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Technical Report – Implementation feasibility of LOTOS-EUROS model in Colombia Domain

Medellin Air qUality Initiative MAUI

MAUI-RT-02

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ABSTRACT

This report presents the feasibility analysis of the LOTOS-EUROS as a tool to represent the atmosphere dynamic over the Colombia domain. For determinate de feasibility of the model, is implemented the methodology described in the report MAUI-RT0001. In the same way, are presented different challenges and opportunities to the implementation of the model.

INTRODUCTION

One of the most used and studied Air Quality Models at present is the LOTOS-EUROS (Mues et al., 2014). The LOTOS-EUROS (LOng Term Ozone Simulation- EURopean Operational Smog model) is a chemical transport model that models in three dimensions the air pollution in the lower troposphere. This model was developed in 2004 by TNO and RIVM/MNP organizations, in Netherlands, unifying the previous developed LOTOS and EUROS models. At the beginning it was developed like a model focused on ozone, but actually, the LOTOS-EUROS (versión 1.8) allows calculate concentrations of ozone, particulate matter, nitrogen dioxide, heavy metals and organic pollutants with a standard model resolution of approximately 36x28 km. (Sauter et al., 2012).

The LOTOS-EUROS has widely used in different projects located around the world, whereby it shows the capacity of the model. As well, it is within the framework of the project MACC II, that is looking to produce the forecast at European continent level in air quality, meteorology and solar radiation (Marécal et al., 2015). The MACC II project uses the network of satellites and sensors denominated COPERNICUS along with LOTOS-EUROS (among other air quality models) to make the predictions of air quality. Likewise, the LOTOS-EUROS is used in Netherlands to predict Ozone concentrations and PM in national territory. This project is named SmogProg and is used by Dutch authorities as official forecasts, it is directly published to the institutions and population in the country (Hendriks et al., 2013), but the LOTOS-EUROS model has not been only implemented in Europe, actually is part of the project PANDA, that collect a set of models and looks for modeling and predicting pollutants concentrations in Chinese territory. Comparable, in the north of Africa is settled the Regional Center for Northern Africa, Middle East and Europe, which uses the LOTOS-EUROS to monitoring and predicting the air quality in Northern Africa, Middle East and Eastern Europe. As with in America continent the model has been implemented by Brazil to monitoring and predicting Ozone concentrations, Nitrogen Dioxide and PM 2.5 while was taking place the FIFA World Cup.

BACKGROUND

LOTOS-EUROS MODEL

The dynamics of the pollutants in the model LOTOS-EUROS is regulated by processes of chemical reactions, diffusion, drag, dry deposition and wet, emissions and aversion (Sauter et al., 2012; Van Loon, Builtjes, & Segers, 2000). The LOTOS-EUROS dynamic is given by:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} + V\frac{\partial C}{\partial y} + W\frac{\partial C}{\partial z} = \frac{\partial}{\partial t}\left(K_h\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_h\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) + E + R + Q - D - W \tag{1}$$

With *C* the concentration of a pollutant, U, V and W, are wind components in West-East, South-North direction and vertical direction, respectively. K_h and K_z are horizontal and vertical coefficients by diffusion of turbulence. *E* represents the entrainment or detrainment due to variations in layer height. *R* represents generation and consumption rates of pollutant by chemical reactions. *Q* is contribution by emissions, *D* and *W* are loss by dry and wet deposition process, respectively.

The main equation of LOTOS-EUROS dynamic is composed by different operators, each one models different components of pollutants behavior. The operators that compose the LOTOS-EUROS are: i) the transport operator, ii) the chemistry operator, iii) the dry deposition operator and iv) the wet deposition operator. Emissions and values related with meteorology are directly taken from data sources as satellite or measuring devices located in the land surface.

The transportation operator consists in the dynamic of advection in three dimensions, horizontal and vertical diffusion and entrainment. The horizontal advection is described by horizontal winds (*U,V*) that are inputs to the model. The vertical wind component (*W*) is calculated by the model through the convergence and divergence of the horizontal winds. The horizontal diffusion coefficient (K_h) is calculated through an empiric constant η and the speed tensor deformation *Def*, as is shown in equations (2) and (3):

$$K_h = \eta|Def| \tag{2}$$

$$|Def| = \sqrt{\left[\left(\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y}\right)^2 + \left(\frac{\partial U}{\partial x} - \frac{\partial V}{\partial y}\right)^2\right]} \tag{3}$$

The chemistry operator models everything related to the production and consumption of components by different chemical reactions in the atmosphere. Due to the complexity of LOTOS-EUROS, to handle a complete mechanism of chemical reactions could cause an unmanageable model. To avoid this problem, the LOTOS-EUROS can use one of two mechanisms of simplified reactions, Carbon Bond-IV (CB-IV) or CB99. The CB-IV uses 9 primary components directly issued to the atmosphere and a total of 81 reactions to determine secondary species produced in the atmosphere. The second mechanism belonging to the LOTOS-EUROS is the CB99, which is a variation of the CB-IV. The CB99 uses 42 chemical species and 95 reactions, including 13 photolytic reactions.

The dry deposition is divided in two phases, the dry deposition of gases and the dry deposition of particles. The dry deposition of gases is modeled through the transfer of gases between the land surface and the atmosphere, result of the difference in concentrations and resistance between them. In the dry deposition of particles the scheme used depend of the given use to the land over is made the analysis. This scheme confer flexibility and dynamism in the aerosol size, although due to simplicity is taken two sizes of reference 0.7 and 8.0 μm.

The operator of wet deposition is modeled through the belowcloud scavenging process. The belowcloud scavenging process uses a sweep coefficient Λ [s^{-1}] that describes the mass transfer speed of a pollutant from the air to the raindrops. The value of the sweep coefficient depends of the considered component. Nevertheless, in general the decrease in concentration C [μg / m3] is calculated as:

$$\frac{\partial c}{\partial t} = -\Lambda C \qquad (4)$$

The contribution to the flow of wet deposition ΔD [$\mu g/m^2$] is described by:

$$\Delta D = C_0(1 - e^{-\Lambda t})\Delta z$$

Where C_0 is the initial concentration and Δz [m] is the height of a cell in the resolution grid.

The LOTOS-EUROS model is considered on a large scale due to the solution of the equation (1) is executed for different components and in each point belonging to a grid on the region of analysis. Because of this process the vector of states has large size (in the order of thousand).

The LOTOS-EUROS model has the next outputs:

1 Volume mixing ratio of O_3 in humid air
2 Volume mixing ratio of NO_2 in humid air
3 Volume mixing ratio of NH_3 in humid air
4 Volume mixing ratio of SO_2 in humid air
5 Volume mixing ratio of HNO_3 in humid air
6 Volume mixing ratio of CO in humid air
7 Volume mixing ratio of N_2O_5 in humid air
8 Volume mixing ratio of CH_2O in humid air
9 Volume mixing ratio of isoprene in humid air
10 Volume mixing ratio of PAN in humid air
11 Mass concentration of NO_3 in humid air
12 Mass concentration of SO_4 in humid air
13 Mass concentration of ammonium dry aerosol in humid air
14 Mass concentration of TPM25 in humid air
15 Mass concentration of TPM10 in humid air
16 Tendency of atmosphere mass content of ozone due to dry deposition
17 Tendency of atmosphere mass content of sulfur dioxide due to dry deposition
18 Tendency of atmosphere mass content of sulfate dry aerosol due to dry deposition
19 Tendency of atmosphere mass content of nitrogen monoxide due to dry deposition
20 Tendency of atmosphere mass content of nitrogen dioxide due to dry deposition
21 Tendency of atmosphere mass content of nitric acid due to dry deposition
22 Tendency of atmosphere mass content of nitrate dry aerosol due to dry deposition

23 Tendency of atmosphere mass content of ammonia due to dry deposition
24 Tendency of atmosphere mass content of ammonium dry aerosol due to dry deposition
25 Tendency of atmosphere mass content of carbon monoxide due to dry deposition
26 Tendency of atmosphere mass content of formaldehyde due to dry deposition
27 Tendency of atmosphere mass content of sulfur dioxide due to wet deposition
28 Tendency of atmosphere mass content of sulfate dry aerosol due to wet deposition
29 Tendency of atmosphere mass content of nitric acid due to wet deposition
30 Tendency of atmosphere mass content of nitrogen monoxide due to wet deposition
31 Tendency of atmosphere mass content of nitrogen dioxide due to wet deposition
32 Tendency OF atmosphere mass content of nitrate dry aerosol due to wet deposition
33 Tendency of atmosphere mass content of ammonia due to wet deposition
34 Precipitation

The output concentration for each pollutant is calculated through five vertical layer. The height of this vertical layer depend of the mixing layer. In the Figure 1 is shown an example of the layers height.

