Emissions Inventory for the Metropolitan Area of Vitoria, ES, Brazil using SMOKE System

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ABSTRACT

Large industrial facilities were installed in the northeastern region of Metropolitan Area of Vitória, Espírito Santo, Brazil. These facilities were built to enable production and port exportation of goods from the ore, steel and pelletizing industries, but the main wind direction in the area carry the gases and particles emitted to the most populated sector of the city. This problem has led to legal disputes between residents and companies, generating additional costs for the enterprises in the form of mitigating actions and upsetting the populace, which has to deal with the impact of the industrial emissions, including breathing the polluted air. Emission inventories are a fundamental input to atmospheric chemical transport models (CTMs). This study presents an adaptation of the official emission inventory for anthropogenic sources covering Great Vitoria Area (GVA) for the reference year 2009 using the SMOKE (Sparse Matrix Operator Kernel System). The SMOKE model is used to compile a high spatially and temporally resolved emission inventory. The bulk of the pollution is due to motorization, facilities, and residential activities. The inventory provided by the local environmental agency has been adapted and tested with the air quality model (AQM), Chemistry Model Air Quality (CMAQ).

1. INTRODUTION

"Atmospheric emission models supply one of the most important pieces of data required by dispersion models for reactive pollutants: the amount of pollutants emitted in each point of space at a given moment, i.e. the emission inventory. Emission models are also essential to estimate the emissions of atmospheric pollutants in a given area: their type, origin, amount emitted and the distribution in time and space. The elaboration of emission inventories on a regional or local basis is a necessary step when setting up plans to control the level of pollutants, especially in areas of high formation of photochemical oxidants." (Costa et al., 1996, p. 1).

Emissions inventories are developed and updated throughout the world. Their quality has greatly improved in recent years due to significant efforts in data compilation of technology-based and activity-based emission factors, and the development of more robust estimation methodologies.

"Currently, there is a remarkable tendency in the different states towards the development of high-resolution emission models (1 km^2) following bottom–up approaches" (Baldasano et al., 2008, p. 2). This tendency can be found in Aérovalo et al., 2004 (1x1 km^2), Guttikunda et al., 2013 (1x1 km^2), Kannari et al, 2007 (1x1 km^2), Markakis et al., 2010 (2x2 km^2) and Baldasano et al, 2008 (1x1 km^2). In the United States (U.S.) there are several inventories for specific pollutants with different grids nationwide. "Emission inventory preparation is a critical stage in an air quality model (AQM). The generation of input information from regulatory emission inventories compatible with requirements of eulerian chemical-transport models needs a computationally efficient, reliable, and flexible emissions data processing system. The SMOKE was developed in the United States and redesigned by the US Environmental Protection Agency

to support air quality modeling activities in the framework of the USEPA Models-3 system." (Borge et al., 2008, p. 1) [3]. In South America, particularly in Brazil, there is no nationwide emission inventory adaptable as input for photochemical air quality models. The GVA (fig. 1 and 2) is one of the few regions in the country where there is an hourly emission inventory, provided by IEMA-ES, for point, area and highways sources. This work aims to adjust this inventory to SMOKE format, with high spatial (1x1 km^2) and temporal (1 hour) resolution grids. Pollutants used include those composed of particles with diameter less than 10 mm (PM_10) and SO_2 (sulfur dioxide) gas.

Fig.1. Vitoria position in the South America.

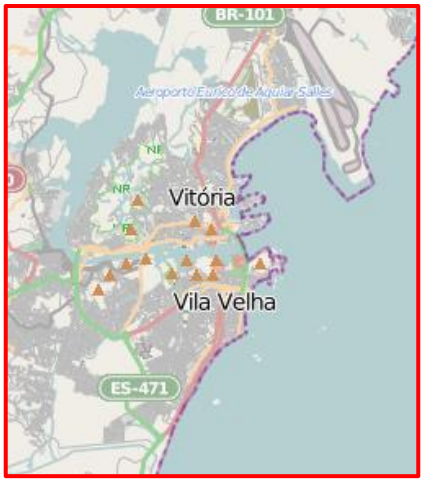

Fig. 2. SMOKE domain.

