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SOFIA: AN INTEGRATED COMPUTATIONAL MODEL FOR AIR QUALITY

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Abstract. *This paper presents a numerical model for predicting air pollutant concentrations in a 3D geo-referenced framework. The model (**SofIA** = Software de Impacto Atmosférico) is based on a Gaussian dispersion criterion. A wide range of sources arising from a typical urban study area are included in it, i.e. mobile sources, residential and commercial emissions, open burning, dust resuspension and stack releases. As output, the model gives the concentration fields for the considered pollutants, and both short-term and long-term exposures.*

In order to show the model capabilities, the simulation of the air quality in a megacity is presented. Model calibration and validation procedures are discussed. Although the available database to feed the model is reduced both in quality and quantity, a relatively good agreement between measurements and predicted concentrations is found. In this way, it is shown that the model is able to represent the main characteristics of the local air quality.

The impacts of potential mitigation measures on the local air quality are also presented, including long-term NO_x *and* PM_{10}*. Predictions for the period 2000-2012 are presented.*

Finally, some recommendations about model improvement are discussed.

1 INTRODUCTION

The availability of relevant and accurate environmental information is essential for environmental policy-makers. In particular, most of the megacities around the world have from moderate to very serious problems related to air quality, so the correct prognosis about the impact of mitigation options is of prime importance.

As first-cut approaches to modeling air quality inputs for health/economics analyses two properties are ideally required:

- A portable, user-friendly modeling system that can be adapted to new cities
- A modeling approach that provides a good compromise between complexity and efficiency

There are not modeling systems fulfilling those properties. Nevertheless, in order to quantify the mentioned impacts a wide range of air quality models have been developed [1].

The selection of a particular numerical tool depends basically on the quality of the available data required to feed and to validate the model. When only a few data are available a zeroth order approach is recommended (i.e., crude estimates based on macro variables). Alternatively, a first order approach could be used (i.e., “roll-back” or source apportionment methods) [2].

More sophisticated tools are based on dispersion criterions. In this field, the simplest systems are the box models [3]. Second order approaches use dispersion modeling, which need meteorology, emissions inventories and greater computational resources. The new trends can be grouped in the nth order approaches, which need detailed and accurate inputs and have hefty computational requirements (i.e., US-EPA Mesoscale Models3).

Here we present a computational system based on the Gaussian dispersion (second order) approach. Taken into account that traffic is in general the main pollution source in big cities, a special treatment is performed to simulate mobile sources according to the available input data. All kind of sources arising in a typical polluted city are included in the model.

To show the model capabilities, the case of the Buenos Aires City is presented. The model is calibrated and validated, and some prognosis related to green house gases (GHG) emissions reduction are presented.

2 *SOFIA* MODEL

2.1 Theoretical background

Under an Eulerian framework, the concentration of any pollutant in the atmosphere can be described by the following advection-diffusion-reaction (ADR) equation:

$$\frac{\partial c}{\partial t} + \mathbf{u}.\nabla c = \nabla.\left((\nu + \nu_t)\nabla c\right) + R + S \qquad (1)$$

with

c : concentration
t : time
$\mathbf{u}$: atmospheric velocity field
ν : molecular viscosity of the air
ν_t : turbulent eddy viscosity
R : reaction rate
S : source/sink of pollutant

Equation (1) was obtained considering air incompressibility and performing a Reynolds average of the Navier-Stokes equations. Also, it was considered that the pollutant is passively transported by the atmosphere (i.e., the pollutant's presence does not modify the velocity field).

Here we consider the following simplifying assumptions, based on the uniformity of turbulence:

- The flow is stationary and it is characterized by a main direction of motion (the wind direction)
- The effective viscosity (the sum of the viscosities defined in eq. (1)) has non-null components only on the plane that is perpendicular to the wind direction

Then, for the case of a point source equation (1) reduces to:

$$u\frac{\partial c}{\partial x} = \nu_y \frac{\partial^2 c}{\partial y^2} + \nu_z \frac{\partial^2 c}{\partial z^2} + R + Q\delta(\mathbf{r} - \mathbf{r_0}) \tag{2}$$

with

u : wind velocity
x,y,z : Cartesian coordinates, assuming that x is in the wind direction and z is the vertical direction
ν_y, ν_z : Effective viscosity in the corresponding y,z directions
Q : Emission rate of pollutant
$\mathbf{r}$: Position vector
$\mathbf{r_0}$: Source location

