Simulation Tools to Analyze the Impact of Industries Installation

Gerson A. L. Nunes, Camila D. Thomasi, Márcio M. Jugueiro, Alexander Gularte, Diana F. Adamatti

Centro de Ciências Computacionais, Universidade Federal do Rio Grande

Av. Itália km 8 Bairro Carreiros, Rio Grande, Brazil

{dfrabu, camilathomassi, marcio.juguero,alexgularte, dianaada}@gmail.com

ABSTRACT

IThis paper presents a simulator that analyzes the impacts of the pollutants emission of a new industry insertion on a specific region (in our studies, at Rio Grande City – Brazil). This simulation calculates the atmosphere pollutants concentration and the user can chose between three pollutants dispersion models to simulate: a hypothetic model, ISC model or CALPUFF model, all of them were integrated to GIS.

Indexing terms/Keywords

Social simulation, pollutants dispersion, air quality control, ISC, CALPUFF.

Academic Discipline And Sub-Disciplines

Computer Science; Management of Natural Resources; Pollutants Emission

SUBJECT CLASSIFICATION

Computer Science

TYPE (METHOD/APPROACH)

Computational methods to simulate the pollutants emission in a specific study case.

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INTRODUCTION

 The natural resource management can be understood as a way to manage the use of lands, waters, plants and animals, aiming at the quality of life without compromising future generations. This topic has gained increased visibility with the growing concern about sustainable development (Camara et al., 1997).

The structuration of environmental policies in a national and international levels is essential to natural resources management, and softwares can contribute to the detail of these policies, helping in their implementation, maintenance and monitoring of their consequences and effects (Mattos, 2009) (Thomasi et al., 2011).

According to Fuller et al. (2007), there are three major computational challenges related to natural resource management: management and communication data; data analysis; and optimization and control. Resources management depends on Geographic Information Systems (GIS), in order to have interactivity, high performance, embedded computing and geographic distributed computation.

The problems created by excessive emission of pollutants are not recent and they had significantly increased due the fast industrial growth. An alternative is to take some preventive measures by knowing the risk of the installation of a new industry on a region.

The natural resources management requires that the government, citizens and other actors interact through the support of computing. In this context the simulation appears as a mechanism that plays real systems using computational tools, and support to prevision of future consequences and to assist in decision making (Freitas Filho, 2001) (Scire et al., 2000).

Using computational tools is an alternative to predict risks. By this way, these tools can create new possibilities for the control of air quality, because the simulations are able to predict the atmosphere concentration of pollutants.

In this context, the GIS are emerging as robust tool, helping to organize and to have a better understanding about the results, because they have methods/objects to view, manipulate, synthesize and edit the georeferenced data (Camara et al., 1997).

In our first studies, GIS is used in a hypothetic model, where the pollutants dispersion is simulated by a structure similar to a automata cellular (Nunes et al, 2010)(CONAMA, 1990). After, we use GIS to evaluate the dispersion radius of total suspended particles and to analyze the potential risk of contamination of coastal ecosystems near to the industrial zone in Rio Grande city (Brazil) (Thomasi et al., 2011) (Moraes, 2004), using the stationary model ISC (EPA, 1995) (Saraiva and Krusche, 2001). However, a non-stationary model (Scire et al., 2000) (Matlab, 2011a) provides a more realistic evaluation because the meteorological factors are under flotation most of the time. In this way, we are developed a simulation that calculates the pollutants concentration in the atmosphere, using the CALPUFF non-stationary Gaussian model (Scire et al., 2000) (Matlab, 2011a), to analyze the pollutants emission impacts of a new industry insertion in a specific region (in our studies, in Rio Grande City – Brazil) (Thomasi et al, 2012) (Matlab, 2011b).

The main goal of this paper is presented simulation tools, where the three models above described work together, in a graphic interface, that makes easier the use of them.

The paper is organized as follows: Section 2 presents the basic concepts of air pollution, the dispersion phenomenon and the requirements to air quality control. In Section 3 the tools used to implement the simulator are described. In Section 4 is shown complete simulator tool and the results. Finally, Section 5 presents the conclusions and future works.

POLLUTANTS EMISSION IN THE ATMOSPHERE

Some concepts of pollutants emission must be explained to better understand the models of pollutants dispersion:

Atmospheric Pollution
Chemicals, even toxics, are not necessarily considered atmospheric pollutants, because to cause damage they have to reach a certain concentration. In this way, an atmospheric pollutant is any form of matter, that a given quantity, exceeds the limits (defined by a control agency), and it transforms the air improper (Scire et al., 2000) (CONAMA, 1990) (Matlab, 2011a)(Vallero, 2008).

Therefore, the atmospheric pollution occurs when the air contaminants injure the well-being and health of people, and it cause harm to the environment (CONAMA, 1990)(Vallero, 2008).

The Dispersion Phenomenon
The dispersion mechanisms of pollutants in the atmosphere are governed by fluctuations in wind fields and turbulence (Moraes, 2004) (Vilhena et al.,, 2005).

The main meteorological factors that influence the atmospheric dispersion phenomenon are wind, temperature, pressure and terrain. The meteorological factors in the region can contribute in a positive or negative way in the mixing of contaminants with clean air. These factors could cause a quick or slow dispersion pollutants.

According to Saraiva and Krusche (2001)(EPA, 1998), the main damaging weather conditions to the pollutants dispersion in our study region are: high pressure associated with light winds, low temperature and high humidity.

Air Quality

The air quality standards are a control strategy used to indicate the maximum concentration of pollutants that could be issued to preserve the health and well-being of the population, flora, fauna and the environment in general (CONAMA, 1990) (Vallero, 2008).

The pollutants group responsible for controlling air quality, basing to their frequency in the environment, is composed of: sulfur dioxide (SO2), particulate matter (PM), carbon monoxide (CO), ozone (O3) and nitrogen dioxide (NO2). In this work only SO2, CO and NO2 are considered to evaluate the emission of air quality.

