

H13-199

AIR QUALITY PHOTOCHEMICAL STUDY OVER AMAZONIA AREA

Lucio SILVA DE SOUZA^{1,2} Luiz LANDAU² and Luiz Claudio PIMENTEL¹¹Department of Meteorology, Institute of Geosciences, Federal University of Rio de Janeiro (DMET/IGEO/UFRJ), Rio de Janeiro, Brazil²Laboratory for Computational Methods in Engineering, Alberto Luiz Coimbra Institute, Graduate School and Research in Engineering, Federal University of Rio de Janeiro (LAMCE/COPPE/UFRJ), Rio de Janeiro, Brazil

Abstract: Urban-scale air quality modeling over Brazil has been advancing in recent years with several modeling studies of air quality in the metropolitan areas of Rio de Janeiro and Sao Paulo especially. Extending these photochemical modeling applications to the continental scale in order to study regional transport of pollutants throughout South America is the focus of this presentation. This work presents the initial results of a photochemical modeling system composed of MM5-SMOKE-CMAQ that focuses on the Amazonia region of Brazil. These results focus on biogenic and biomass burning emissions in Amazonia and the impact of these emissions on regional and local air quality. A combination of global and local anthropogenic emissions data, satellite-derived biomass burning inventories, and biogenic emissions calculated with the MEGAN model were used to estimate emissions over the mother domain at grid resolution of 37-km. The mother domain covers most of South America. We modeled August 2005 because it was the driest period in the region over the last 50 years. Due to a lack of surface-based air quality monitoring data in Amazonia, we are exploring model evaluation techniques using satellite-based air quality products. This paper focuses on the development of the input data to the CMAQ air quality model, including initial and boundary conditions, meteorology, and emissions. Preliminary CMAQ results are also presented along with qualitative comparisons against satellite networks for some air pollutants. Results are consistent with theory of O₃ formation and were compared with MODIS TERRA satellite data available.

Key words: Amazonia photochemical air quality, SMOKE emissions processing, CMAQ forecast for Brazil.

INTRODUCTION

Air Quality forecast over Brazilian Amazonia Area is still a theme of uncertainties. The lack of emissions inventories and air quality monitoring networks for that area still remain a problem for those interested in studying this theme. On the other hand, Amazonia has been experiencing a stronger change process due to economical growth. The main metropolitan Areas are Manaus and Belem and only these two urban complexes have a total population of 4,152,000 inhabitants, while in the total legal Brazilian Amazonia area (composed of 9 states) the population is about 20 million (IBGE, 2000).

Changes in the land use by deforestation (controlled or not) compose one of the main actors for that scenario changing. The called "Arc of deforesting" is a proof of those changes and has stronger correlation with the agriculture and livestock expansion for that region. The figure 1 shows the "arch" that has been under control from the authorities and is nowadays called "Arch of sustainable development".

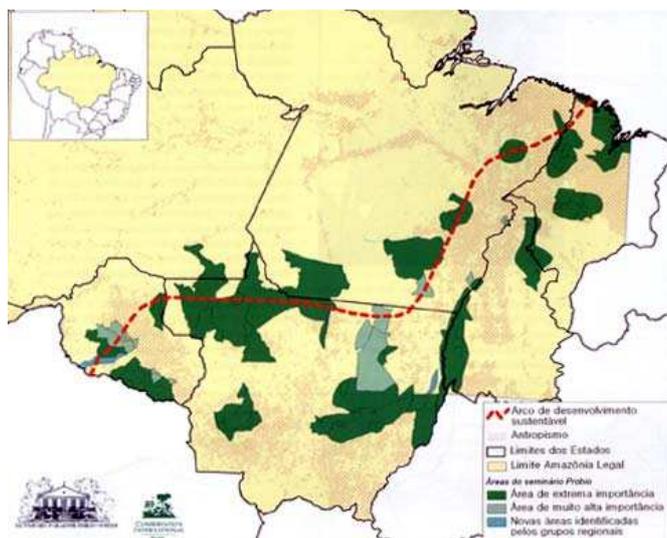


Figure 1 – Arc of Deforesting (2002)

Over Amazonia there's a Petroleum and Gas Natural plant in the southwest of the Amazonas State and a refinery at Manaus metropolitan area. These two petroleum facilities are responsible for feeding that area with fossil fuels and altogether with land use changes due to biomass burning and economic growth confirm the need for air quality studies in North Brazil Region.