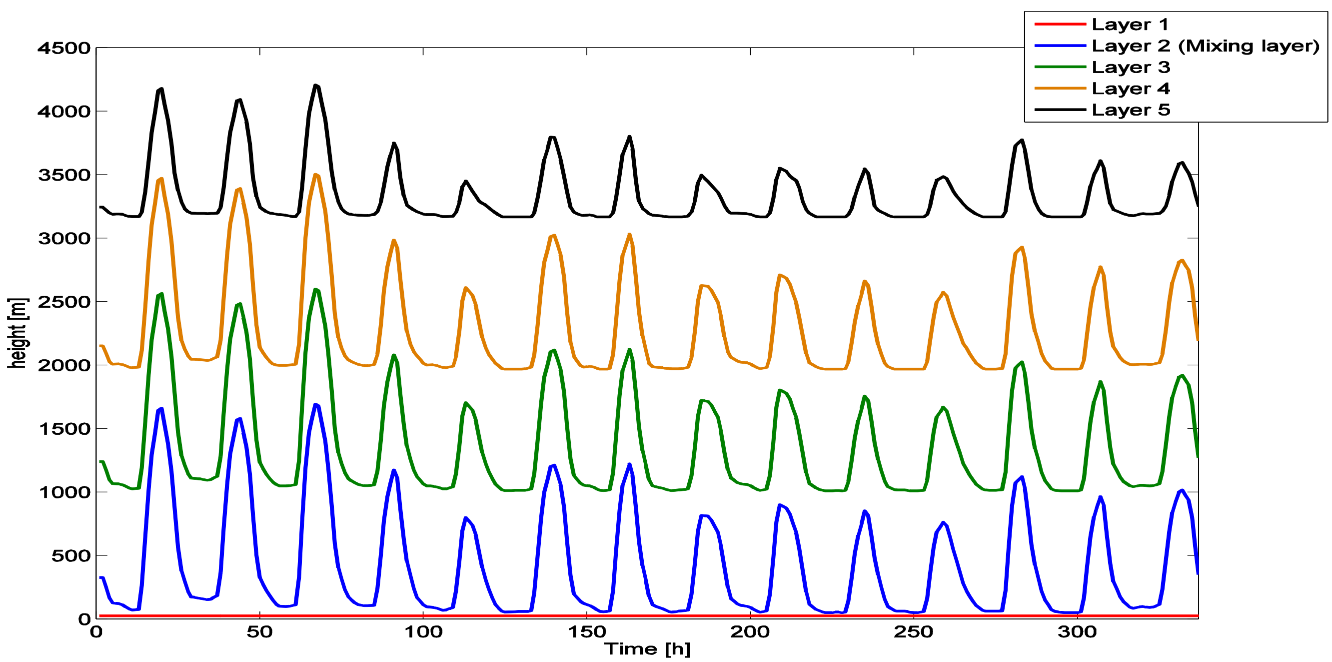

Figure 1. Vertical layers of LOTOS-EUROS.

MODEL EVALUATION

For the model evaluation was implemented the methodology presented in the report MAUI_RT001 and was used the data from MACC1 project as control data. The comparison between LOTOS-OUTPUTS outputs and MACC1 project was made in one point close to the Aburrá Valley, in the surface layer. For the analysis was selected de volume mixing ratio of O_3 and NO_2 in the period of Abril 1-2015 and March 1- 2016. The point of comparison is shown in the Figure 3.

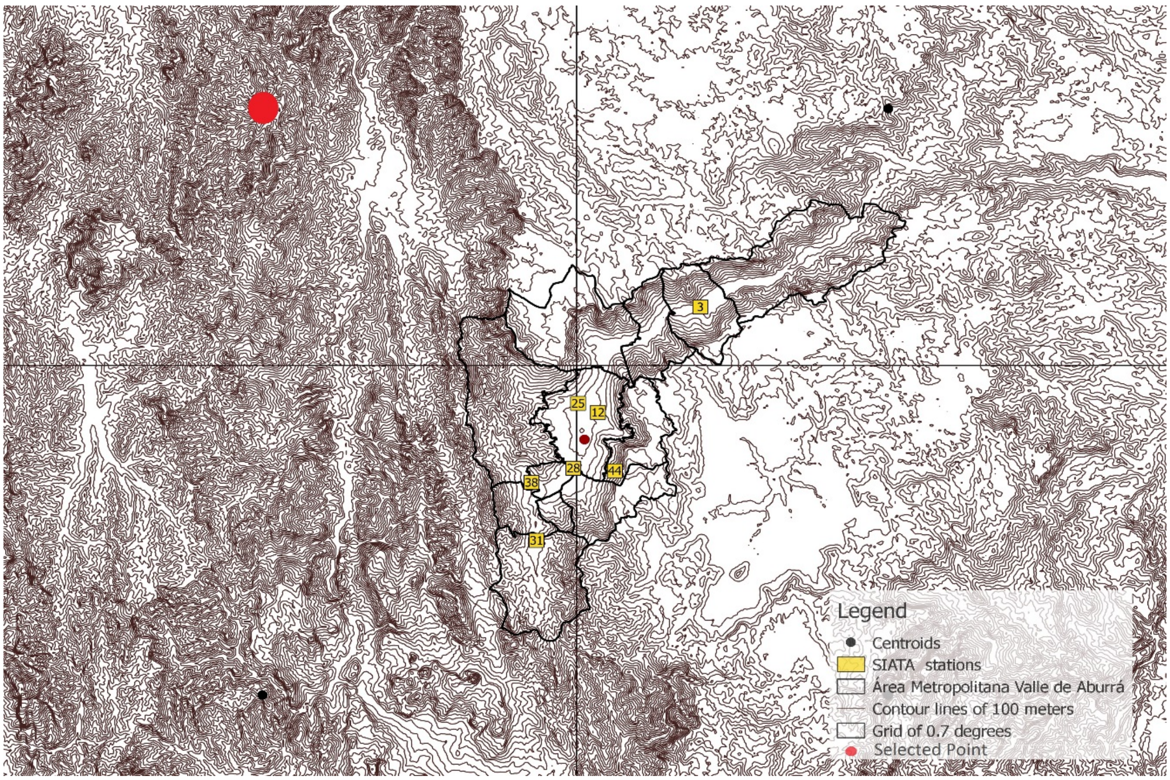

Figure 2. Selected Point for the comparison.

SPECTRAL ANALYSIS

Foe each substance is calculated the frequency spectrum for LOTOS-EUROS outputs and MACC 1 project. The corresponding spectrum and a comparison between the both sources of data are shown in the figures 4, 5,6,7,8 and 9. For the comparison figures the magnitude was normalized between 0 and 1.

