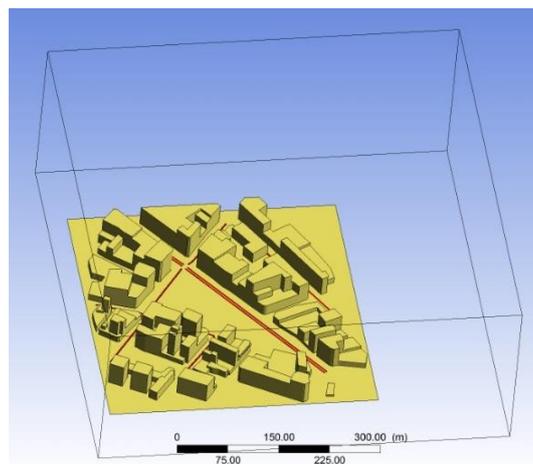


Figure 2: Computational domain (Elaborated using SolidWorks 2015 from IPP data).

In case of don't have a territory information system and be able to perform a simulation in whatever place, a 3D geometry scenario can be got using sophisticated tools like photogrammetry, LiDAR system, or more simply using packages like Google Earth Pro in combination with geographic software like ArcGIS.

2.3 Pollutant Mass Flow

The amount of polluting compounds emitted by exhaust pipes of vehicles are dependent on the fuel and engine type used, and the mode and operation conditions (i.e., cold or hot start and stabilized conditions) (US EPA). Because of this, the time of a given trip has a strong relation with the emission levels of pollutants.

Emission factors are reported each year by the Environmental Company of the State of São Paulo (CETESB), and should be used to get accurate estimates. However, knowing the difficulty in obtaining data on the complete distribution of vehicle fleet flow in each track, which deserves a separate study, Cancelli & Dias (2011) suggest the use of emission factors for a simplified division of vehicle categories, based on CETESB data.

Due to the lack of information of the vehicle fleet, it was decided to make an own counting of vehicles in the tracks considered. The quantity of a certain pollutant emitted over a given period of time on a road was calculated with the following equality:

$$E_i = F_{r,j} \cdot F_{e,i} \cdot L \quad (6)$$

Where

E_i is the amount of pollutant i emitted (g),

$F_{r,j}$ is the total number of vehicles of category j which circulate in the road of interest during a certain time,

$F_{e,i}$ is the pollutant emission factor i (given in $g \text{ km}^{-1}$) and

L is the total length of the road for which it is desired to estimate the amount of pollutants emitted (km).

De Oliveira, et al. (2015) evaluated exhaust emissions (CO , NO_x and SO_2) for alcohol, gasoline and diesel vehicles by static tests with cold and hot starts, and in the idling mode of the engine. It was also noted that Otto cycle vehicles normally operate close to the stoichiometric ratio, while diesel-cycle vehicles operate with excess air, thus reducing CO emissions and increasing NO_x emissions in this type of vehicle. Based on all of this information, an approximate mass flow of each trace elements of exhaust gas pollutants were calculated to each track.

3. RESULTS

3.1 Flow Field

In order to represent a fully developed flow in the ABL, were used alternative values for the constants of the $k-\varepsilon$ turbulent model, found in field experiments (Kim & Baik, 2004; Santos, 2009).

Panofsky & Dutton (1984) presented a summary of field studies and concluded that the value of the ratio between the TKE and the friction velocity square is $k/u_*^2 = 5.48$ for a great variety of conditions in the atmospheric layer. Consequently, the value of C_μ should be 0.033, this value is less than 0.09 (used in the standard $k-\varepsilon$ model) and 0.0845 (used in the RNG $k-\varepsilon$ model). In addition, equation 3 must be satisfied. These facts were considered by Yi Yang et. al. (2009) to model the equilibrium ABL, in the theoretical derivation of a set of boundary conditions for the input and using the standard $k-\varepsilon$ turbulent model in an empty domain, obtaining good results.

A characteristic of these boundary conditions is that the new expression for k allows us taking into account the decrease of k with height, which corresponds better to wind tunnel results and full-scale measurements, while the profile of k by Richards and Hoxey (1993) is constant with height.