2. METHODOLOGY

"The SMOKE modeling system (Houyoux et al., 2000; UNC Carolina Environmental Program, 2005) was created by the MCNC Environmental Modeling Center (EMC) to allow emission data processing methods to integrate high-performance-computing (HPC) sparse matrix algorithms. This software is based on a parallel approach to emissions processing and was redesigned and improved with the support of the United States Environmental Protection Agency (USEPA), for use with EPA's Models-3 Air Quality Modeling System." (Borge et al., 2008, p. 2-3). This article creates a SMOKE format files for the GVA emissions inventory.
In the adaptation of the Great Vitoria Area (GVA) emissions inventory for SMOKE, emission sources of pollutants were divided in two types: point and area sources. Sources, whose features required them to be classified as point sources by the model such as font height, diameter of the chimney, emitted gases temperature, stack gas exit velocity, etc., were so classified. Area sources were composed of regions exposed to various materials and urban roads, commercial and residential emissions. SMOKE can accommodate many formats of inventories of area sources ($ARINV) and point sources ($PTINV). In this article, Inventory Data Analyzer (IDA) format was used. Simulation was performed in the period from 15 to July 31, 2012.

Chemical Speciation
SMOKE can process gaseous pollutants such as carbon monoxide (CO), nitrogen oxides (NO_x), volatile organic compounds (VOCs), ammonia (NH_3), sulfur dioxide (SO_2), any particulate matter (PM), PM with diameter equal to or less than 2.5 micra (PM2_5) or equal to or less than 10 micra (PM_10), as well a variety of toxic pollutants such as mercury, cadmium, benzene and formaldehyde. Actually, SMOKE has no limitations on the number or type of pollutants it can

process. SMOKE can also accommodate a variety of chemical mechanisms. From the perspective of emissions inventory, chemical mechanism is the mapping of pollutants from emissions inventory, deployed for species of interest required in AQM. PM2_5 and VOC speciation, i.e., the percentage of each chemical component on these pollutants, were derived from North American references (SPECIATE V4.2 database, USEPA, 2009) adapted to regional experimental measurements. In the absence of specific information, the relationship between NO/NO_x was considered equal to 0.62 for all categories of nitrogen oxides emissions.

Temporal Allocation

Industrial chimneys sources typically operate 24 hours a day including weekends and holidays. However, many sources are intermittent, which creates the necessity to describe their hourly emission profile. Urban roads were portrayed by following the traffic flow of GVA's main bridge (named Third Bridge).

Spatial Allocation

"The choice of method for spatially allocating regional emission inventories into grid cells depends on the source characteristics and resolution size." (Zheng et al, 2009, p. 5). For large industrial plants, emissions from chimneys were treated as point sources and allocated directly to the grid cell where the plant is located based on their geographic coordinates (latitude and longitude). For allocating GVA regional on-road source emissions, Geographic Information System (GIS)-based road network information as spatial surrogates was adopted. This approach has been shown to provide more reasonable spatial allocations of regional mobile source emissions, especially at higher resolutions (Zheng et al, 2009c).

3. RESULTS

Emissions Summary

Point sources in GVA are located mostly in an area called Shark Point, located to the north of the region's most populated area. In GVA, point source emissions represent 15.86% of PM_10 total emissions, 16.34% of PM2_5, 76.04% of SO_2, 48.64% of NO_x, 49.54% of CO and 6.92 % of NMVOC. Emissions from diffuse sources are 9.51% of PM_10 total emissions, 10.24% of PM2_5, 22.59% of SO_2, 17.98% of NO_x, 0.84% of CO and 39.43% of NMVOC. Road emissions, considering particle resuspension, tire wear, exhaust fumes and evaporation represent 74.63% of PM_10 total emissions, 73.42% of PM2_5, 1.37% of SO_2, 33.38% of NO_x, 49.61% of CO and 53.65% of NMVOC. None of these percentages take into account biogenic emissions.