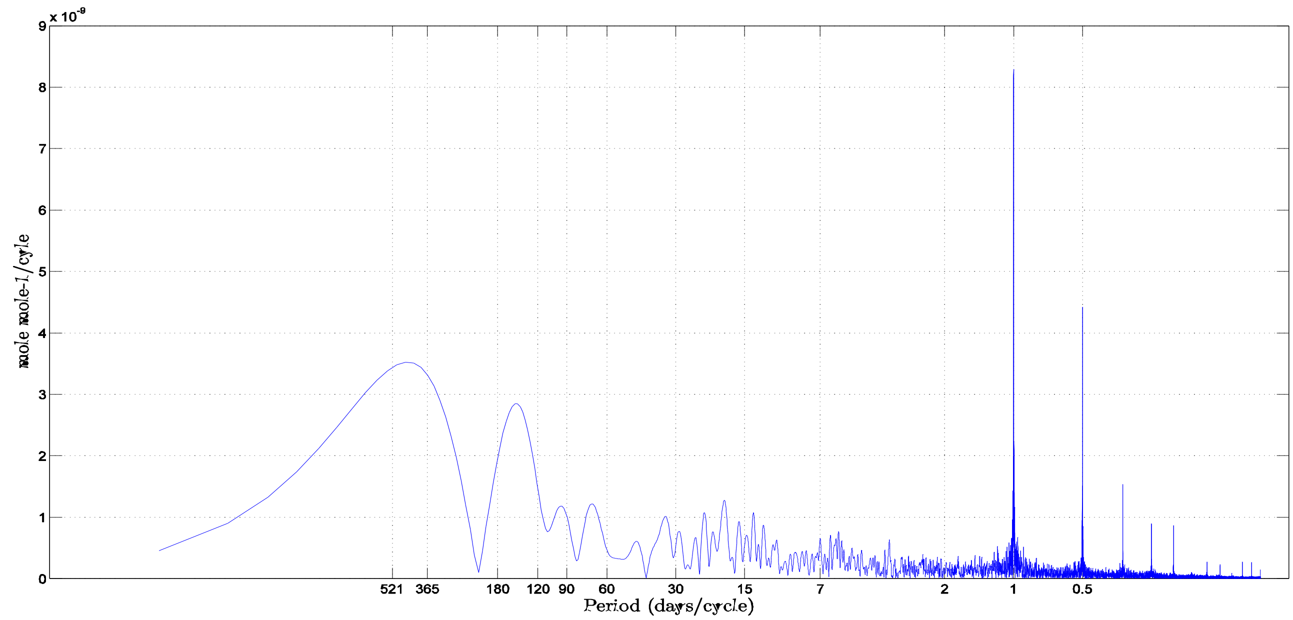

Figure 3. Frequency spectrum of O_3 by LOTOS-EUROS

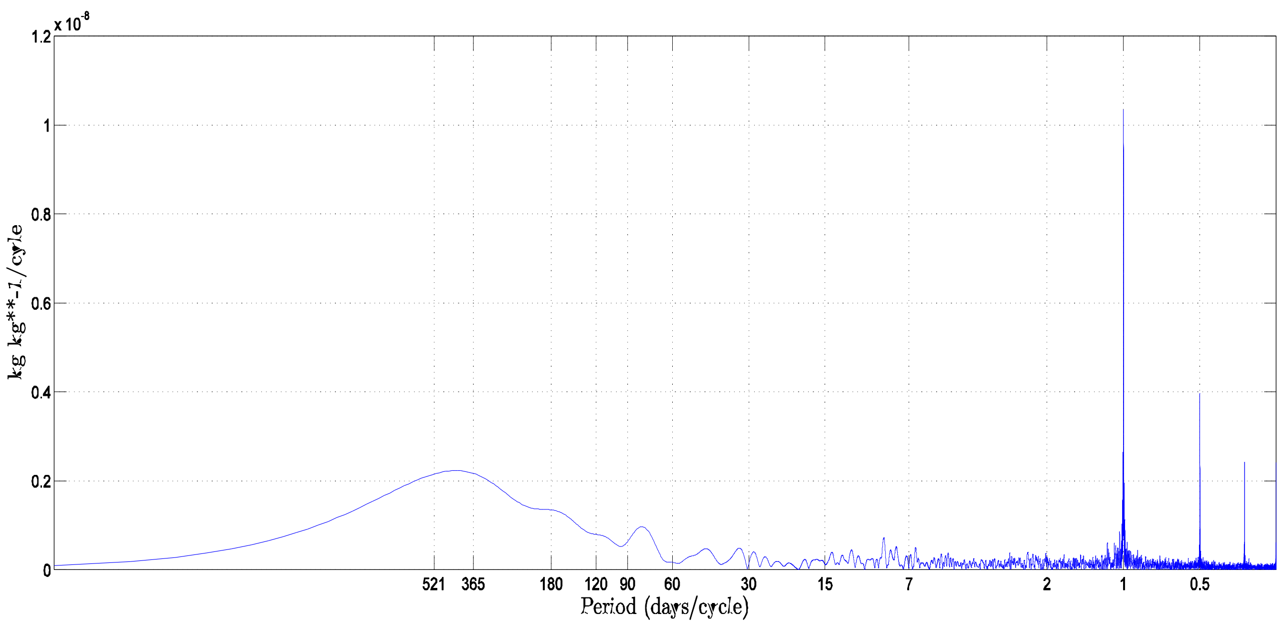

Figure 4. Frequency spectrum of O_3 by MACC1

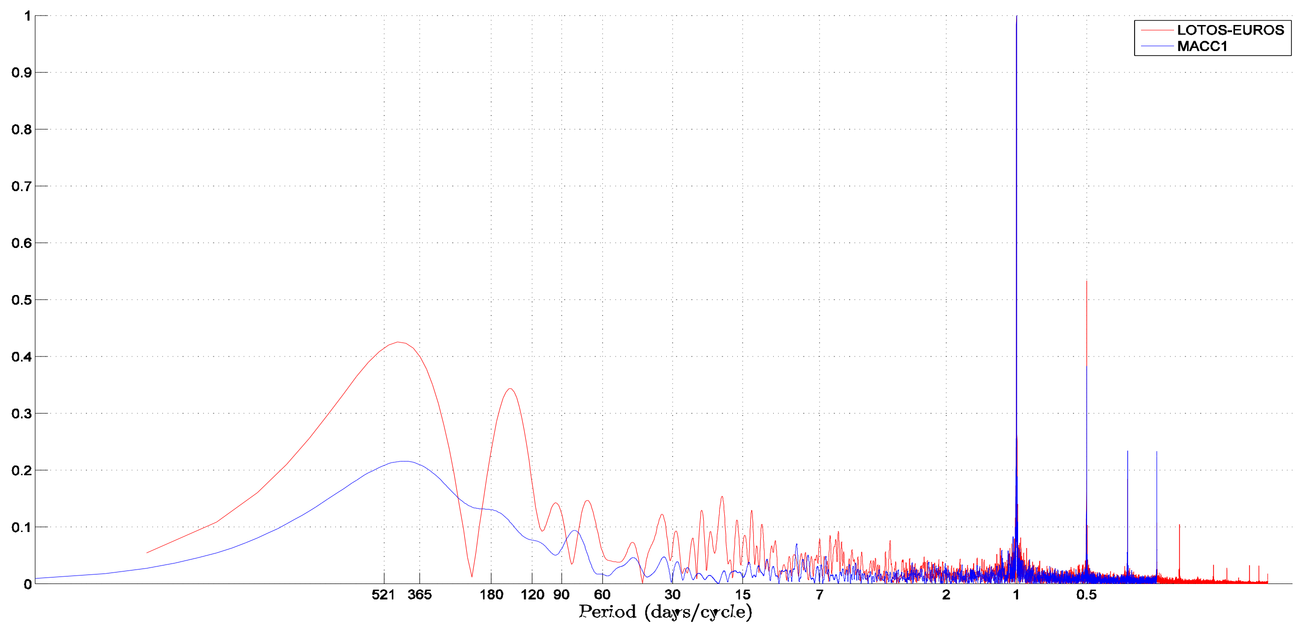

Figure 5. Comparison between LOTOS-EUROS and MACC1 frequency spectrums for O_3.