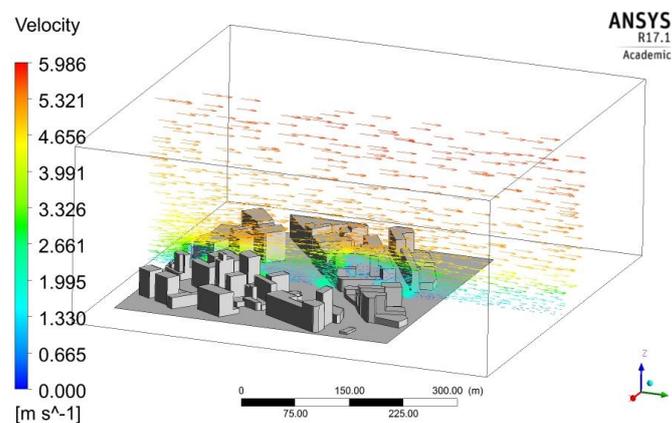


Figure 3. Velocity vector field in the central vertical plane (0 m, y, z).

The new turbulence input boundary conditions derived by Yi Yang et. al. was applied in our case study. Then the result of the velocity field was used to calculate the concentration field.

In Figure 3 and 4, the velocity vectors are shown, where the recirculation's predicted numerically in the canyon regions and the downstream flow of the buildings in vertical and horizontal plane respectively can be visualized in detail. Clearly it is seen that there is a massive airflow along the streets, which follows the prevailing direction of the wind.



Figure 4. Velocity vector field in the horizontal plane (x, y, 5 m).

3.2 Concentration Field

The scenario for the analysis of the dispersion of pollutants is presented in this section. Only the dispersion of CO, NO₂ and SO₂ were simulated since they comprise the pollutants for which more information was available, while other pollutants such as hydrocarbons and particulate matter did not have sufficient information of their sources, besides requiring other considerations such as resuspension, evaporations and secondary formation, which would make the analysis more complex.

The concentrations and TKE field generated by the modeling were superimposed on a plane perpendicular to the Conde de Bonfim Street (road with the highest vehicular traffic) for better visualization and analysis of the results, as shown in Figure 5.

The pollutants emitted by vehicles were implicitly represented as terms of mass source in the region of the first volume elements above each route considered. For this, the mass flow values calculated according to item 2.3 were used.

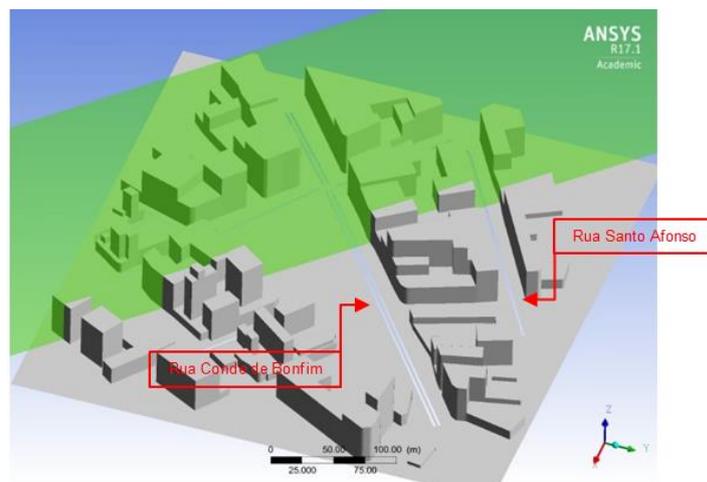


Figure 5. Baseline for representation of results.

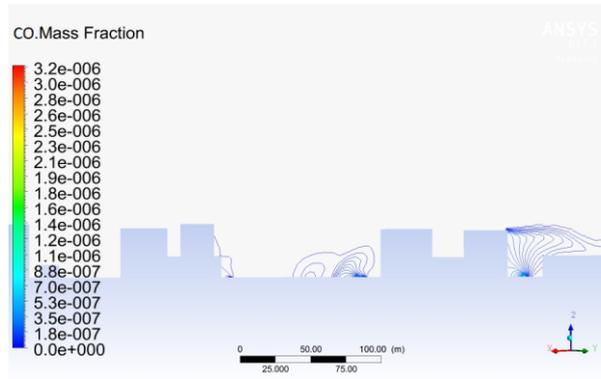


Figure 6. Concentration field of CO (ppm) with implicit TKE source of $5 \text{ kg m}^{-1} \text{ s}^{-3}$.

As already discussed, the contaminating gas released into the atmosphere has different physical conditions in comparison with the surroundings of the environment, such as higher temperature and especially higher TKE generated by the movement of the vehicles, being an important factor in the dilution of the pollutants. Therefore, a source of TKE equal to $5 \text{ kg m}^{-1} \text{ s}^{-3}$ was incorporated above the streets to implicitly simulate the mechanisms of turbulent mixing in the streets. Figure 6 shows the face of the TKE field with the inclusion of the TKE source above the street.