Excessive exposure to pollutants causes damage. Therefore, the great importance of the emissions control is to preserve the life quality of people and also the environment preservation (Scire et al., 2000) (Matlab, 2011a). According to the resolution of CONAMA – The Brazilian National Environmental Council (CONAMA, 1990) (Vallero, 2008), there are specific levels of emissions that are allowed, ranging from the lowest level of "attention" to the higher level of "emergency", as shown in Table 1.

Table 1. Standards of air pollution by Brazilian national environmental council (CONAMA, 1990).

Parameters	LEVELS		
	ATTENTION	ALERT	EMERGENCY
Sulfer Dioxide - SO2 (µg/m3) - 24h	≥ 800	≥ 1.600	≥ 2.100
Carbon Monoxide - CO (µg/m3) - 8h	≥ 17.000	≥ 34.000	≥ 46.000
Nitrogen Dioxide - NO2 (µg/m3) - 1h	≥ 1.130	≥ 2.260	≥ 3.000

USED TOOLS

This section describes the used tools to develop the simulator. These tools were chosen because of their availability, documentation, generation and manipulation of maps iteratively.

MATLAB

The MATLAB (Matlab, 2011a)(Lakes, 2011) is a programming language with several libraries that allow us to perform a series of scientific calculations, statistics, solution of linear differential equations, engineering calculations, etc. Moreover, it has specific libraries to work with neural networks, filtering, bioinformatics, telecommunications, imaging, digital signal processing, automation, GIS and others.

In this work, to automate the processes of file management, data import, creation, manipulation and presentation of maps and their respective layers, we have chosen the GIS library (called "mapping toolbox"). This library was also important to perform post-processing data of the CALPUFF model and results analysis.

Mapping Toolbox

The mapping toolbox (Matlab, 2011b)(Nunes et al., 2010) is a library of specific functions that allow us analyzing geographic data, create and manipulate maps. It imports both vector and raster type data. It also has support to the most common file formats, such as shapefile, GeoTIFF and DEM SDTS. In addition, it is possible to import data from WMS servers (Web Map Service). Thus, the developer can customize his application in subsection, side view, intersection and other methods.

The toolbox features allow us to develop customized solutions for various geographic problems. Some of these features allow that different layers data can be easily manipulated and presented in the same map.

Other features that also deserve attention are those that allow you to convert different types of coordinates, facilitating the use of data from different sources and to allow you to save all creation and manipulation of files that can later be analyzed by users of GIS software.

GIS - Geographic Information System

The GIS (Geographic Information Systems) (Vallero, 2008)(Thomasi et al., 2012) are softwares that manage, view and manipulate geographic data computationally. They allow that each set of data can be presented in different layers.

The layers are composed by a set of features of geographic objects. These objects have an infinite variety of shapes, but they can be represented basically by three different kinds: polygons, lines or points. Polygons represent things that have limits such as countries, states, cities or lakes. Lines represent narrow things such as streets, roads, rivers or railroads. Points are used to small things such as buildings, hotels, schools, fire hydrants or poles. The union of polygons, lines and points generates the vector data.

Therefore, GIS are used for better understanding the patterns, relationships and trends in the data. Many times, those information are not obvious to find in databases.

Graphs

According to Goodrich et al (2002), graphs represent the relationship between pairs of objects in a set. They are composed by nodes (vertices) and connections (edges). A graph is a data structure that can be used in a lot of applications. In our studies, they are used to create and manipulate the maps of the GIS.

To implement a graph, it is necessary an auxiliar data structure. We choose the adjacency matrix to do that, because it shows the possible relationships between the vertices. To investigate the relationship between the nodes of the graph, all positions of the adjacency matrix must be analyzed. If a particular position has the value 0, we consider that there is no connection between nodes i and j. Otherwise, we say that a relationship exists between them.

THE SIMULATION TOOLS

The goal of the simulator is to provide the best location for insertion of a new industry, allowing prior knowledge of the risks and, in this way, help public and private sector in the making-decision, in Brazilian context. For that, all simulator was implemented in native language, Portuguese.

Some steps are the same for all models available in the simulator such as Maps manipulation and Impacts generation. Other steps are specific to each model. Maps manipulation is used to read, write, manipulate and display vector files. The objects insertion lets us choose the geographic location where the industries are inserted, and also their initial parameters of the simulation.

Impacts generation is used to plot the concentration of each point, according to its latitude and longitude around the industry. In this step a shape file is created and it contains the junction of industries and pollution points, basing in initial map inserted.

The basic inputs to start the simulation are: the map file (shape) of the interest region, the parameters of the industry to be inserted and the name of an output file (shape).

Firstly, maps are read, manipulated and presented. Before simulating the impacts, the insertion of objects (industries) is done. Finally, the all results are stored in an output file and it could be presented in graphics.

When the simulator is initialized, the user should choose the model (Hypothetic, ISC or CalPuff), as presented in Fig. 1. Afterwards, s/he should define the output name to identify the simulation (Fig. 2).
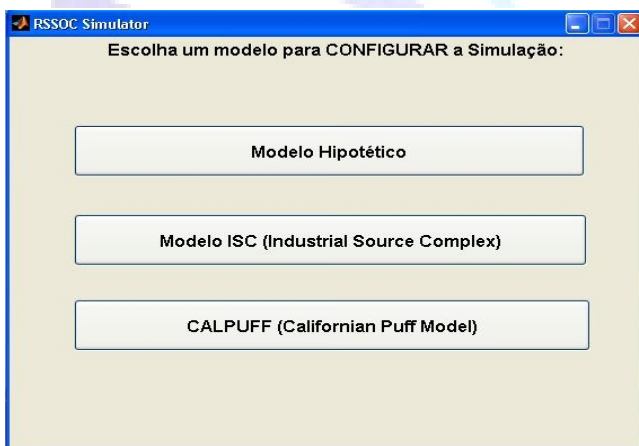

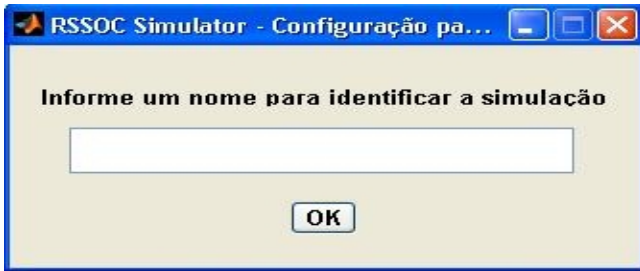**Fig. 1. First screen of the simulator, where the user should choose the pollution model.**

Fig. 2. The user should inform the output name to identify the simulation.