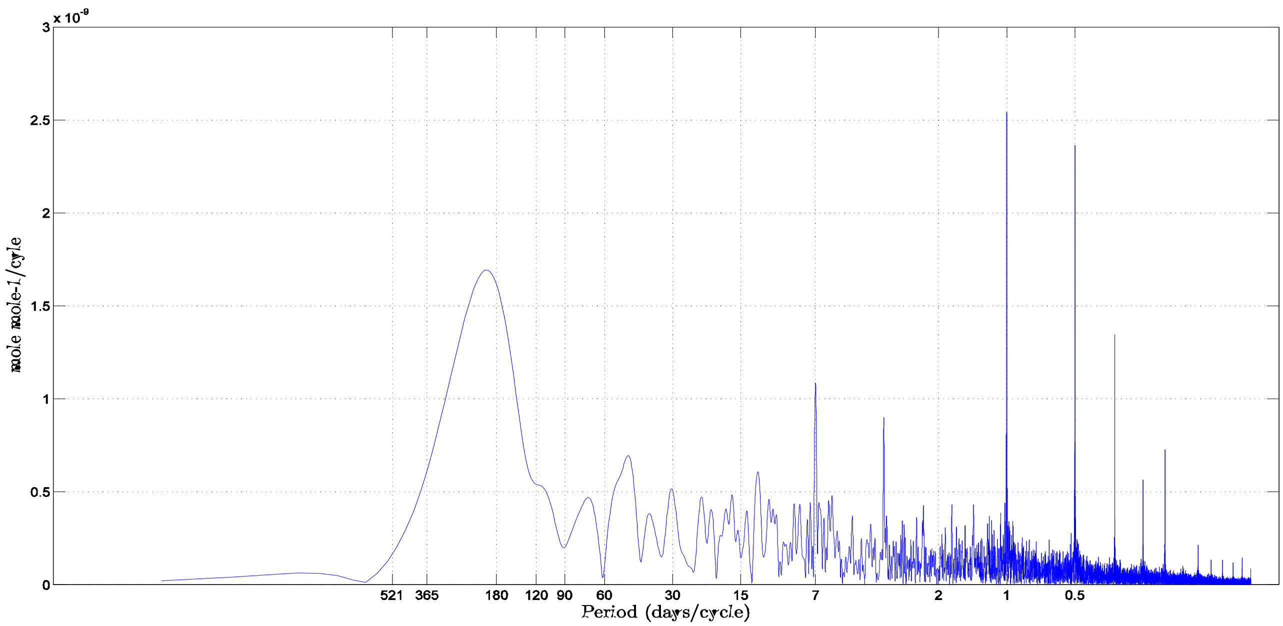

Figure 6. Frequency spectrum of NO_2 by LOTOS-EUROS.