Equation (2) allows obtaining the classical solution for the three-dimensional field downwind of the point source:

$$c(\mathbf{r}) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left[-\frac{(y-y_0)^2}{2\sigma_y^2}\right] \exp\left[-\frac{(z-h_e)^2}{2\sigma_z^2} - \frac{(z+h_e)^2}{2\sigma_z^2}\right] \exp\left[-\frac{k(x-x_0)}{u}\right] \tag{3}$$

where the reaction rate is assumed that represents a first order reaction, the terrain is considered flat and fully reflective, and

x_0,y_0 : source location in the x-y plane
h_e : effective plume height
σ_y, σ_z : standard deviations of the Gaussian plume in the y,z directions
k : reaction coefficient

The standard deviations are defined experimentally, through field studies of plume dispersion. Here we use those proposed by Hanna et al. [4], which depend on terrain properties and stability class.

2.2 Boundary conditions

The computational domain is a 3D volume covering the city and its suburbs. In the case of gases, the terrain is considered fully reflective, while in the case of particulate matter (PM) partial or total absorption and dust resuspension are allow.

The space overhead the city is considered infinite, with the exception of the presence of any inversion layer. In the last case a reflective lid is imposed. All horizontal reflective boundaries are simulated through the use of the virtual source method.

The vertical boundaries are considered as transparent, so the pollutant plumes can cross them with no accumulation of mass into the domain.

2.3 Point sources

The industrial activities typically contribute to air pollution level through stack releases. When the scale of the study covers a whole city, those releases can be simulated directly using equation (3).

In those cases, the effective plume height takes into account both the near field zone (i.e. the zone where the buoyancy and initial momentum are dominant) and the far field zone (i.e. the zone where plume dispersion is controlled by atmospheric conditions) [5]. When a water body is close to the stacks, the effects due to thermal internal boundary layer development (such as shoreline fumigation) are included [5].

2.4 Non-point sources

Non-point sources can be simulated either by:

- Integrating equation (3) over the emission domain
- Using virtual (equivalent) point sources
- Discretizing the emission domain through multiple point sources

We adopt the third option. The main traffic network (highways and avenues) is represented through line sources. In general, traffic data at neighborhood scale is scarce or null, so we represent this important emission source through area sources. Into each domain the emission rate is considered uniform, simulating the diffusive character of the mobile sources emission. Domestic and commercial pollution is also represented using area sources.

2.5 Reaction modeling

In the case of PM_{10} only primary emissions are considered, that is, no secondary aerosol formation is accounted for.

The deposition process is mainly due to two phenomena:

- Dry deposition, due to gravitational settling
- Wet deposition, owing to the rain scavenging

Both of them can be modeled as first order reactions. In the first case, the reaction coefficient is calculated as a function of the deposition velocity. For wet deposition, the first order decay constant is obtained using the scavenging coefficients reported in the literature [6].

2.6 Computational System

To obtain the air pollutant concentration field, all the mentioned contributions are integrated using the superposition principle. This procedure is done by the computational system ***SofIA*** (Software de Impacto Atmosférico). ***SofIA*** includes in a single tool the preprocessing of input data, the calculation of the stationary concentration field and the post-processing to obtain the desired output (short term or long term pollution fields), as schematized in figure 1.

Geometrical data (traffic network, source location, area source definition) can be obtained from a Geographical Information System (GIS). Meteorological input is performed directly from the local station measurements, and the (hourly averaged) atmospheric conditions are then internally computed. A detailed emissions inventory is needed to obtain the emission rates. In the case of mobile sources, the net emissions are then computed using (internally) a distribution traffic model.

Although this framework is relatively simple, the calculation procedure in the case of long-term simulations is very time-consuming due to the high number of point sources needed to simulate a whole city.