Hypothetic model

This is our first model, an academic model to pollutants dispersion. All algorithms and formulas were created by our group and they are hypothetical. They serve to prove that it is possible to propagate the environmental impacts caused by construction in the region and their neighbors. The basic rules pollution spread are defined by (1).

$$Pol_x = Pol_{index} \cdot \sum_{i=0}^{n} \left(\frac{B_i}{P_x} \cdot Pol_i \right) \qquad (1)$$

Where:

Polx represents the pollution that we want to calculate. Polindex is a constant representing the maximum pollution rate that comes from neighbohood, Bi is the bordary length between the regions, Px is the region's total perimeter. Poli is the existing pollution in neighbour. The idea is incremeted the neighborhood pollutions, basing to the neighboring borders and boundaries of the region. The result of this sum is multiplied by the maximum pollution index of pollution, and it is propagated by the neighbors.

Fig. 3 presents the graphical interface to this model, where the user informs the input file (shape) and all industries locations (latitude and longitude points) as well as the percentual of pollutions in each industry.
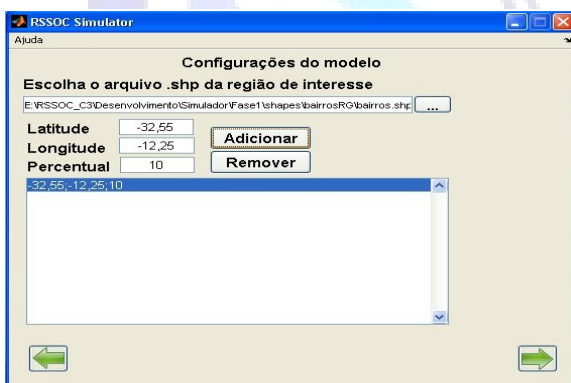

Fig. 3. Graphical interface to hypothetic model.

ISC (Industrial Complex Source) Model

The Gaussian model ISC (Industrial Source Complex) enables the emissions modeling from a wide range of sources present in a typical industrial complex.

According to EPA (1995, 1998), the basis of the model is linear and stationary Gaussian plume that, with some modifications, is used to model emissions from sources in a simple point - the stack. The equation shown in Figure 4 is used to calculate the pollutants concentration emitted from point sources.

$$x = \frac{Q.K.V.D}{2.\pi.U_s.\sigma_y.\sigma_z} \exp\left[-0.5\left(\frac{y}{\sigma_y}\right)^2\right] \quad (2)$$

In Equation (2), the equation shows that the concentration x depends on several factors. Q is the rate of emitted pollutants (g/s), K is the coefficient of expansion used to convert the calculated concentrations in desired units, the term vertical V represents the vertical dispersion caused to reflection (it can be or not enable), D is the decay, σy and σz are the standard deviations of the lateral and vertical concentration distributions in meters, Us is the wind speed in the stack height and Y is the crosswind distance.

As ISC model allow just one pollutant source (one industry), the Fig. 4 presents the graphical interface to insert all factor (described by equation 1) in the simulator.

Fig. 4. ISC Model Graphical interface.

CALPUFF Model

The last one model implemented in the simulator is a non-stationary pollution dispersion model, called CALPUFF. The non-stationary models can be Eulerian, Lagrangian and Gaussian. The Eulerian and Lagrangian models have a high computational cost due because they need to solve complex equations. It requires parallelization to obtain a satisfactory response time. In other hand, the Gaussian models do some simplifications that it allows a faster response, making it attractive for real time applications.

CALPUFF is a non-stationary Gaussian model that allows the prediction of risks caused by one or more industries in a specific period of time, varying the weather conditions in space and time (EPA, 1998).

Calpuff model is recommended by U.S. EPA (Environment Protection Agency) due to be working with a micro-region and it can handle complex three-dimensional wind fields. It is easy to setup and run for point sources with multiple parameters.

The Gaussian models do not have accuracy when we use a complex topography or emissions near the ground. In our experiments, these factors are not relevant because the simulated region has a flat terrain and their emission sources have a certain distance from the ground. The work aims to develop a tool to help the community and responsible entities in decision-making, visualization and evaluation of possible risks caused by the pollution emission from industries, without the concerned of accuracy.

The proposed simulator integrates the Gaussian CALPUFF model to MATLAB in order to automate their execution. The Matlab Mapping Toolbox saves and presents the output data in a vector layers and it can be manipulated in GIS softwares.

The Modelling of Proposed Simulator

With CALPUFF model, we want to predict what will be the risks in a specific region by the pollutants emission caused by the insertion of one or more industries. The result of the simulation is a layer with georeferenced points containing the concentration of certain pollutants. The simulator calculates the pollutants concentration resulting from one or more emissions.

The simulator is divided in two modules: CALPUFF model execution and maps' manipulation. According to the flow diagram, shown in Fig. 5, the basic inputs to start the simulation are: the shape file containing the map of the interesting region and the output shape file names. The simulation returns the files with georeferenced points.
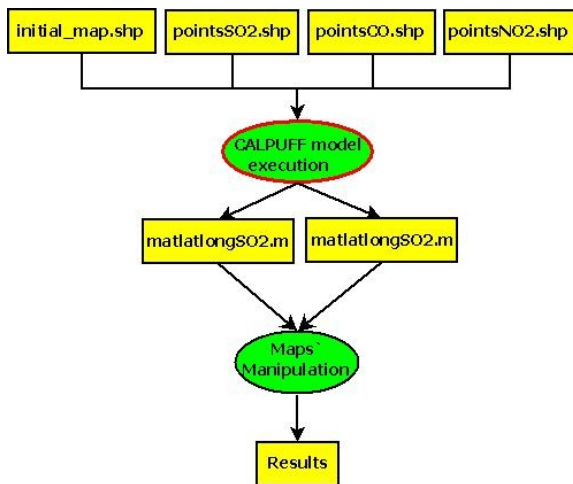
Fig. 5. Data Flow Diagram to use the CALPUFF non-stationary Gaussian model.