The system composed of MM5-SMOKE-CMAQ is implemented for Brazil with coarse horizontal resolution of 37 km (165 x 165 points), and 23 vertical sigma levels. The SMOKE model was fed with Biomass burning data from GFED inventory, part of the GEIA (www.geiacenter.org). The Biogenic Emissions were obtained from MEGAN model (Guenther *et al.* 2006) with resolution of 1 km. These two emission components might be in charge of photochemistry in that area, particularly if the

simulations are focused at regional scale. Shipping Emissions, main point sources and National Roads were inserted from GIS global database as well and were treated as area sources at SMOKE.

OBJECTIVES

The main objective of this work is focused on the implementation of the system composed of MM5-SMOKE-CMAQ models of Brazil and its surroundings. The additional objectives might be discussions of the initial results for air quality photochemical forecast over the Brazil Amazonian area as well as illustrating the emission inventories framework to perform that modeling for South America. The lack of a public national emission inventory and air quality based ground monitoring network makes this work a challenge by adapting global to regional inventories and assimilation of them by the SMOKE model. The results shown in this paper refer to our coarse domain. The problem identification of this task as a whole might also be considered as an objective.

METHODOLOGY

The system is run in a 64 bits machine with 8 processors and our compiler is intel XEON 3.0 GHZ. Tests linked to processors and/or compilers and computational efficiency are not our focus at this moment.

The dry season 2005 was the most intense in the last 50 years over the Amazonia area and, this season has been linked to the anomalies of Sea Surface Temperature (SST) that was one of the main causes of the intense hurricane season over the North Atlantic and Caribbean area that year (CLIMANALISE, 2005). This SST anomaly implied in a very unstable atmosphere, driven by upward vertical motion in the Northern Atlantic and, as a response to that upward motion, the downward motion was directed to Northern Brazil. This motion blocked the convection mechanism, the dominant raining regimen over that area, causing significant problems to the people and environment at that area.

The PSU/NCAR mesoscale model (hereinafter MM5) is used to feed the SMOKE-CMAQ system with hourly meteorological data. The MM5 outputs are processed throughout the Meteorology Chemistry Interface Processor, hereinafter MCIP, that perform the changes needed in the original MM5 outputs to the use at SMOKE-CMAQ. This tool is available together with SMOKE and CMAQ (www.cmascenter.org). The model is run with GFS-NCEP global data ($1^\circ \times 1^\circ$), with a mother domain horizontal resolution of 37 km and two nested grids (12.3 and 4.1 km) and the outer grid is centred at the geographic South America centre, while the two other domains at Brazilian Amazonian Area. The smaller is centred in the Petroleum and Natural Gas Facility, southwest state Amazonian (BOGPM), the biggest Petroleum and Natural Gas facility at Brazil North Region. This MM5 run is composed with 24 vertical layers, in which 8 of them are at the boundary layer. The MM5 parameterizations schemes are disposed at table 1.

Table 1 – MM5 Parameterizations.

Cumulus	Grell (1993) domain 1 and 2 ¹ ,
Clouds Microphysics	Dudhia (1989)
Radiation	Dudhia (1989)
Landuse	Landuse model NOAH LSM (Chen and Dudhia, 2001)
PBL	Mellor and Yamada (1974, 1982)

The SMOKE model (www.smoke-model.org) is used to provide emission inventory data as input to CMAQ model. Generally SMOKE processes the emissions from typical emission inventories formats into the one required by the CMAQ model (www.smoke-model.org). At this work, SMOKE was used to process emissions from the GFED biomass burning global emission inventory (www.geiacenter.org), with $1^\circ \times 1^\circ$ horizontal resolution, year base 2005 and a total monthly mean extracted and processed to daily basis. These data processing is done with support programs available altogether with SMOKE and CMAQ at the web portal (www.cmascenter.org). Also in SMOKE it is possible to set up the average day emissions once informing that the input data are on a monthly basis by setting this information into one of the SMOKE run scripts, which was done for this work as described earlier. In the case of National Mobile Roads emissions, these data were extracted from GIS Brazil National Geographic Institute (IBGE, 2000) and the emission factors are informed according to the available GIS global database. The mobile sources are processed into a week basis and the holidays tool isn't set for this run. The shipping traffic and emissions are extracted from GIS information and also processed on a weekly basis. In all SMOKE steps, the meteorological information processed through MCIP must be inserted on each type of source processing in the run scripts and is inserted on the merge script, the one that makes the processing for all types and creates gridded emissions in moles/s as required by CMAQ model. The chosen chemical mechanism is CB05 and at this moment, chemical mechanism isn't the focus of this work. The results of the innermost domain aren't shown in this written work because they are under map projection errors that have still been a source of numerical work from both UFRJ and UNC - Chapel Hill, USA groups. Shipping emissions and the main National Brazilian Roads (only federal roads) were also provided as area sources at SMOKE model.