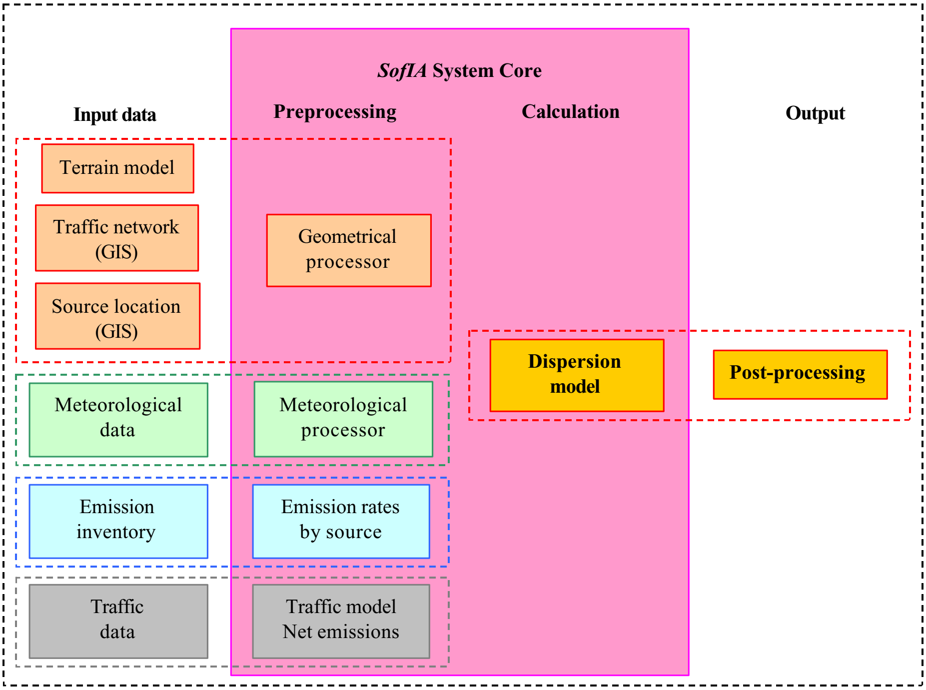


Figure 1: Schematic representation of the computational system *SofIA*.

3 APPLICATION TO BUENOS AIRES CITY

3.1 Motivation

The main aim of this study case is to implement the computational system ***SofIA*** to predict both the air pollutant concentrations and the impact of potential mitigation measures on the air quality of the Buenos Aires City.

The first mentioned point involves the calibration and validation procedures. The output is the long-term level for the two pollutants considered: NO_x and PM_{10}.

In order to quantify the impact of implementing green-house-gasses reduction emission policies on local air quality, some calculations are made for short-term NO_x and long-term $PM_{2,5}$.

3.2 Air quality in Buenos Aires

The Buenos Aires Metropolitan Area (BAMA) is located in the Argentinean coast of the inner part of the Rio de la Plata River, over the flat terrain that makes up the so called "pampa húmeda" (see figure 2). The high population density, the relatively high level of motor vehicle ownership, the large number of public transport vehicles, the high concentration of truck traffic, and the major industrial and thermoelectric complexes all contribute to air and noise pollution levels. Among them, traffic is the most important.

Due to favorable meteorological and topographical conditions, air pollution in Buenos Aires is not as severe as that of other Latin American megacities such as Mexico, Santiago de Chile, or Sao Paulo. Air pollutant concentrations are generally low due to winds blowing over the flat terrain. However, the winds are not sufficient to disperse vehicular air pollution in narrow, heavily traveled streets during weekday commuting and business hours.

As there is not an air quality monitoring system in BAMA, descriptive data about the current and historic situation of the air quality are limited [7].

3.3 Modeling strategy

The computational model is applied over a rectangular working domain of 67 km in the W-E direction by 56 km in the N-S direction (see figure 2).

This domain is discretized horizontally using regular cells of 250 m by 250 m, that is, a total of around 60,000 computational nodes by vertical level. At each node of the grid the concentrations are calculated. The spatial steps were determined based on the knowledge that, in general, the pollution levels at a distance of the order of 1 km from line sources are below the air quality standards.

For simulation of mobile sources two situations were considered:

a) The main traffic network (composed of highways, avenues and main streets) was represented by line sources fitting in each path section. Using a GIS platform the main traffic network presented in figure 3 was performed. It contains a total of 870 segments covering 2150 km of roads. For each segment the necessary input data are traffic density and composition by mean.
b) The spread traffic (i.e. the traffic in the secondary streets at neighborhood level) was represented by area sources. In this way, a coarse graining of the study domain was performed, dividing the study area in a total of 164 sectors.

For the sake of simplicity the same division by sectors was used to simulate domestic and commercial, spread traffic and open burning sources. In all the cases the emission characteristics were considered uniform into each individual sector.