In the CALPUFF model execution stage all the settings and procedures for their execution are made and these steps are explained in greater details later.The output of this module has two georeferenced matrices containing latitude, longitude and pollutants concentration in the points. These matrices will be the inputs of the next step (maps manipulation) and they have the function of read, write, manipulate and present the vector files. Three structures are created, one for each pollutant to control the air quality: SO2 (sulfur dioxide), CO (carbon monoxide) and NO2 (nitrogen dioxide), containing the attributes shown in Table 2. The elements of these structures are filled with the input values. After this procedure, three layers are created, one for each pollutant, which are the simulator output files.

The last step is the creation of the georeferenced matrices that have the concentrations and converted UTM coordinates to latitude and longitude coordinates for each gridded point.

The plume, in these models, is represented by a set of discrete puffs of polluting material (Moraes, 2004), as shown in Fig. 6.
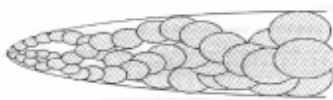

Fig. 6. Representation of plume in CALPUFF model.

Table 2. Structure of points

Attribute	Type	Description
Geometry	*string*	Geometry of the point;
BoundingBox	[2x2 *double*]	Extreme of the point;
X	[1xN *double*]	X coordenates set in the point;
Y	[1xN *double*]	Y coordenates set in the point;

POLLUTION	*double*	Calculted pollution level by Gaussian model;
LOCAL_X	*double*	X coordinate of the location of the center point;
LOCAL_Y	*double*	Y coordinate of the location of the center point;

The puffs mass is dispersed according to a Gaussian distribution. The transport is made according to the trajectory of its mass center and the local wind vector speed (Moraes, 2004).

The wind changes every hour, changing also the puffs path to the wind flow. While the puff is transported in the air, its pollutant concentration decreases. If the puff finds out other receptor, a new pollutant material is increased to it (EPA, 1998).

The Equation (3) is the basic equation to provide the contribution of a puff on a receiver (Scire et al., 2000). To discover the total concentration of a receiver, it is necessary to add the concentration of neighborhood puffs of a particular receiver.

$$ C = \frac{Q}{2\pi\sigma_x\sigma_y} \ g \ \exp\left[-d_a^2/\left(2\sigma_x^2\right)\right] \exp\left[-d_c^2/\left(2\sigma_y^2\right)\right] $$

(3)

Where C is the ground-level concentration (g/m3), Q is the pollutant mass (g) in the puff, σx is the standard deviation (m) of the Gaussian distribution in the along-wind direction, σy is the standard deviation (m) of the Gaussian distribution in the cross-wind direction, σz is the standard deviation (m) of the Gaussian distribution in the vertical direction, da is the distance (m) from the puff center to the receptor in the along-wind direction, dc is the distance (m) from the puff center to the receptor in the cross-wind direction, g is the vertical term (m) of the Gaussian equation (Thomasi et al., 2011).

CALPUFF Model Execution
The CALPUFF model execution in the simulator is responsible for setting up all files and parameters needed to run the model. With this analysis, is possible to observe the entire operation of the system.

Initially, the terrain configurations are made based in a file that has the x and y coordinates of all terrain and elevation. To obtain these information is necessary to run the TERREL.

TERREL is a preprocessor to create the terrain elevation data from multiple databases to a grid specified by the user (Scire et al., 2000). This preprocessor has a control file where the scanned files are assigned. According to the flow diagram in Figure 7, the first thing is to obtain the terrain and topography grid, using files available in WebLakes (Lakes, 2011). The next step is to configure these files as input to the control file terrel.INP.

Once that is done you can run the module runTerrel. This preprocessor provides as output a formatted file containing the coordinates in UTM X, Y and Z (elevation of the land).
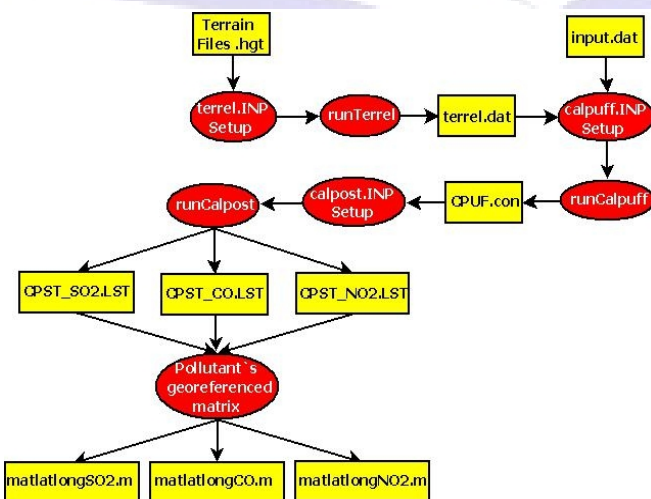

Fig. 7. Steps of CALPUFF model execution.

After obtaining the characteristics of the terrain, the next module is responsible for the CALPUFF Model control file configuration/setup. In this module, two files are needed as input: the terrain file (terrel.dat) and the region weather setting file (input.dat). The terrain file is provided from the preprocessor TERREL and the region weather file is a formatted file containing: day, month and year of data, simulation hours (0-23 hours), wind direction in degrees, air temperature (° K), Pasquill stability class (Scire et al., 2000) and the urban and rural mixing heigths (m). With these inputs and the configured control file calpuff.INP, it is possible to run the execution module of the CALPUFF (runCalpuff). This module generates its output as a binary file (conc.dat) that contains an average grid of pollutants concentrations, which were simulated in a period of time.