¹ Not applied for horizontal resolutions under 10 km

The biogenic emissions were extracted from MEGAN model (Guenther *et al.* 2006) and the outputs are inserted into SMOKE with horizontal resolution of 1 km. When biogenic emissions come from MEGAN model, SMOKE model do not process its information because the outputs are ready for CMAQ input, but SMOKE helps on the grid distribution of them. Meteorological information for MEGAN is also required and is processed at the same manner as for SMOKE model with MCIP converser.

The CMAQ model (Byung *et al.* 1998) is run with 37 km horizontal resolution centred at South America centre exactly as for MM5 and SMOKE. The task of running isn't complex as it is for SMOKE and its support programs because once the emissions files from SMOKE are available, CMAQ tends to run properly with correct shell scripts manipulation and chemical mechanism choice through the modeller. In our study the focus with CMAQ is to inform that this model might be used for South America, having solved the numerical structural problems (map projections, compilers, etc...) in the code. The CMAQ initial conditions were run to use the default profile Initial Conditions (IC's), the Plume in grid option isn't set, the meteorology is set with 3D met fields as requested to nested grids and the mechanism conversion is set according to CB05. The Boundary Conditions (BC's) were also run with the default profile input, including Plume in Grid profiles from IC's dynamics and concentration generation, and the same other settings as described for IC's. The photolysis rates are run at JPROC program and set as the meteorological information has been disposed from MM5-MCIP. The JPROC, which performs the photolysis rate, is highly influenced by meteorological conditions. No Global Chemical Model is used to feed the coarse domain borders in this work. This is a task that is still under development.

The main problems linked to this system became apparent when converting the meteorological data into MCIP converser to feed SMOKE with meteorological data. There is a structural problem with MCIP code that didn't support the Mercator recommended projection for tropical areas, then it was necessary to configure the model by using Lambert Conformal projection, besides this one isn't the best for our area of interest. It should be noticed that the same problem was found when assimilating the GIS information into the SMOKE, as for the surf zone coastal area. Nowadays, it has been a joint effort with the staff of CMASCENTER to develop a MCIP version in order to support Mercator projection.

RESULTS

Briefly a discussion of the emission results for the Julian day 216 (August 4th, 2005). The maps on figure 1 show the top emissions and concentrations obtained for this day and are at the same scale as in "a" and "b". These biogenic emissions were extracted from MEGAN model and the Area Anthropogenic emissions were processed with SMOKE model, both also as described earlier.

According to figure 2 is possible to see that the top biogenic emissions occur late afternoon and the anthropogenic is related to the biomass burning activity, which is a regular action to renew the soil for the next crop. This biomass burning might or might not be controlled by the authorities. All emission maps are presented in mol·s⁻¹, the required unity for CMAQ input. The scales are set to be the same for all pollutants processed.