The concentration profile for the CO, in the base plane above Santo Afonso Street, shown in Figure 7, allows us to observe that the incorporation of the TKE source influences the horizontal dispersion in the first meters above the ground.

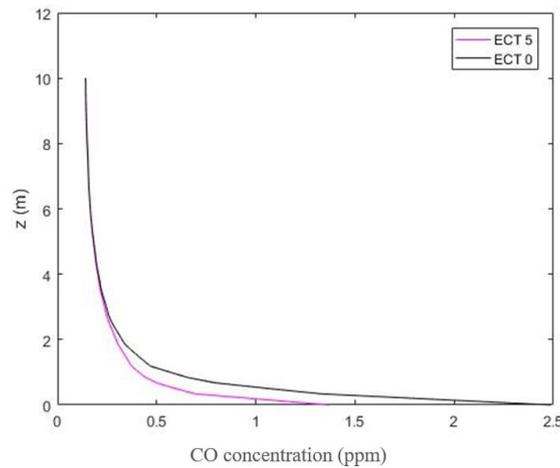


Figure 7. CO concentration profile in the base plane, above Santo Afonso Street, with and without TKE source.

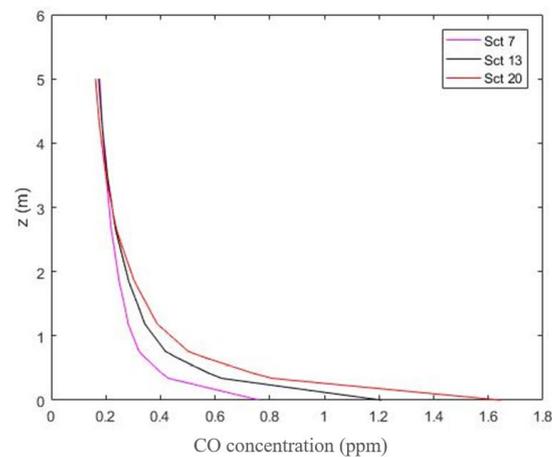


Figure 8. CO concentration profile in the base plane, above Santo Afonso Street, for $Scv = 0.7, 1.3$ and 2.0 .

Several experimental studies suggest that the optimum value for the Turbulent Schmidt number (S_{ct}) ranges from 0.3 to 1.0 according to the flow characteristics. Boçon (1998), concluded that the imposition of a smaller turbulent diffusivity coefficient on the system, results in less diffusion of the plume; while higher diffusions are obtained with the increase of this parameter. This phenomenon can be clearly visualized in Figure 8 which shows the concentration profile for CO in the base plane above Santo Afonso Street performed to Turbulent Schmidt numbers equal to 0.7, 1.3 and 2.0, for which the concentration field changes slightly horizontally in the first meters above the ground.

3.3 Model Validation

It is desirable to compare the results of the simulation with experimental data for several points of the domain, in order to determine if there is a good agreement, and to validate the simulation. However, we only have one measuring point at the monitoring station. Table 1 shows the average concentration of CO, NO₂ and SO₂ measured at the Tijuca station and those simulated numerically during the months of May, June and July. When comparing the results, it was possible to verify that the numerical simulation underestimated the concentration values by a factor of 16 for CO, 20 for NO₂ and 22900 for SO₂.

Table 1. Comparison between mean concentration of CO, NO₂ and SO₂ measured and those simulated at the Tijuca station site.

Pollutant	Average Concentration (ppm) - Tijuca Station	Simulated Concentration (ppm) at Tijuca Station site	Ratio between the measured value and the simulated value
CO	6.39×10^{-1}	4.03×10^{-2}	1.59×10^1
NO ₂	7.49×10^{-2}	3.75×10^{-3}	2.00×10^1
SO ₂	2.19×10^{-3}	9.55×10^{-8}	2.29×10^4

According to the air quality index (IQA) proposed by CETESB (2010), the air quality at the monitoring site is good with respect to the pollutants CO, NO₂ and SO₂. However, as can be seen in Figure 9, there are sites where the concentration of pollutants may be much higher than the concentrations measured at the monitoring site, especially near emission sources and in canyons where there is no good dispersion.

Although the field of study is small, it is clear that the simulation supports the choice of locations for the development of a sensor network to make a more elaborate match between the predicted concentrations in the numerical simulation and the observed concentrations.

In the simulation the transport of the pollutants is predominantly due to the turbulent flow, this would make us think that the face of the concentration field for the three pollutants considered in the study should be similar, but this is not so because the composition of the vehicular flow in each way and another sources that could not have been considered.