To calculate the concentrations, the conc.dat file must be executed in CALPOST postprocessor (Scire et al., 2000). For that, firstly, the calpost.INP configuration module should be setted with the runCallpuff. After it, the runCalpost should be executed to the number of species issued. In this work, we have issued three species: SO2, CO and NO2. As output files are provided CPST_SO2.LST, CPST_CO.LST CPST_NO2.LST and these files provide the concentration values in each grid point.

Our simulator combines several graphic interfaces in all the CALPUFF model steps above described. As can be seen, the full process is rather complex. The Figures 8, 9, 10, 11, 12 and 13 show these interfaces. It could facilitate the use of the CALPUFF model for less experienced users in the pollutants dispersion and meteorology areas.
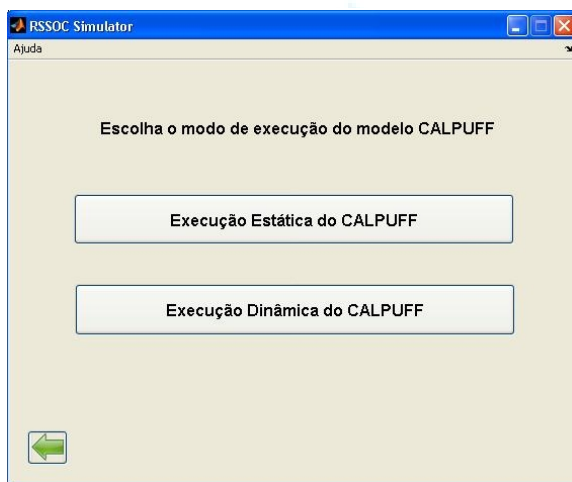

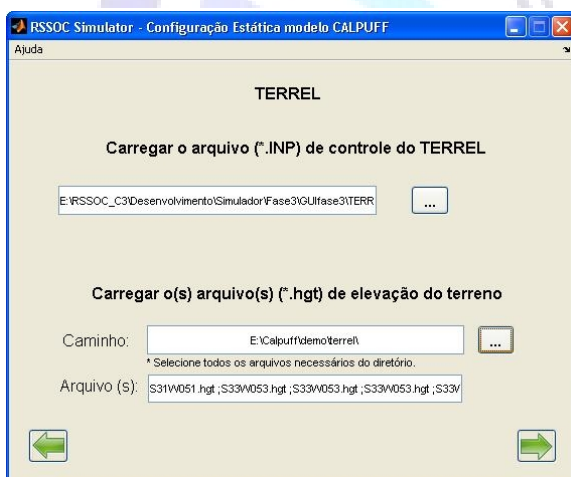**Fig. 8. First CALPUFF graphical interface: Dynamic or Static execution.**

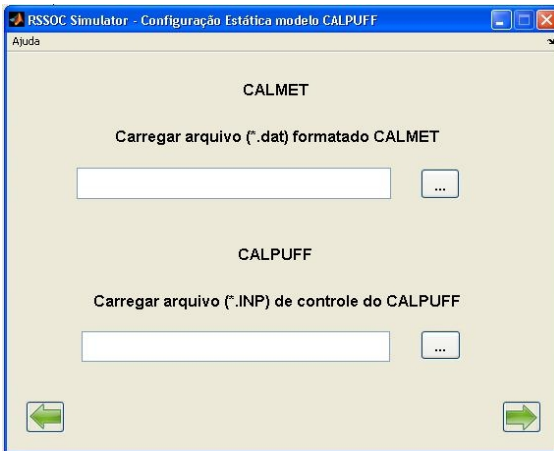**Fig. 9. Graphic Interface to inform files to TERREL pre-processor.**

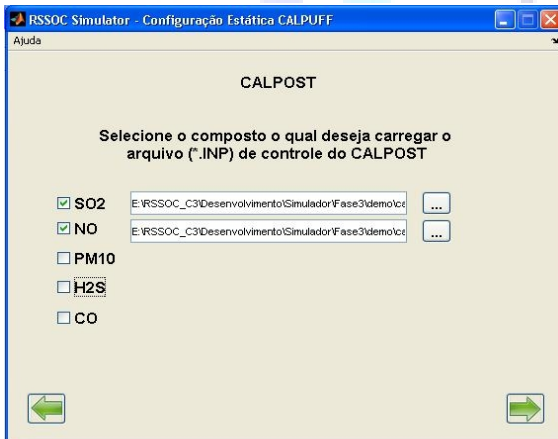**Fig. 10. Graphic Interface to inform meteorological and configuration input files to CALPUFF module.**

Fig. 11. Graphic Interface to inform files to CALPOST module.

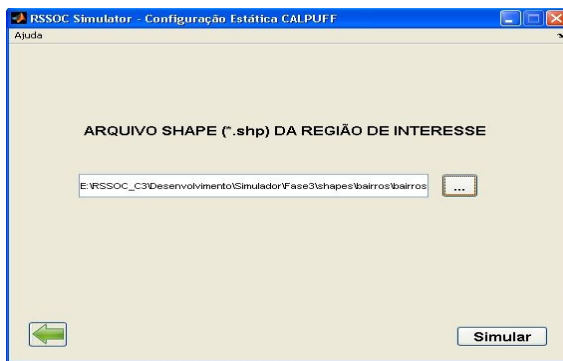**Fig. 12. Graphic Interface to inform the industry position to simulation.**

Fig. 13. Graphic Interface to inform the interesting region shape file.

SOME RESULTS

The last step of the simulation is to present the results. In our tests, we have chosen the industrial zone in Rio Grande city, in southern Brazil, to evaluate the model. The city has a large number of industries which emit a large quantity of pollutants in the atmosphere.

The simulator allows the user customizes the industry features to be inserted, according to their emission profile. The following features can be modified according to the desired simulation scenario: latitude and longitude, elevation, height and diameter of the stack, speed and temperature of the pollutant output and emission rates of pollutant source.

Our tests involve ISC and CALPUFF simulator. The meteorological data in the ISC simulator are: wind direction and speed, air temperature, and Pasquill-Guifford-Turner stability class (Scire et al., 2000).