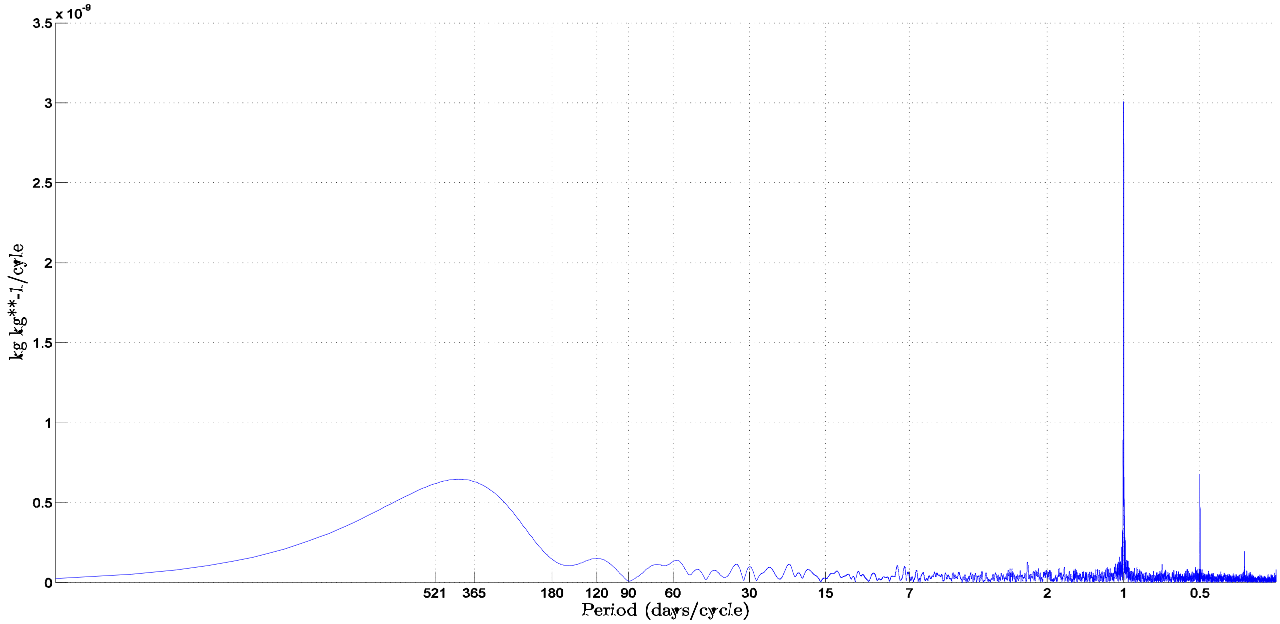

Figure 7. Frequency spectrum of NO_2 by MACC1

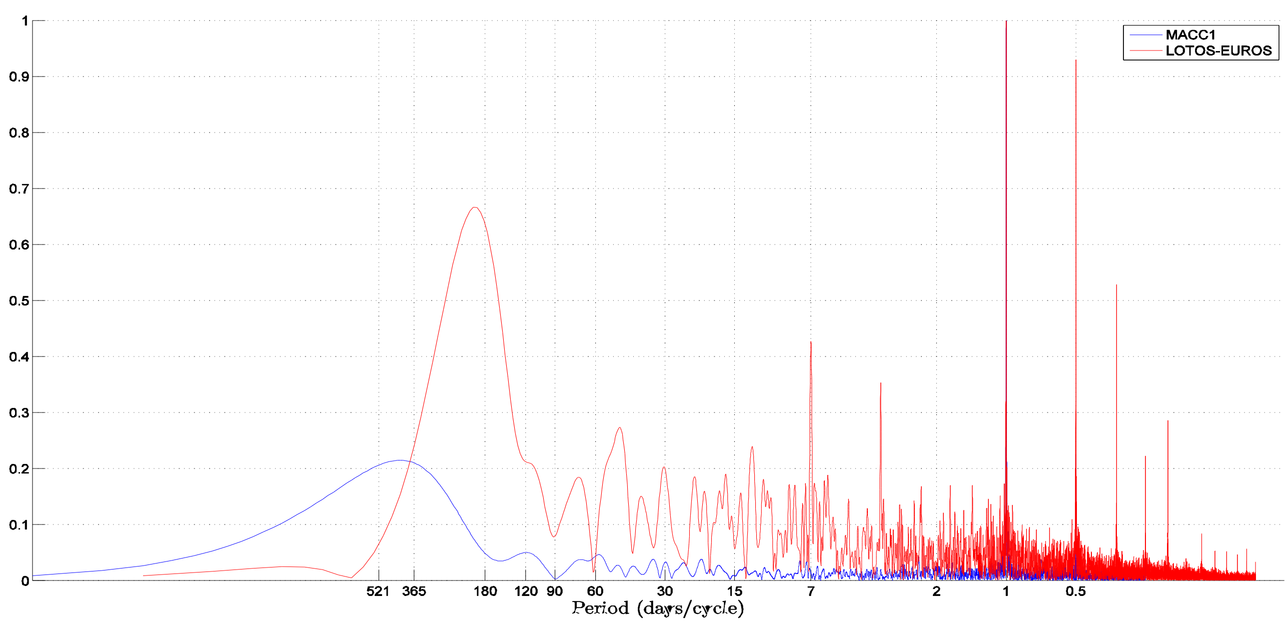

Figure 8. Comparison between LOTOS-EUROS and MACC1 frequency spectrums for NO_2.

With Figures 4-9 it can be concluded that the model is able to reproduce the main frequency for both substances (one-day period). In the case of ozone, the model shows a frequency behavior similar to that of the MACC 1 project, but with a bias in the magnitude of the frequency components. On the other hand, for the NO2 and unlike the main frequency, the frequency spectrum of LOTOS-EUROS and MACC1 are different. The frequency spectrum of LOTOS-EUROS for NO2 for example has an important component in the 7-day period, which is not evident in the MACC spectrum.

DAILY CYCLE ANALYSIS

Due to that for both substances analyzed the most important cycle is the daily cycle, is very important analyze it. The daily cycle, variation of the substance concentration throughout the day, is of vital importance as it allows to detect critical moments, and associate this moments to possible causes, man-made or not.