There are three thermal power stations into the study area. These complexes have a total of 18 stacks, with heights from 12 m to 154 m. All these stacks are simulated as point sources. The thermal effect of the Río de la Plata River is taken into account.

Meteorological data are available through the National Service. The details on the other input data are described elsewhere [7] and omitted here for the sake of brevity.

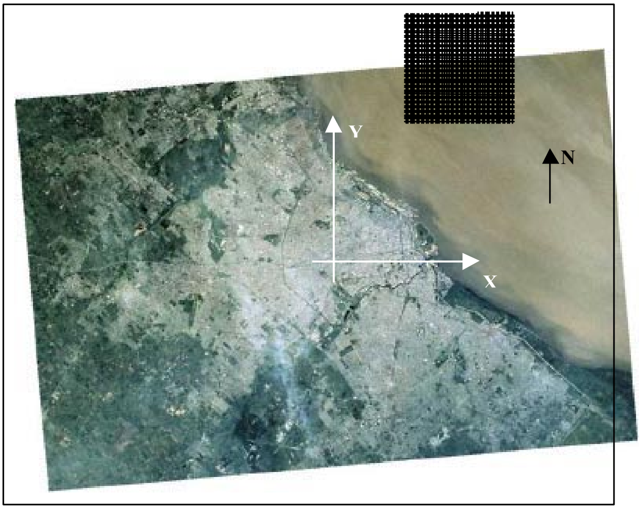


Figure 2: Study area: the black rectangle indicates the model horizontal boundary. A computational grid detail (right top) and the coordinate system (center) used by the model are shown.

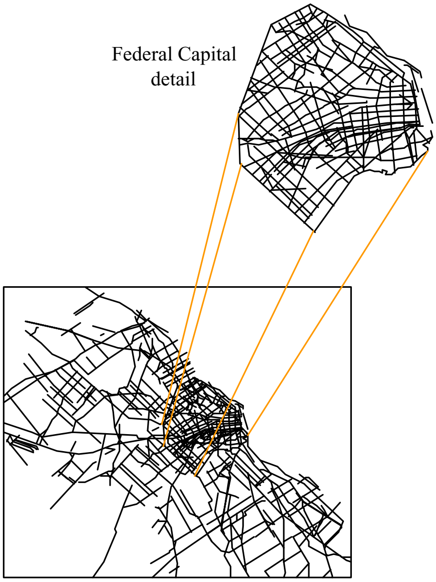


Figure 3: BAMA's main traffic network.

3.4 Model calibration and validation

Data on PM are scarcer. In winter 1997 a monitoring campaign included measurement of PM_{10} at three stations during around a month. In fall 2000 a relatively short monitoring campaign performed daily averages of PM_{10} in ten stations. Those data were used to calibrate the model [7]. The calibration procedure consisted in adjusting the emission factors associated to fugitive dust entrainment from paved roads. The adjustment between measured data and model results for 1-day average shown in figure 4 is obtained. A quite good agreement is reached, with exception of two stations, where the model overestimates the concentrations.

Once the model was calibrated, their long-term predictions were compared with long-term measurements. This sort of validation presents the reasonable agreement between them shown also in figure 4.

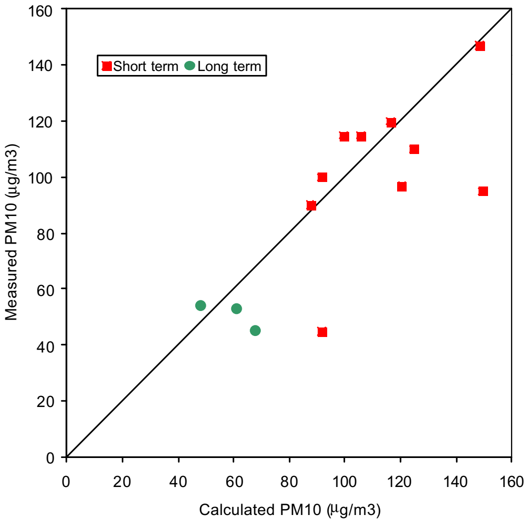


Figure 4 – Model calibration for PM_{10} concentrations. The black line indicates the expected value.