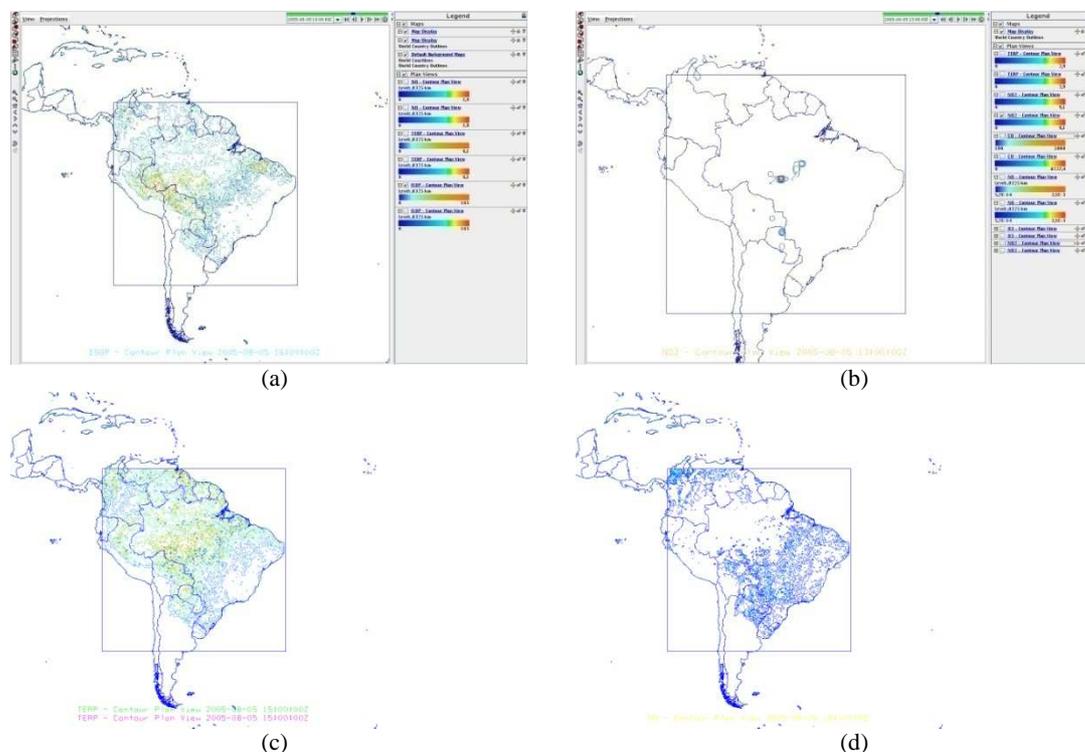


Figure 2 - Megan - Biogenic highest Emissions for (a) Isoprene; (c) Terpene and (d) NO – SMOKE Area Anthropogenic emissions (b) NO₂

The CMAQ runs outputs are illustrated on figure 3. CMAQ was run as described earlier and the results show the top concentrations for each pollutant set in this run. It is possible to identify the high concentrations observed at south-western and centre Amazonian area. These highest concentrations are linked to biomass burning and stronger biogenic emissions as processed at SMOKE and MEGAN respectively. Besides neglecting important emissions sectors, the system is able to forecast the main area in Amazonia for air quality studies. The output units are all in ppmV.

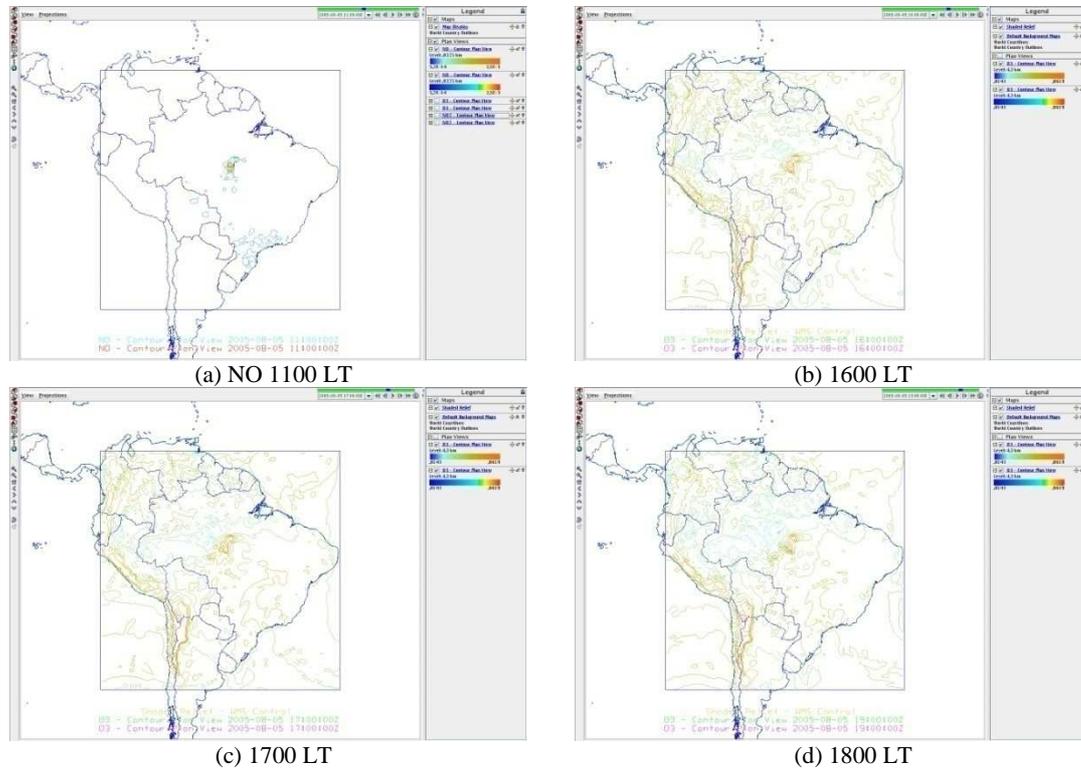


Figure 3 – CMAQ outputs top concentrations for (a) NO; and O₃ in (b), (c) and (d). The results are shown in Local Time (LT)

The Satellite images from MODIS imagery (TERRA and AQUA) are shown in sequence (figure 3) for the same period as for CMAQ outputs. According to MODIS data it is only possible to observe some high concentrations over South America Centre with TERRA sensor, as the low resolution of this sensor (1° X 1°) might be one of the reasons for this poor imagery quality.