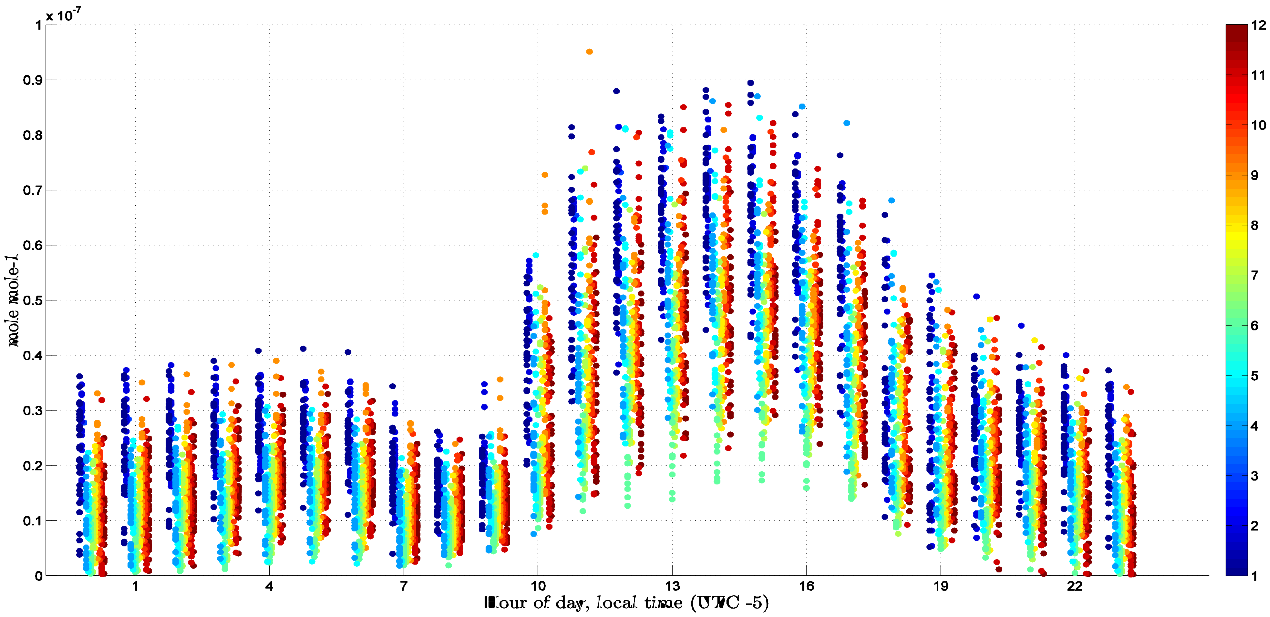

Figure 9. Daily cycle for O_3 by LOTOS-EUROS

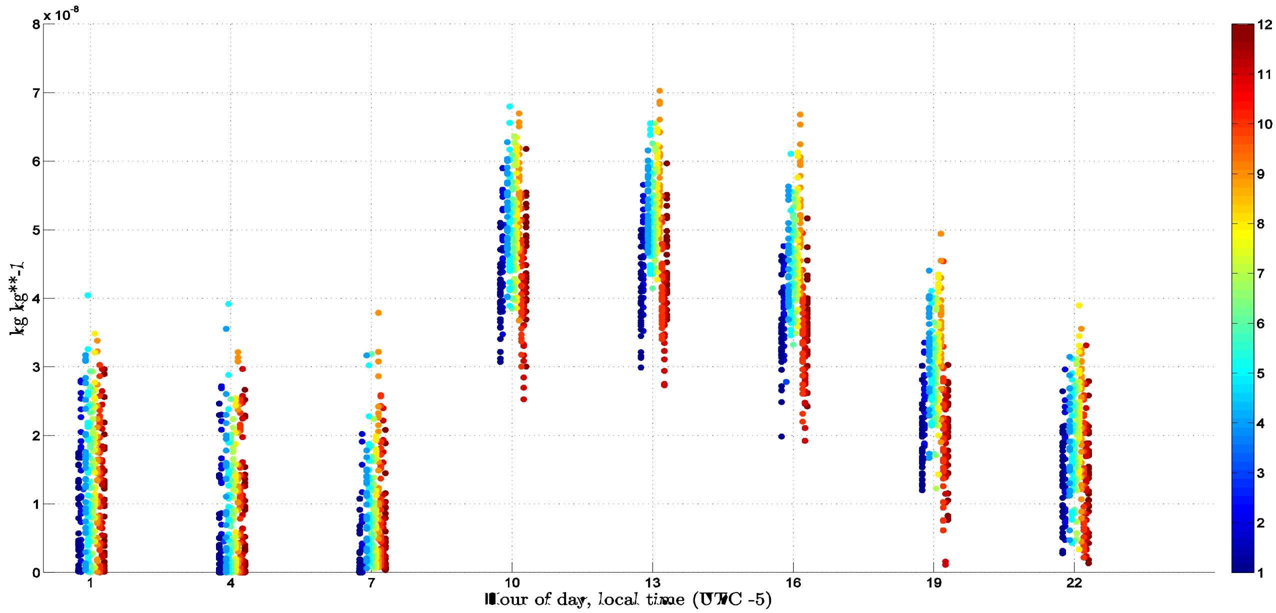

Figure 10. Daily cycle of O_3 by MACC1

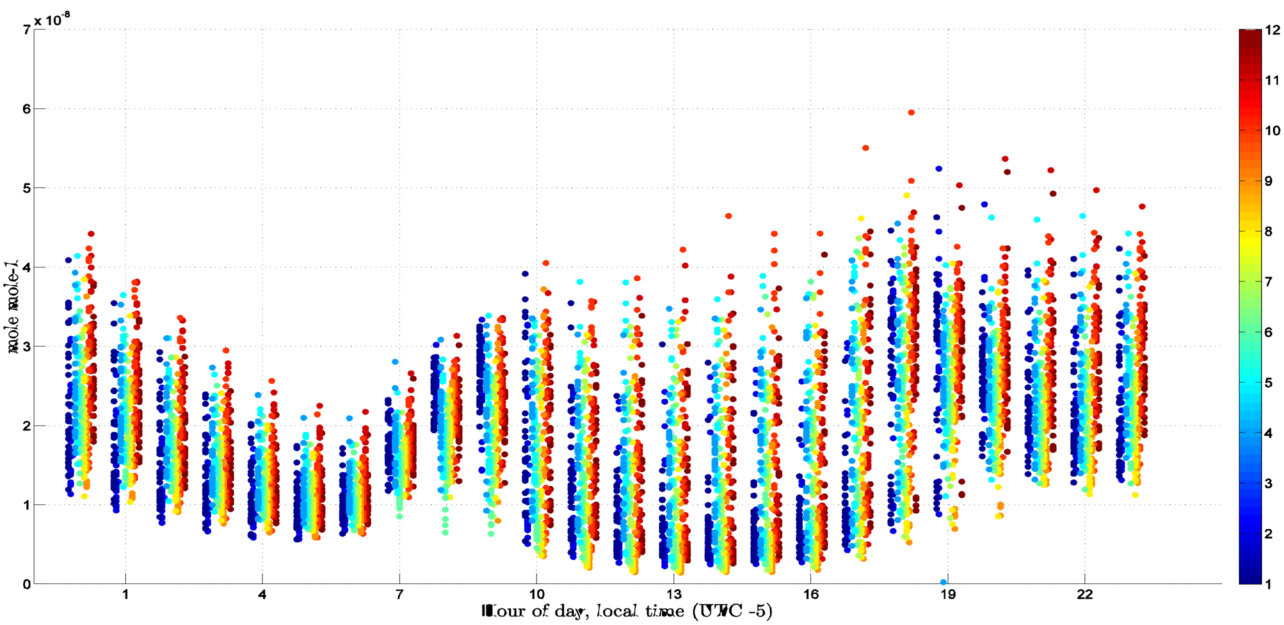

Figure 11. Daily cycle of NO_2 by LOTOS-EUROS

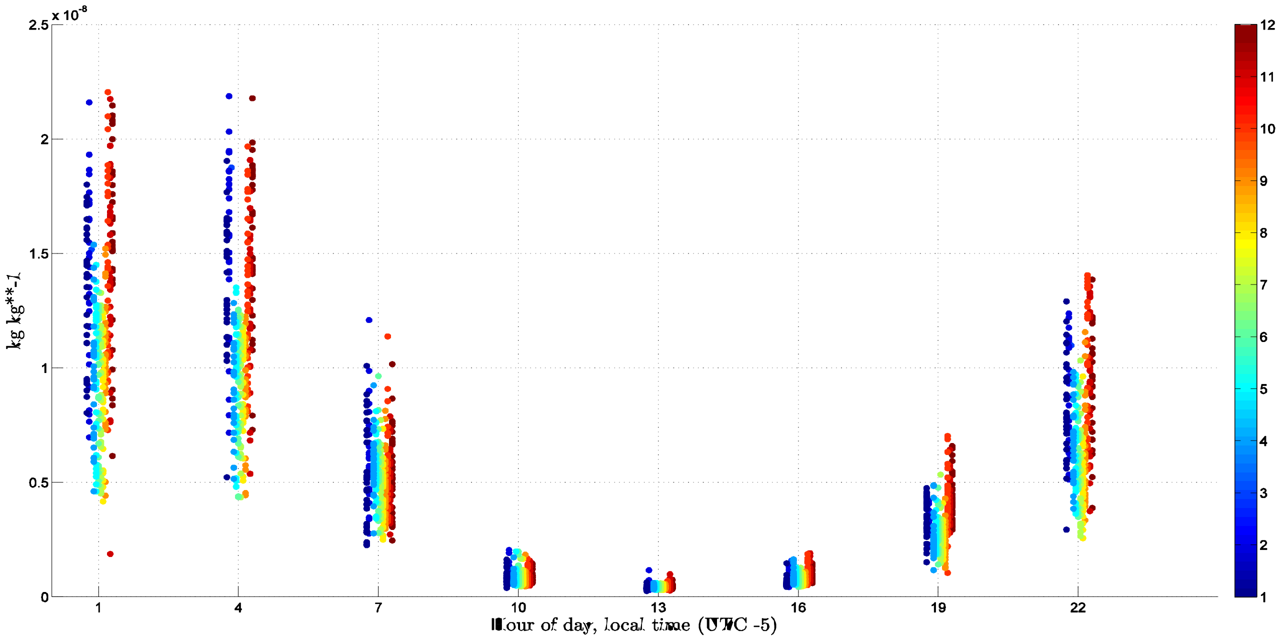

Figure 12. Daily cycle of NO_2 by MACC1

In addition to the time information of the day, the color is associated with the corresponding month. This allows to identify the variations of the daily cycle associated to the annual cycle. LOTOS-EUROS has a one-hour time resolution and MACC1 has a three-hour time resolution. For Ozone, the daily cycle modeled by LOTOS-EUROS is very similar to the MACC daily cycle. The highest values occur in the afternoon and the lowest in the period without solar radiation. On the other hand, the distribution of value throughout the year is different, the concentration peaks for MACC are in the period between July and September (the second dry season of the year) but for LOTOS-EUROS are between January and March (the first dry season of the year). In the case of NO2, the daily cycle of both data sources is completely different. LOTOS-EUROS could not represent the daily behavior of NO2. In general, LOTO-EUROS data are more scattered than the MACC1 data.

TEMPORAL DISTRIBUTION ANALYSIS

As discussed in the previous section, the concentration levels of the different substances change depending on the time of day and the time of year. Also, as the development of the variables under study is generally unknown, it can be understood as a stochastic process. Thus, the analysis of the distribution is required. Additionally, it is inferred that these are not stationary processes, so the variation of the distributions versus time must be taken in consideration. To evaluate these aspects, the following analysis is proposed:

- Define a time window of arbitrary duration, which is used to segment the variable of interest.
- Calculate the histogram of the windowed data.

- Move the window through the time domain, obtaining the empiric distributions for each position.
- Concatenate the histograms to obtain the temporal distribution matrix (moving histogram).

The temporal distribution of O_3 and NO_2 by LOTOS-EUROS and MACC1 are presented in the figures 14-18.