In the case of NO_x, the monitoring campaign performed during fall 2000 involved 1-hour averages, and maximum values were reported. Those data were used to contrast with maximum concentration values arising from the model, as shown in figure 5. Although the simulation does not represent exactly the campaign conditions (i.e. no traffic data were taken those days), the comparison shows a relatively good agreement. Differences between measured and calculated values range from 0.2% up to 78%, with a m.r.s. relative dispersion value of 11% (equivalent to 34 μg/m^3).

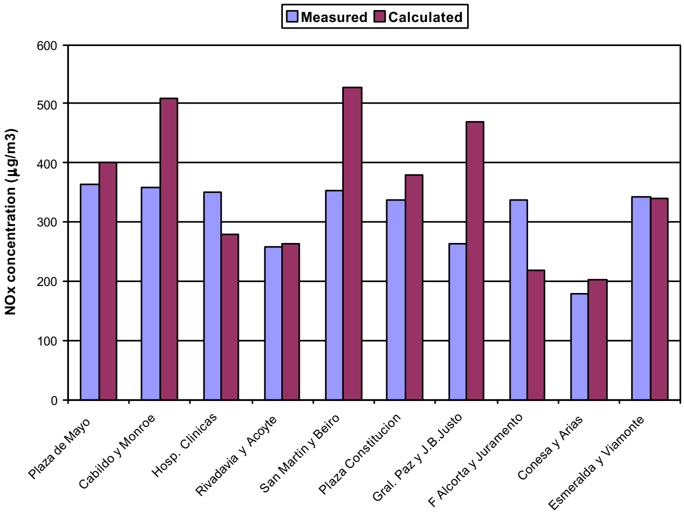


Figure 5 – Comparison between monitoring campaign and model results for NO_x maximum hourly concentration in 10 stations (fall 2000).

3.5 Mitigation strategies

Several mitigation measures that are likely to be serious options to be included in any GHG mitigation scenario for Argentina were analyzed independently. These options specifically include:

- Penetration of compressed natural gas (CNG), consumption improvements, and a little of modes substitution in the transport sector [8]
- Rational use of energy by reducing energy consumption, and indeed electricity supply [9]

Here we present some results combining the most relevant options listed above: the resulting scenario is called Integrated (Strategies) Scenario (IS). Prognoses from 2000 to 2012 were performed. The impact of such policies implementation is calculated as the difference (in space and time) of pollutant concentration between the IS and the Baseline Scenario (BS), which represents the "business-as-usual" evolution of the economy, technology innovation, etc.

3.6 Model Results: NO_x

For BS, the model result corresponding to the annual average NO_x concentration field is presented in figure 6. BAMA presents maximum concentrations in the Federal Capital (FC) downtown area with a concentration gradient spreading and decreasing inland from the river coast.

FC shows higher concentrations than Greater Buenos Aires (GBA) does, with exception of some places in the surrounding districts, especially in the northern zone. Although the main highway affects the northern zone, the annual average is relatively high due to the frequent winds blowing from SE and carrying polluted air from FC.

Within FC the major concentrations arise from the downtown area and the nearest towns. The southeast part of the city, that follows the Riachuelo riverside, presents a better air quality than the rest of it. In spite of having the most populated district of GBA, the western zone shows better air quality conditions than the northern and southern zones.

It is important to note that the major part of BAMA presents NO_x annual average concentrations below the local standard (100 $\mu g/m^3$), although the hourly one is exceeded frequently.

In order to quantify the contribution of each different source considered, figure 7 shows the annual average concentration fields associated to them. As expected, the main contribution corresponds to mobile sources. The highest levels are due to the concentrated sources (traffic flowing in highways and avenues). Diffusive sources produce the major contribution at neighborhood level, even when those zones are affected by the main network emissions. The thermal power plants show a low annual influence, with significance only at some kilometers around its location.