Domain of Interest

a) Area Sources

Area sources were divided into two types: sources from vehicular emissions and diffuse sources. Vehicular sources were treated considering the proportionality between the vehicle flow and road emissions. The fraction of the area occupied by roads in each cell of the grid was considered an emission source. Since traffic flow is not constant throughout the day, week and month, time functions available in IEMA's report were adopted. Diffuse sources are mainly piles of ore and coal from factories located in the northeast GVA. These piles often occupy, even partially, more than a single grid cell. Thus, it was necessary to proportionally distribute these sources in each cell, i.e. the spatial distribution of diffuse sources in the grid. Figure 3 shows PM_10 emissions and figure 4 shows de SO_2 emissions in domain SMOKE grid with 61x79 km^2.

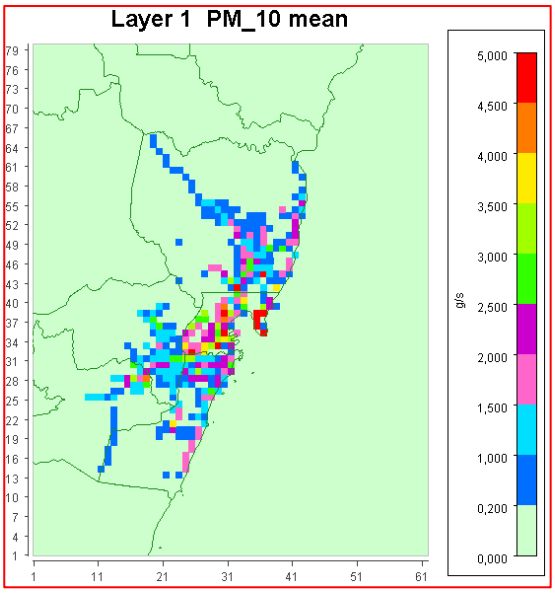

Fig.3. PM_10 emissions from area sources.

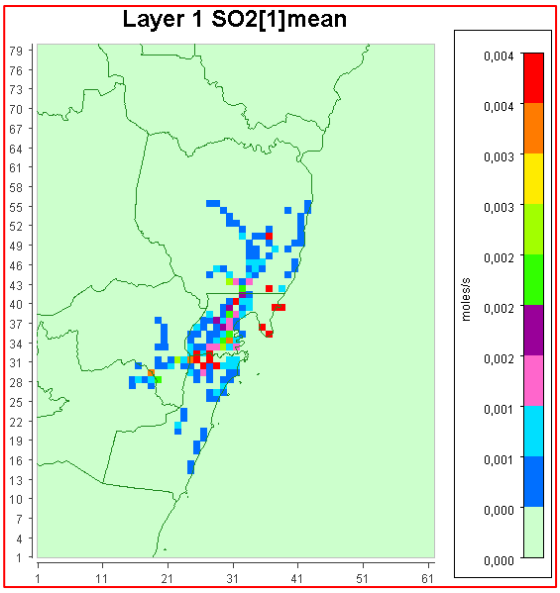

Fig. 4. SO_2 emissions from area sources

b) Point Sources

Chimneys from a large steel mill, a large pelletizing plant and dozens of other smaller factories in GVA were considered point source emissions. An overview of these mean hourly emissions within the grid for PM_10 in layer 1 is shown in Figure 5 and fig 6 show in the layer 7 (between 100 and 140 m. Most large factories in GVA are located northeast of the main residential areas. Since the prevailing winds in the region are also northeast, the populace's main complaint about pollutant concentration refers to industrial pollution.