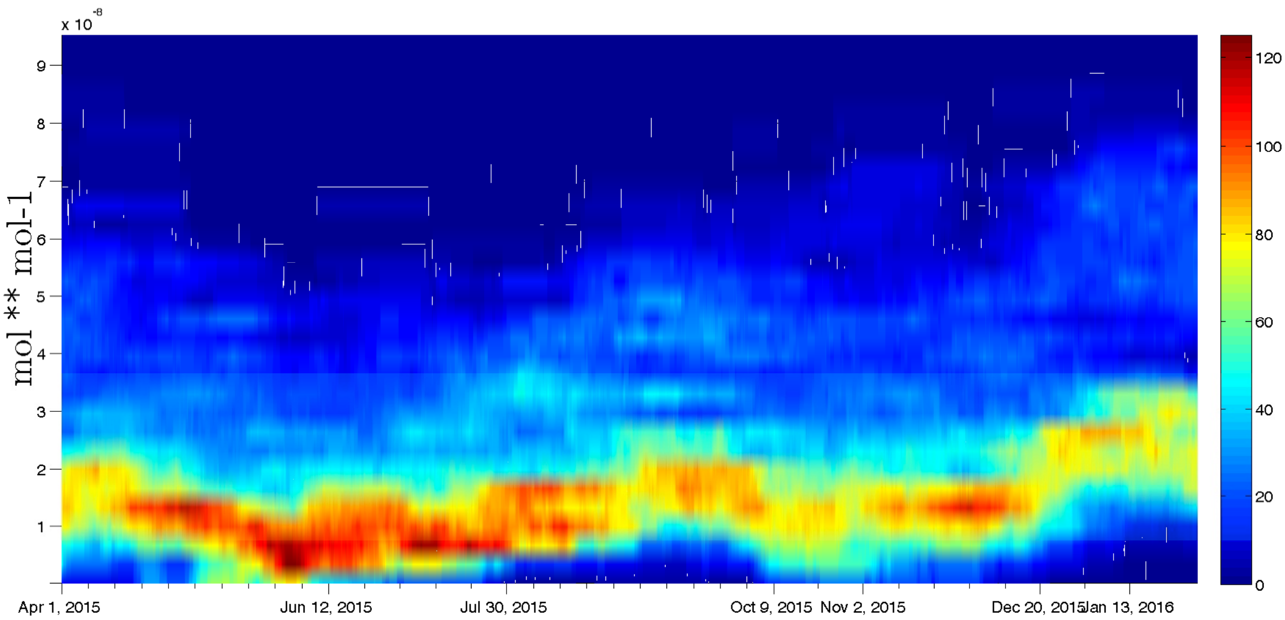

Figure 13. Temporal distribution of O_3 by LOTOS-EUROS.

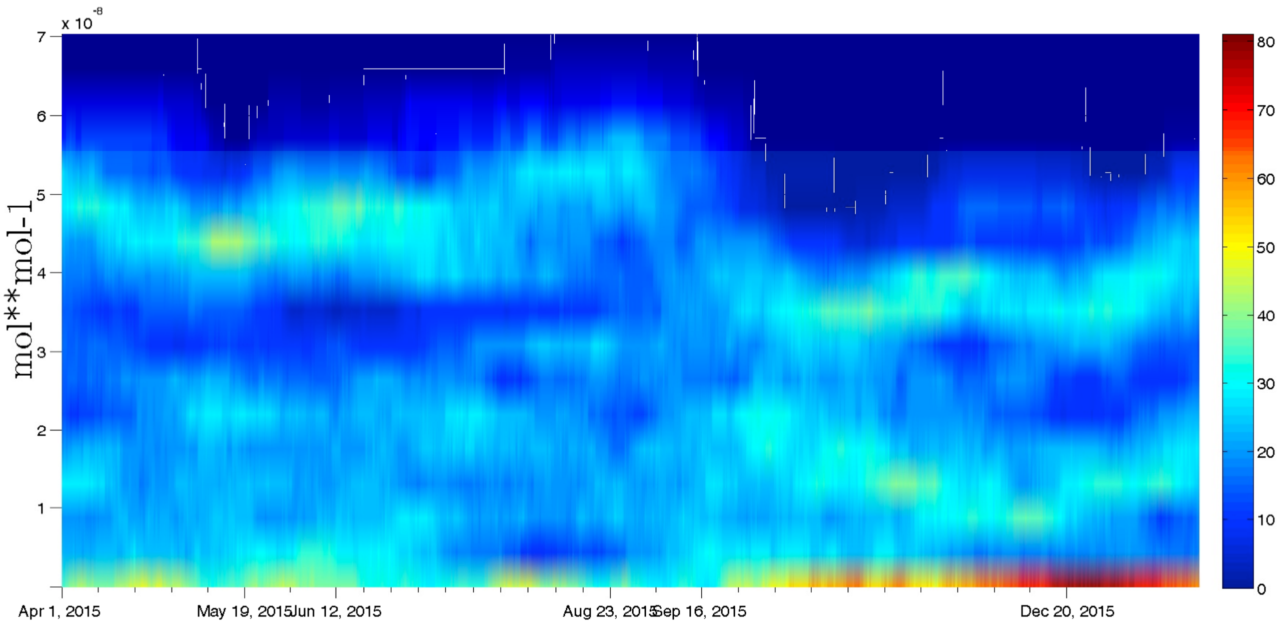

Figure 14. Temporal distribution of O_3 by MACC1.

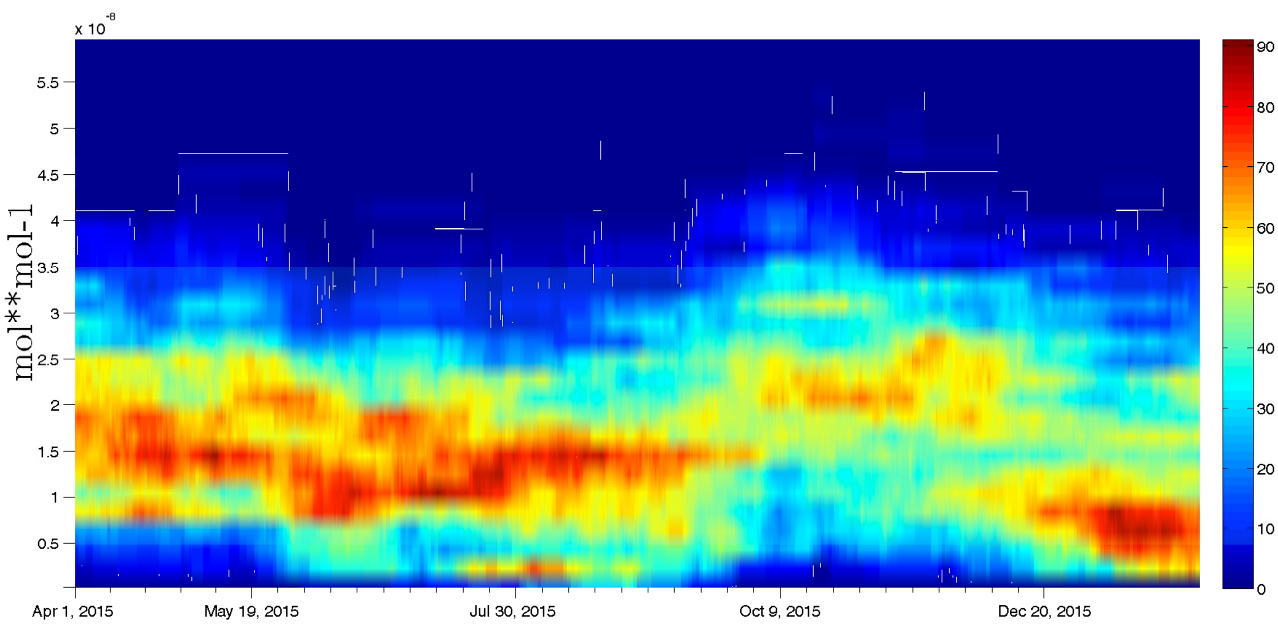

Figure 15. Temporal distribution of NO_2 by LOTOS-EUROS.