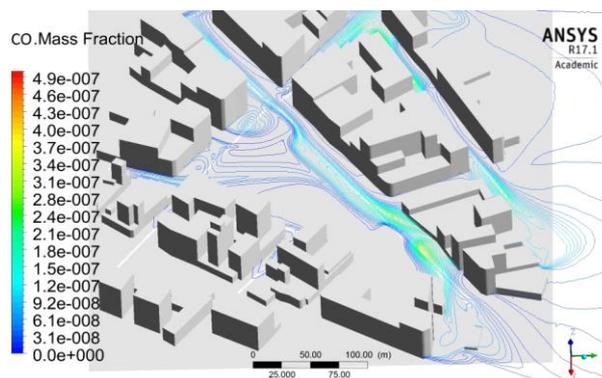


Figure 9. Concentration (ppm) in the plane (x, y, 3 m) for CO.

Figure 10, shows the isosurfaces concentration for CO corresponding to 0.05 ppm, it can be observed that the plumes present a tendency of their displacement in the predominant direction of the wind and that the low height of launching by vehicular sources, and the presence of obstacles (constructions), especially the canyons of the place, make difficult the transport of the plume by the wind. For example, in Santo Afonso Street, "contaminants trapped" is observed in that canyon. While the concentration at this location is not dangerous to the health of ordinary people in transit, it could have negative effects on local residents or people who remain in these places for a long time.

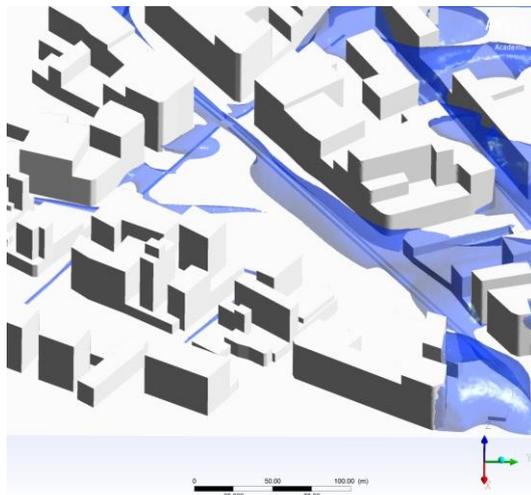


Figure 10. Isosurface concentration for CO at 0.05 ppm.

4. CONCLUSIONS

The area around the Tijuca station was chosen as the study area to investigate the dispersion of pollutants emitted by vehicular sources (CO, NO₂ and SO₂), in a neutral atmospheric condition, which is more common in the winter months.

The present methodology is appropriate for applications with practical significance, in which it is desired to mathematically model the transport of pollutants into the atmosphere, in order to evaluate impacts to the environment and public health from vehicular sources. This is of particular interest in an urban area where buildings make it difficult to disperse the pollutant.

The accuracy of the simulation was limited by the simplification of the domain, and by the lack of meteorology and emission information data, since the emission factors used in this study do not apply directly to the characteristics of the Rio de Janeiro's vehicular fleet. Consequently, due to these limitations, the results of the simulation were affected.

According to the results it was possible to observe that the TKE generated by the movement of the vehicles, influences in the initial dilution of the pollutants emitted in the tracks. Moreover, the best performance of the model, on the Turbulent Schmidt number, could be visualized through the comparison between the simulated concentration profiles. It can be seen that the curves obtained through the simulations with $Sc_t = 1.5$ appear to be more "flat" and with a more elongated base, which resembles more appropriately the natural profiles. This behavior can be explained due to the imposition of a smaller turbulent diffusivity coefficient, causing greater dispersion of the pollutant and greater tendency to horizontal spreading. Finally, in order to significantly increase the quality of the concentration field prediction in a real environment, one of the most important tasks was to sustain an atmospheric boundary layer developed along the computational domain. This was performed developing an appropriate configuration of the boundary conditions, defining the constants of the $k-\epsilon$ model, modifying the law of the wall constants and performing computational mesh tests. The results obtained in the simulations were compared with each other and also with available experimental data from the Tijuca monitoring station, observing good data agreement.

Suggestions for a future work include: to develop an approach which will integrate gas detectors, neural network and gas dispersion models, that can provide a real-time estimation of the gas dispersion, reducing the need to know in detail the information of the emission sources; and to study cases of dispersion of pollutants in domains that represent extensions from larger to more detailed areas, or even whole cities.

5. ACKNOWLEDGEMENTS

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