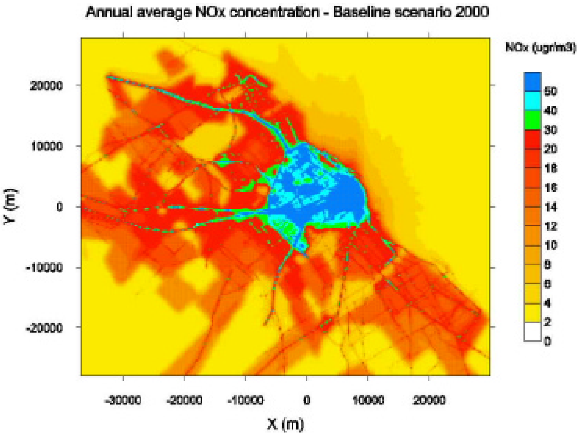
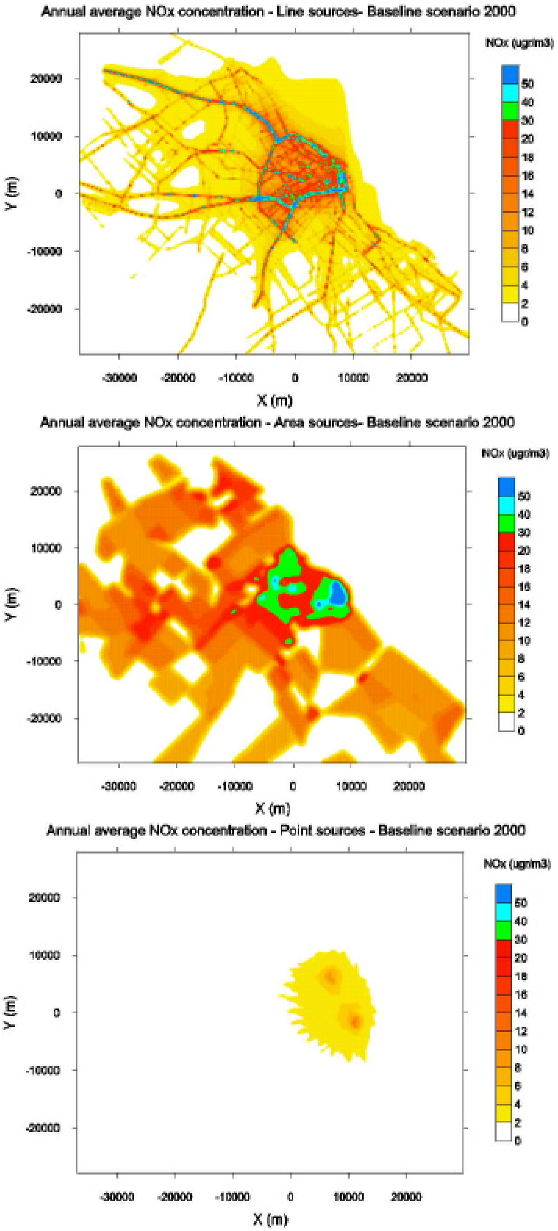


Figure 6 – Model result for NO_x annual average in 2000.



Annual average NOx concentration - Line sources- Baseline scenario 2000

Annual average NOx concentration - Area sources- Baseline scenario 2000

Annual average NOx concentration - Point sources - Baseline scenario 2000

Figure 7 – NO_x contribution by source: Line (upper), Area (middle) and Point (lower).
Blue zones indicate annual average NO_x levels exceeding 50 µg/m^3.

Figure 8 presents the prognoses for both BS and IS in 2012. As expected, a global reduction is observed in IS when compared with BS. Figure 9 presents the difference between the two scenarios. Almost all FC shows a reduction of at least 10 μg/m^3, which is increased to more than 20 μg/m^3 in the central area. In GBA, those zones close to highways and routes decrease their annual average concentrations between 5 and 10 μg/m^3, and in the rest of the districts the reduction is lower than 5 μg/m^3. No increase of concentrations is detected for IS in comparison with BS.

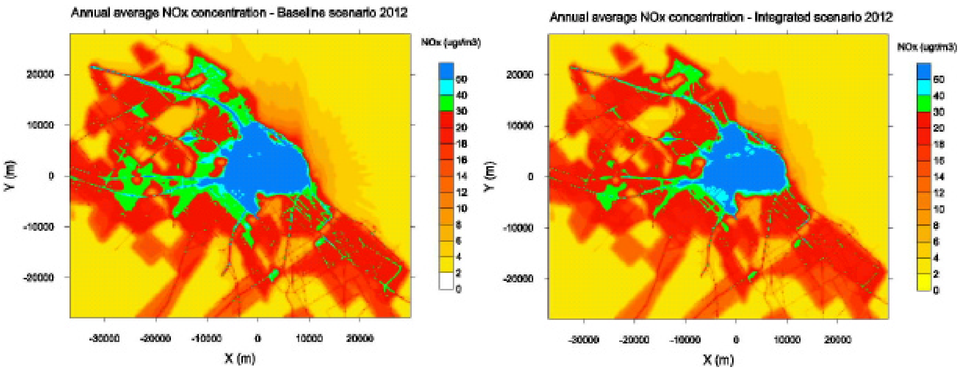


Figure 8 – Model result for NO_x annual average in 2012. BS (left) and IS (right).