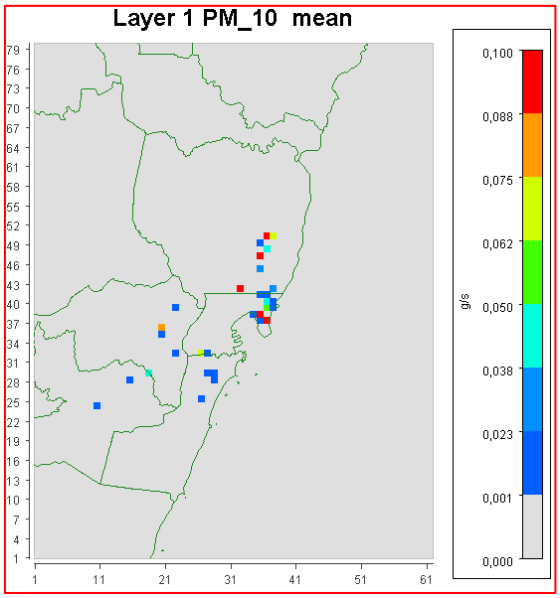

Fig.5. PM_10 emissions from point sources in layer 1.

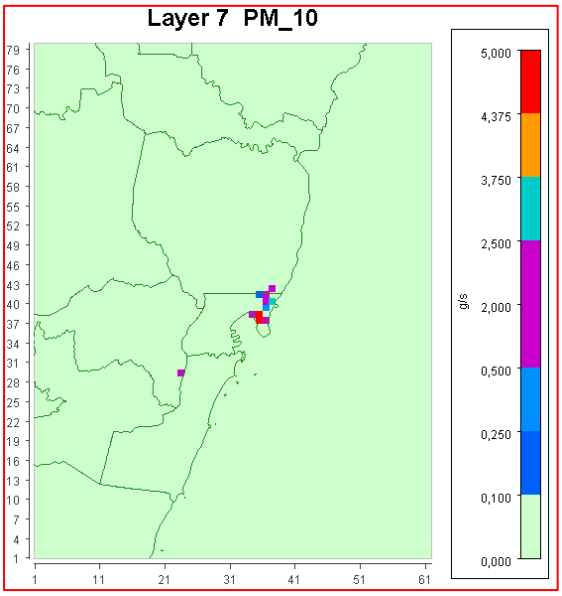

Fig. 6. PM_10 emissions from point sources in layer 7

c) Point and Area Sources

Merging area and point sources, SMOKE creates an emission inventory, which can use in air quality models as CMAQ. This result is shown below. In figure 7 is shown PM_10 emissions and figure 8 is shown SO_2 emissions in layer1 interest domain. Figures 9 and 10 are presented PM_10 and SO_2 emissions in the layer7.

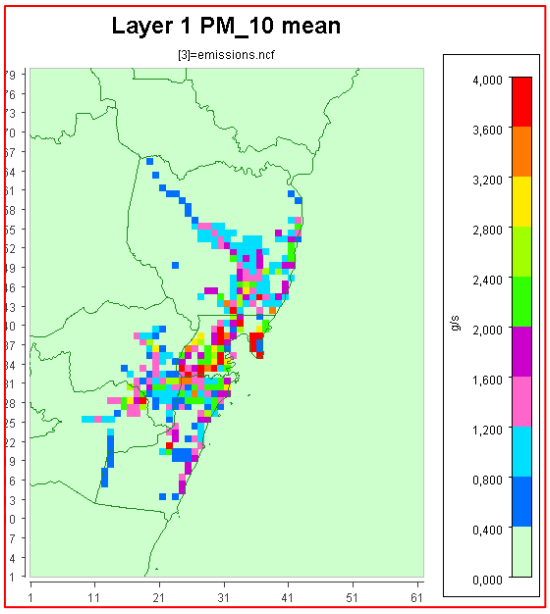

Fig.7. PM_10 emissions from all sources in layer 1.