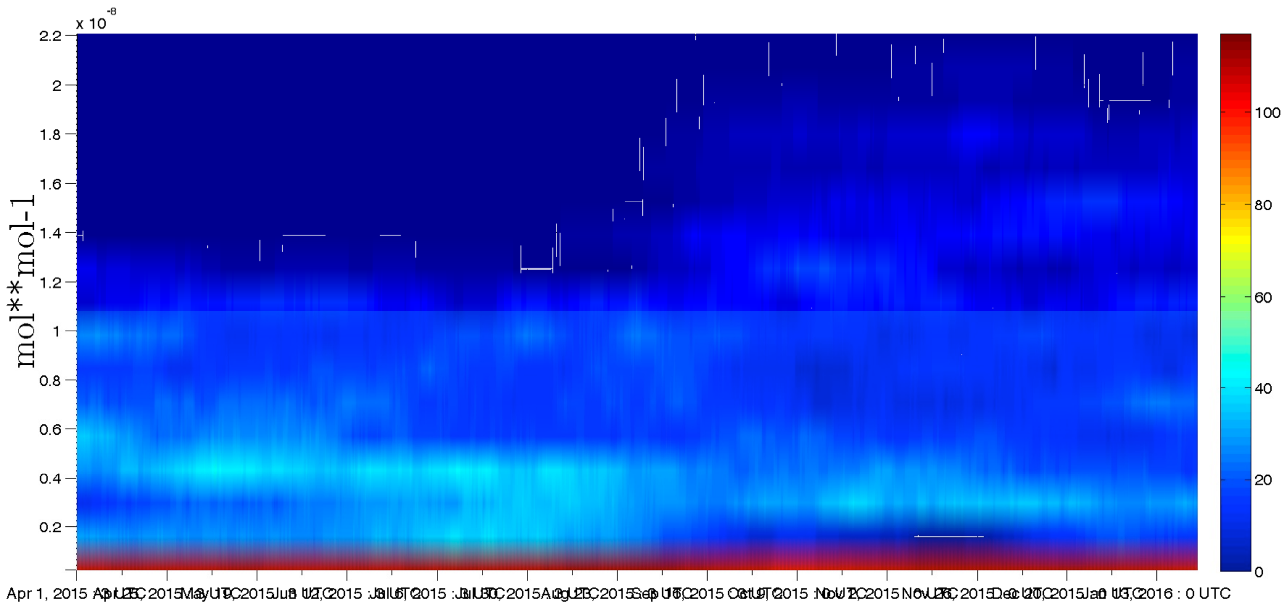

Figure 16. Temporal distribution of NO_2 by MACC1.

ERROR STATISTICS

The error statistics were calculated in the period March 24-April 4, 2016. This period corresponds with the contingency in the region owing to the high concentration of pollutants in the atmosphere over the Medellín metropolitan area. Our objective is to evaluate through the statistical analysis the consistency of error of the physical-chemical results in comparison with the data of the MACC1 Project. To compare the error of the model we used four statistical measures applied to the volume mixing ratio of NO2 and O3 modeled through LOTOS-EUROS. The analysis is based on eight pairs of modeled and measured observations over the selected domain. The evaluation measurements implemented are: the ratio, the residual, the root mean square (rms), and the average correlation coefficient. The selected points to compare the LOTOS-EUROS outputs with data from the Copernicus Project are shown in Figure 18. For each point was calculated the four statistical measures to have a spatial representation of the model error. The total statistical measures for the domain are presented in the Table 1.

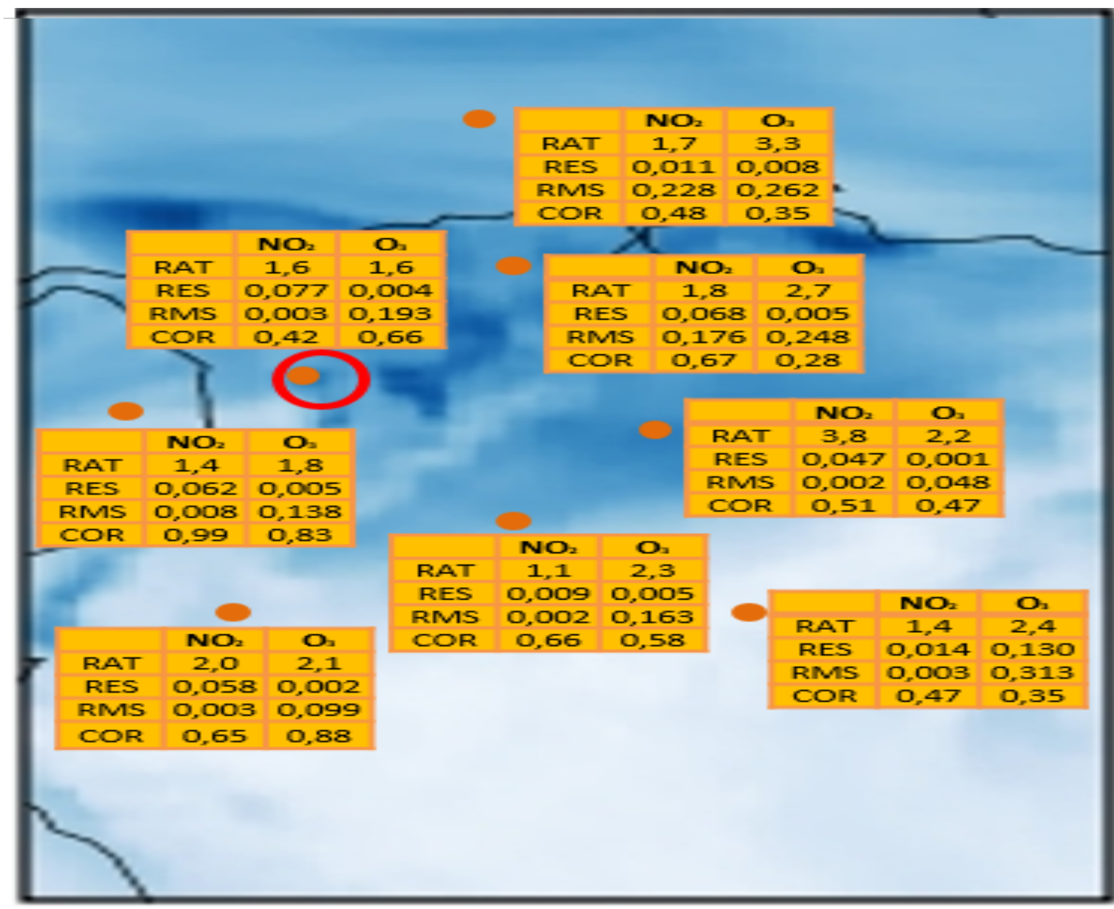

Figure 17. Distributions and statistical measures of the comparison points. The red circle is the Aburrá Valley (Medellín) location.

Table 1. Statistical measures features

Variable	**NO_2**	**O_3**
Ratio	1.8	2.1
Residual	0.003	0.005
rms	0.053	0.183
Corr. Coef	0.62	0.65

According to the Table 1 and the value of the statistics for each point, the model tends to overestimate the concentrations both NO_2 and O_3 for the entire domain. For NO_2, a part of the bias is due to high-modeled concentrations at two points. The other points have a value closer to the regional mean. For O_3 the ratio has a high value for almost all points, presenting a more uniform trend in the region. For both substances, for most points the correlation coefficient is into the range between 0.40 and 0.88, with only a point with a lower value (0.28) and other with a higher value (0.99). The total correlation coefficient for the domain in both substances is considerably high, this means that the model is able to reproduce the temporal behavior of the two substances with an acceptable performance.

CONCLUSIONS

LOTOS-EUROS is a capable tool to represent and simulate the dynamics of the pollutants over the Tropical Andes region. Despite the observed errors in magnitudes, the LOTOS-EUROS model captured the temporal dynamics of the substances analyzed. With the current resolution, LOTOS-EUROS is not able to represent precisely the dynamics of the pollutants in certain cities of the region such as Medellín. Although it is possible to increase the resolution of LOTOS-EUROS, it is necessary to have data for initial and boundary conditions of better resolution. Data assimilation for LOTOS-EUROS with data from ground-based stations and other sources, can improve the accuracy of the model, both for the current scale and for smaller scales.

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