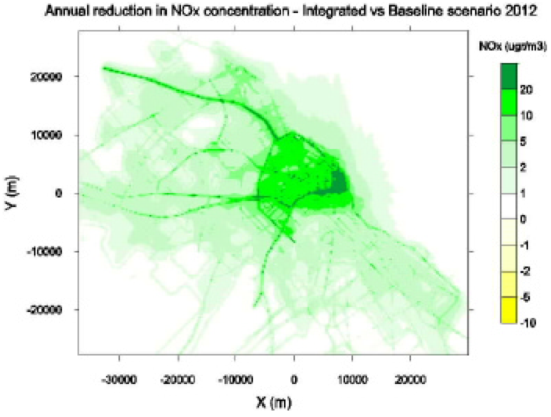


Figure 9 – Annual reduction in NO_x for 2012 (Integrated vs. Baseline scenario).

3.7 Model Results: PM_{10}

The different sources that contribute to PM_{10} annual average in BS are presented in figure 10. Area sources, that include diffusive transit, residential and commercial emissions and open burning, are the major contributors to PM_{10} levels in BAMA, both in FC and GBA. The main network itself produces less pollution than secondary streets owing to its lower emission factors (fast mode) and its better maintenance conditions (lower dust resuspension). Power plant effects are of minor importance.

Figure 11 shows the time evolution in field concentrations for 2012 BS and IS. In the case of BS, almost all FC shows concentrations above the annual standard (50 $\mu g/m^3$), while western and northern zones increase their levels significatively. This trend is helped by frequent winds blowing from E and SE. Note that, due to the same effect, the southern zone does not increase dramatically its level.

The IS shows a very good performance in reducing PM_{10} levels, as is clear from figure 11. It must be mentioned that even comparing this result with the concentration field in the BS during 2000, the pollution levels are lower.

The reduction in concentration between integrated and baseline scenario is presented in figure 12. Some zones in GBA decrease from 5 up to 20 $\mu g/m^3$. Much of FC presents a reduction above 20 $\mu g/m^3$, while the downtown area surpasses 30 $\mu g/m^3$ (with more than 50 $\mu g/m^3$ reduction in the micro-central zone).

4 CONCLUSIONS

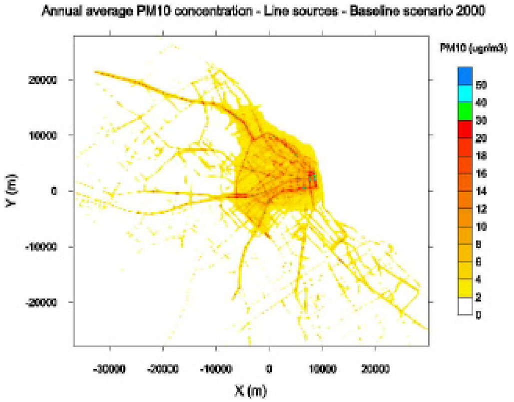
SofIA, the computational system that has been presented here, constitutes the first attempt in modeling the air quality in the whole Buenos Aires Metropolitan Area. The major achievement of the modeling work is the correct simulation of the main features of BAMA's air quality. Then, the proposed modeling strategy can be considered as satisfactory in predicting both the current air pollution trends and concentration levels.

Nevertheless, it is expected that non-negligible deviations between observed and calculated concentrations arise in several zones, as the input data quality varies in a sensitive way from district to district, especially in GBA.

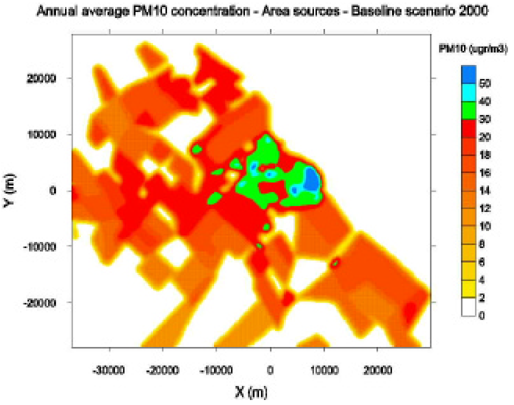
When validating the model, a good agreement between calculations and field data was obtained. It is expected that the average errors between measured and simulated concentrations are greater for each particular scenario than in the differences among scenarios.