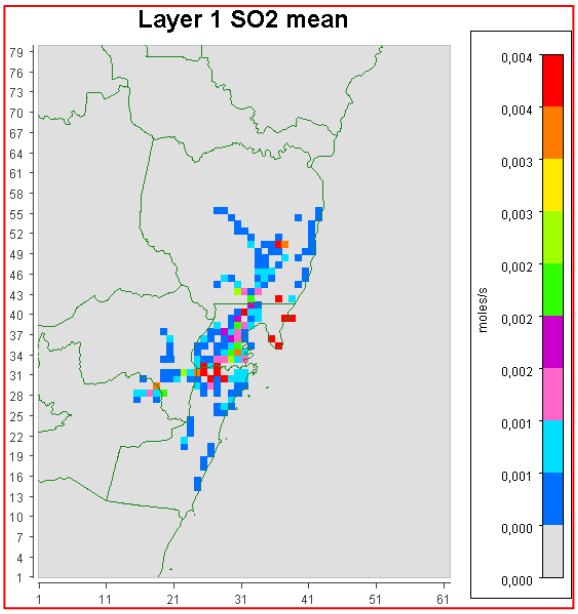

Fig. 8. SO_2 emissions from all sources in layer 1.

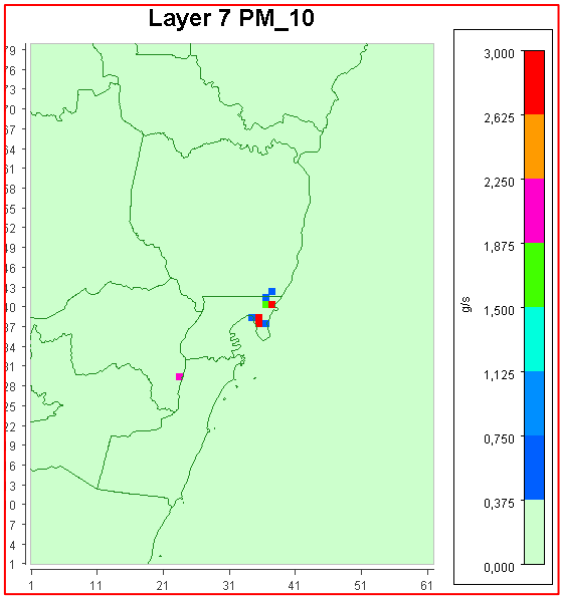

Fig.9. PM_10 emissions from all sources in layer 7.

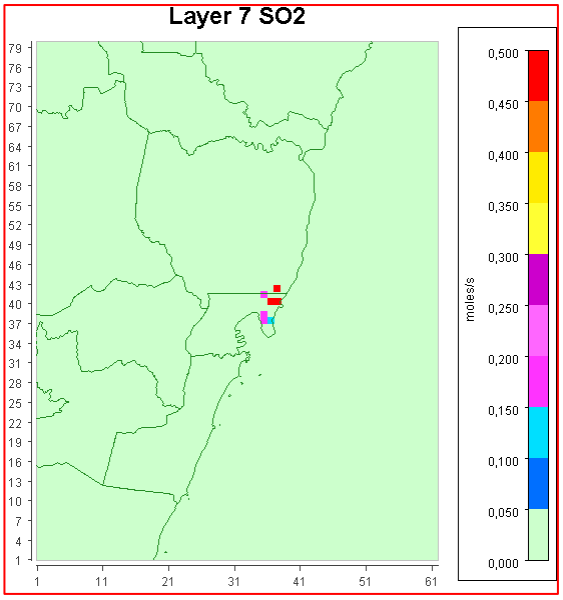

Fig. 10. SO_2 emissions from all sources in layer 7.

4. CONCLUSIONS

Errors on models come from diverse factors such as the spatial variability of pollutants concentration, emission inventory, meteorological data, chemical mechanism parameters and numerical routines (Park et al., 2006). It is no different for this simulation because it is derived from a regional inventory and this inventory has many intrinsic uncertainties. However, this simulation represents an evolution and an incentive for other regions to work in providing and improving emission inventories and chemical speciation of pollutants. An improvement in IEMA's inventory is expected in future versions so that it is more explicit in its chemical speciation, temporal and spatial allocation and, mainly, choice of emission factors. It was

concluded that resuspension values in GVA roads are likely overestimated, which does not invalidate IEMA's effort to provide the emissions inventory for the region.

5. ACKNOWLEDGEMENTS

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