The ISC simulation was done using a single pollutant source during one hour of emissions. The source is located at 52.10452S and 32.11354W and it is characterized by a flow of 500g/s; chimney height of 25 meters; chimney diameter of 5 meters. The meteorological conditions were: pressure of 1010mbar; wind speed of 12m/s; wind direction of 225°; temperature of 25°C and Pasquill-Guifford-Turner stability class was D according to Scire et al. (2000).
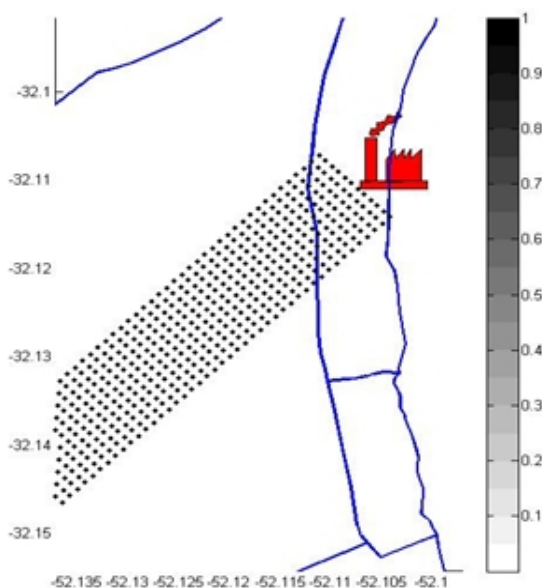

Fig. 14. Some results to ISC model.

Next, we did the tests with CALPUFF simulator. The simulations are more complex due to the one month period, where scenarios were simulated with until 10 pollution sources and all input meteorological variables vary each hour. In our tests, the emission sources are located as presented in Table 3. Fig. 15 shows the geographical industries location. However, some of these industries have more than one pollutant source.

This region has the following characteristics: void elevation, because it is situated at sea level; 25-50 meters of chimney height; 1-2 meters of chimney diameter; output speed 5-10m/s; output temperature 170-208°C; and the following emission rates: 7.4 of SO2, 44.39 of CO and 88.78 of NO2, in g/s to all sources.

According to CALPUFF model simulations we get the results as shown in Fig. 16 and Fig. 17. The Fig. 16 shows the NO2 average pollution concentration along month. The Fig. 17 shows the NO2 maximum concentrations along month.

The pollutants shape file is superimposed on the map of the interesting region, providing a better interface to analyze the results. In this map, the colored contour curves refer to model calculated concentration as shown in Fig. 18.
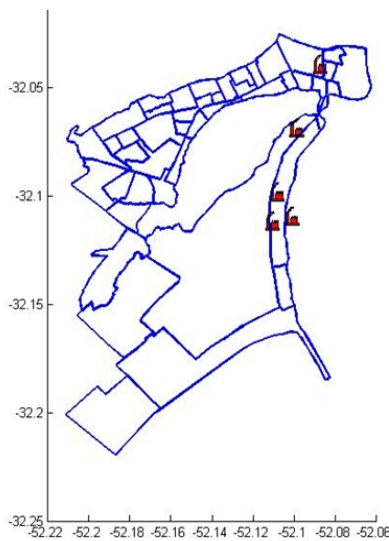

Fig. 15. Industries location

Table 3. Sources location

Source	Latitude	Longitude
1	52.10452 S	32.11354 W
2	52.09105 S	32.04325 W
3	52.11396 S	32.11577 W
4	52.10224 S	32.07274 W
5	52.10291 S	32.07091 W
6	52.09789 S	32.07714 W
7	52.11182 S	32.10231 W
8	52.09111 S	32.04496 W
9	52.10048 S	32.07073 W
10	52.08796 S	32.04377 W

We can analyze the consequences from emissions of the pollutants SO2, NO2 and CO in accordance with current legislation (Scire et al., 2000). CALPUFF model provides more accurate values of pollutants concentration in a specific period and the period could be longer. The highest values are compared with the data in Table I, which presents tolerable limits defined by law in Brazil, CONAMA (1990).

The Fig. 18 shows a moment where the NO2 concentration crossed 1130µg/m3. It means, according with Brazilian's law, that the attention level was achieved. According to the simulated results, the highest CO concentration reached 833.07µg/m³, the SO2 reached 211.23µg/m³ and NO2 reached 1662.6µg/m³ (see Figures 17, 20 and 22).

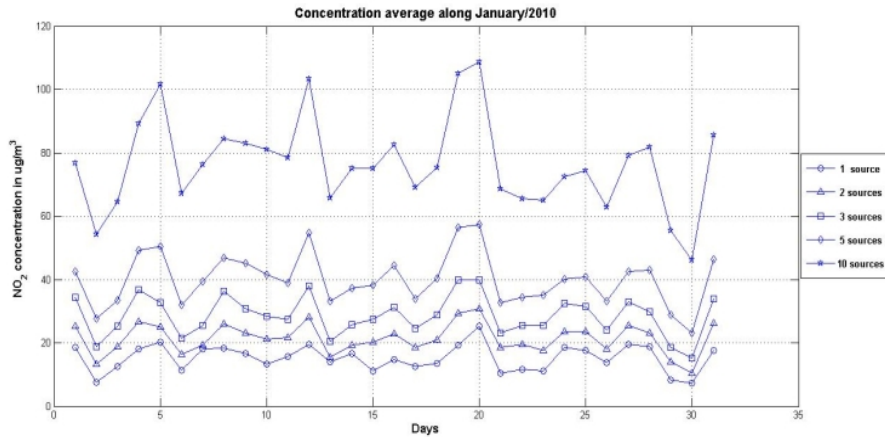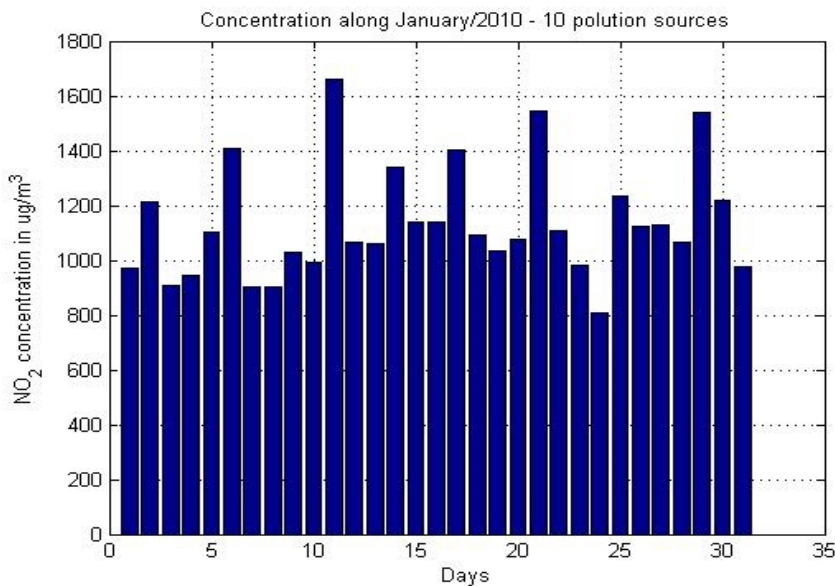**Fig. 16. NO2 mean concentrations along month.**