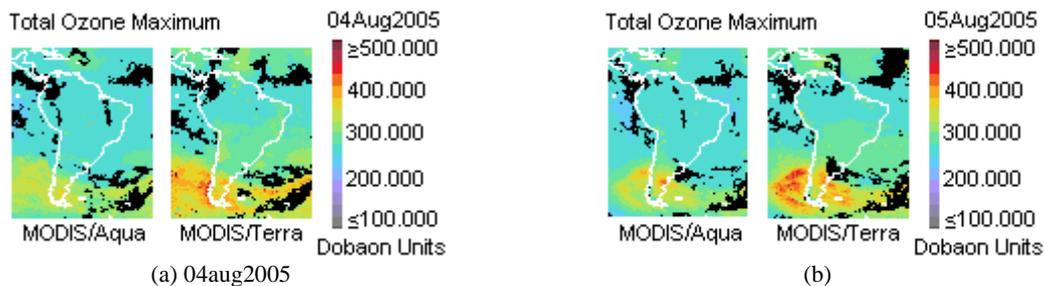


Figure 4 – Satellite Ozone MODIS AQUA and TERRA maximum concentrations for 4th (a) and 5th (b) August 2005

The comparison of modelled data with satellite derived data isn't an easy task. The coarse resolution of the modelling system is 37 km while at the satellite it is 1° (~ 111.1 km). Additionally the measurement units in satellite do not match the modelling outputs. We've been working on the comparison with MOPITT data, but we still do not have Ozone data and for MOPITT CO data provided, highest concentrations registered for that area in August with magnitude of 250 – 300 ppbV are shown.

Conclusions and next steps

The system MM5-SMOKE-CMAQ has been pioneered and implemented in Brazil in a grid that covers almost all South American Countries. The task of feeding SMOKE with global inventories was one of the big challenges of this work. The lack of nationally based emission inventories does not allow another option while studying the ozone formation, especially for Amazonian Area. Besides neglecting important sectors and inventories, the system has disposed the output data according to the expected theory and it might be confirmed through quick comparisons of MODIS and MOPITT data. This system, especially given its characteristics of multi-scale, once complete with data on global and regional issues, and having overcome the structural problems, has great potential both in research and operationally in Brazil.

For the next steps we are working on feeding SMOKE with more GIS based emissions and inserting information about the main metropolitan area inserted on Amazonia. Up to now, we have not had access to the petroleum plant emission data but it is expected to extract some information from global GIS just to provide some signal of this activity in our emission scenario. In the near future, tests for best chemical mechanisms, better meteorological setup and GCM input to the large domain will be provided. Also this domain will work as an input for the grids in Rio de Janeiro and other urban centres in south eastern Brazil area.

The code structural problems found at this implementation have been subject of a joint study with the staff of CMASCENTER and UFRJ. It is important to note that this work has contributed to perform a new MCIP version.

REFERENCES

- Byun, D.W., Ching, J.K.S., 1999. Science algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modelling System; U.S. EPA/600/R-99/030.
- CLIMANALISE, 2005: Boletim de Monitoramento e Análise Climática, (<http://www6.cptec.inpe.br/revclima/boletim/>) Volume 20, Agosto 2005. Accessed from January 2005 to March 2010.
- CMASCENTER, 2010: Community Modeling & Analysis System, (<http://www.mascenter.org/>). Accessed from 2006 to April 2010.
- Guenther, A., T. Karl, P. Harley, C. Wiedinmyer, P. Palmer, and C. Geron, 2006: Estimates of global terrestrial isoprene emissions using MEGAN (Model of Emissions of Gases and Aerosols from Nature), Atmospheric Chemistry and Physics, Nr. 6, 3181-3210.
- IBGE 2000: Brazilian Institute of Geography and Statistics (<http://www.ibge.gov.br/home/>) Accessed from January 2005 march 2010.
- SMOKE-MODEL, 2010: Sparse Matrix Operator Kernel Emissions, (<http://www.smoke-model.org/index.cfm>). Accessed from 2006 to April 2010.