Thus, the prognosis of reductions due to the implementation of mitigation strategies can be considered as calculated with a relatively good precision. From this point of view, ***SofIA*** system becomes a useful tool for environmental analysis, as was illustrated through the study case presented.

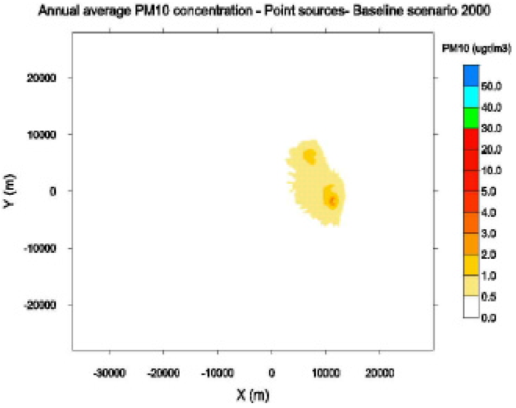
As a general recommendation, the whole input data base should be updated and improved. Finally, in order to run ***SofIA*** in a more realistic situation the enhancement of the computer capacity is recommended, i.e. the use of a parallel version in a PC cluster instead of individual PC.



Annual average PM10 concentration - Line sources - Baseline scenario 2000



Annual average PM10 concentration - Area sources - Baseline scenario 2000



Annual average PM10 concentration - Point sources- Baseline scenario 2000

Figure 10 – PM $_{10}$ contribution by source: Line (upper), Area (middle) and Point (lower).
Blue zones indicate annual average PM $_{10}$ levels exceeding 50 μg/m^3.

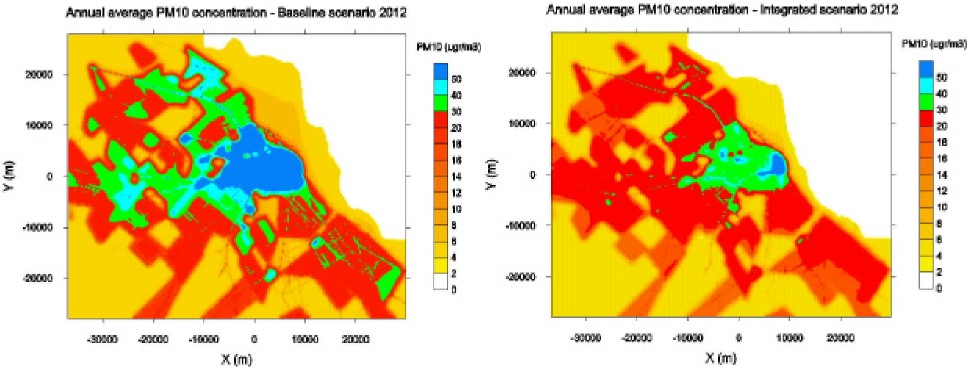


Figure 11 – Model result for PM$_{10}$ annual average in 2012. BS (left) and IS (right).

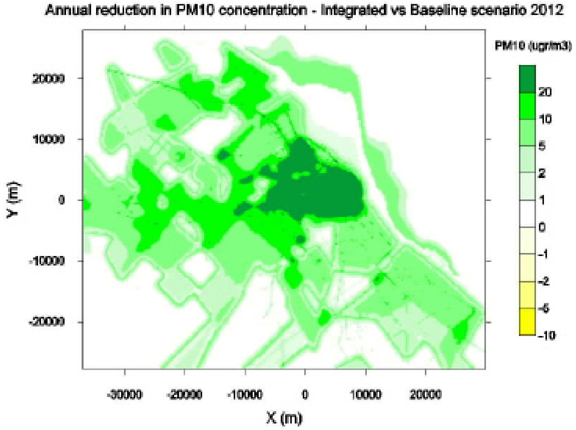


Figure 12 – Annual reduction in PM$_{10}$ for 2012 (Integrated vs. Baseline scenario).

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