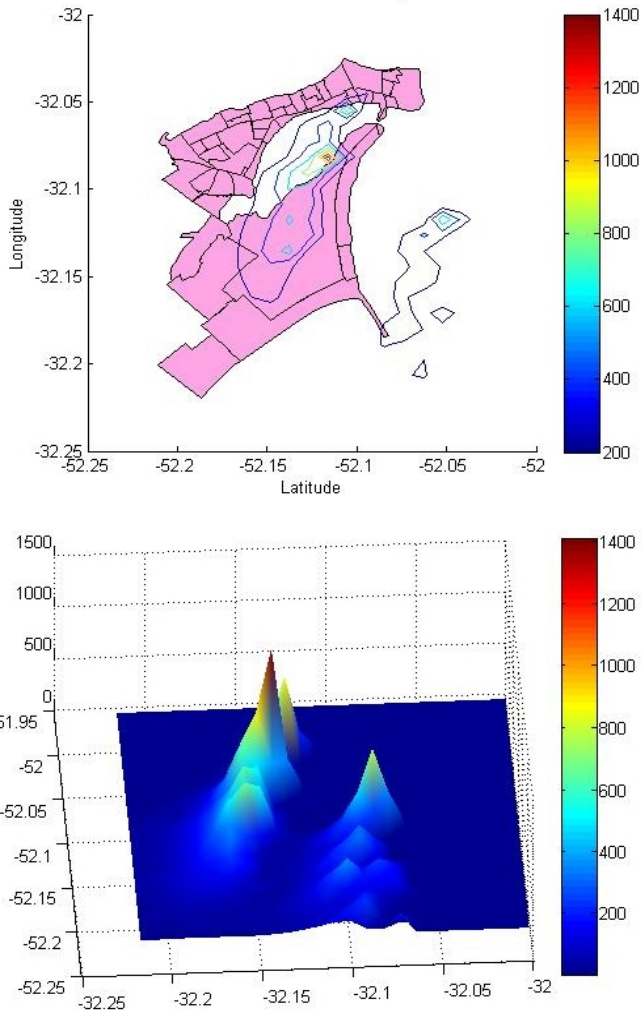
Fig. 17. NO2 maximum concentrations along month.

Fig. 18. NO2 concentration achieving attention level.

The Figures 19 and 20 show the SO2 pollution concentration along month. In the first one, the average concentration and in the second the maximum concentrations.
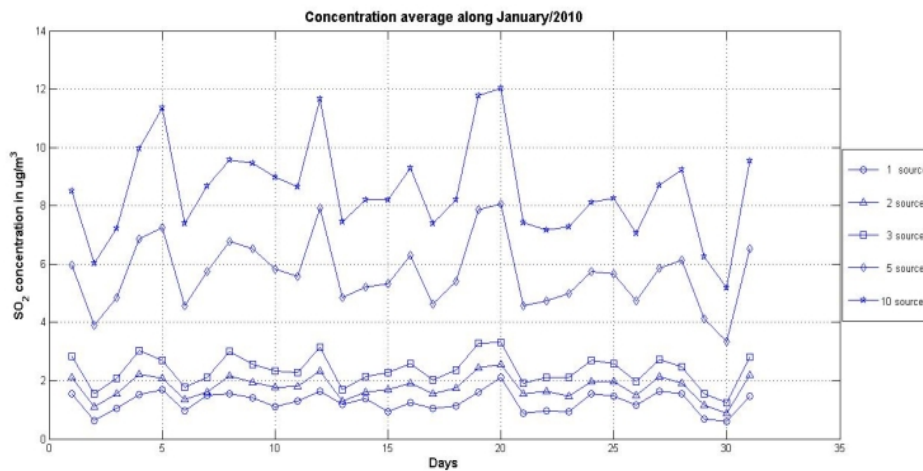

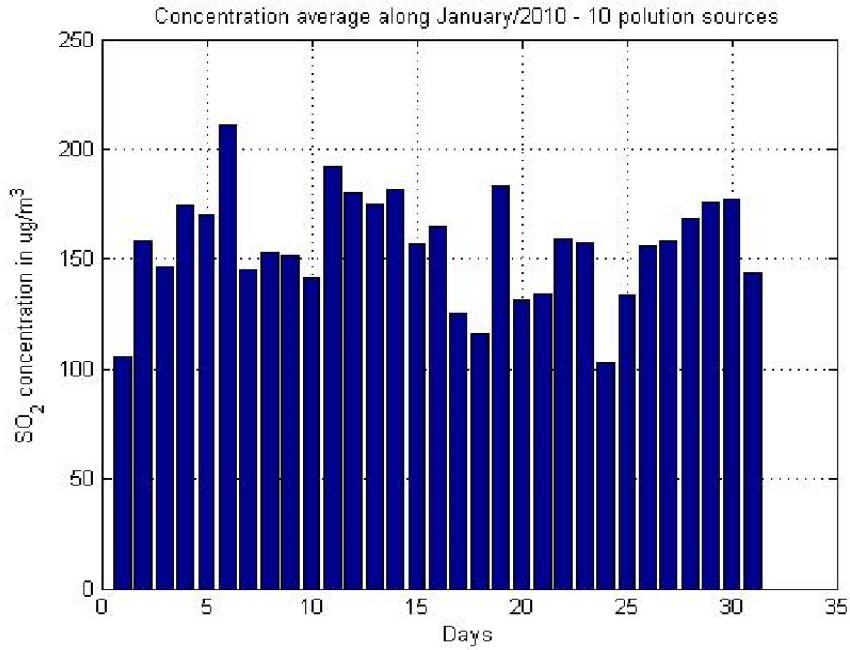**Fig. 19. SO2 mean concentrations along the month.**

Fig. 20. SO2 maximum concentrations along the month.

The Figures 21 and 22 show the CO pollution concentration along month. In the first one, the average concentration and in the second the maximum concentrations.
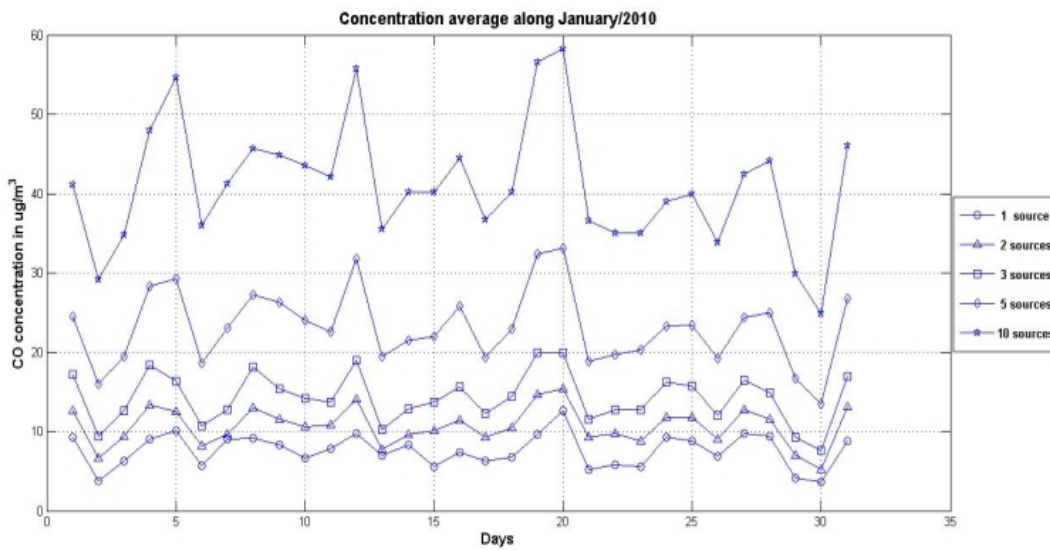

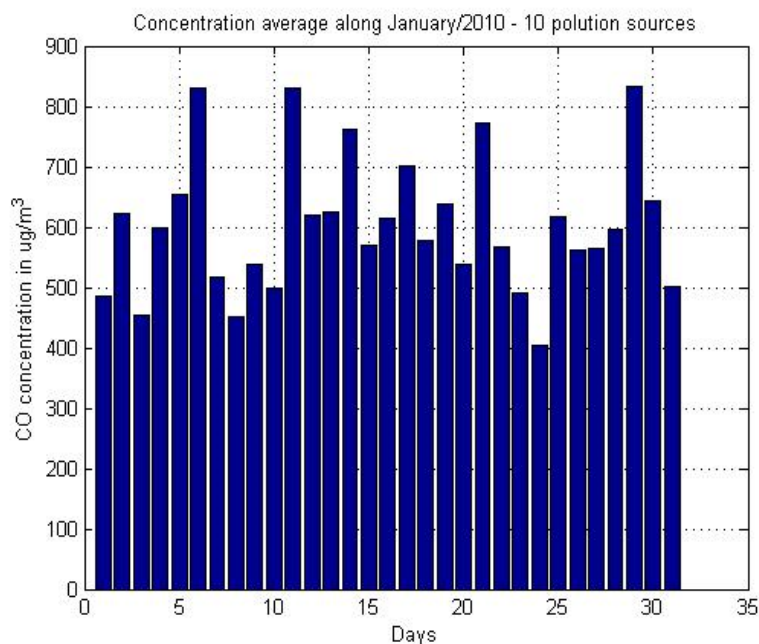**Fig. 21. CO mean concentrations along the month.**

Fig. 22. CO maximum concentrations along the month.

CONCLUSIONS

This paper presented a full simulation tool, where the three models above described work together, in a graphic interface, which makes easier the use of them. The main idea is to analyze the air quality when new industries are inserted in a specific region.

Our case study is the Rio Grande city (Brazil), and it has, historically, problems with air pollution and few works explore this scenario. The second reason to choose this region is because we live here and we believe that computational tools could help a better understanding about environmental problems and improve the people lives.

Our initial tests, using a hypothetical situation, just help to analyze how these models process the data. Our tests used a lower number of emision sources than the reality and the results were concern, because to NO2 concentration, the attention level was achieved. Related to the other pollutants, SO2 and CO , the concentration values still below to attention level, according to Brazilian law.

As further work, we will execute the model for a long period (probably one year) and many emission sources (more than ten). This new scenario will present a more realistic situation, and more comparisons will be done. Furthermore, we want to study the feasibility of including analytical models to the simulator, in order to supply some deficiencies of Gaussian models, so that the results approximate to the maximum of reality.

Other future works evolve the development of a DSS (Decision Support System) to assist communities and agencies involved to correct making-decision, contributing to the learning and analysis of public policies related to the environment.

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