CONTRIBUTION OF ON-ROAD MOBILE SOURCES TO SOA FORMATION IN BOGOTA: A SENSITIVITY ANALYSIS COUPLING WRF-CHEM AND THE TRAFFIC MODEL PTV-VISUM

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1. INTRODUCTION

Organic aerosols, OA, constitute an important fraction of tropospheric aerosols, and are a major component of fine particles ($PM_{2.5}$). In particular, secondary organic aerosols, SOA, can be a dominant part of organic aerosols in polluted areas (EPA, 2016; Seinfeld & Pandis, 2016).

In the city of Bogotá, few studies have investigated the contribution of organics to $PM_{2.5}$. Some studies have focused on the experimental determination of chemical composition of aerosols in the urban atmosphere to elucidate primary from secondary aerosols using receptor models (Hernandez-Gonzalez, Jímenez, Torres, & Holben, 2013; Vargas, Rojas, Pachon, & Russell, 2012). Other studies, like the one conducted by Franco et al., (2015), have characterized VOC's in Bogotá by on-line measurements, finding that diurnal behavior of VOC's is highly influenced by vehicular activity.

To this date, no work has been carried out where photochemical transport models are used to analyze the contribution of SOA to particulate matter concentrations in the city.

In this project we perform a series of sensitivity analysis with the Weather Research and Forecasting coupled with Chemistry model (WRF-Chem) to determine the potential contribution of SOA from mobile sources, to the total sub-micrometer particle mass in the city.

In order to assess the contribution of mobile sources to SOA, emissions are estimated by using spatially distributed activity factors obtained from the traffic analysis software PTV VISUM. This traffic software simulates all roads and their interactions, and is fed with road characteristics and estimation of origin-destination matrixes, its outputs are vehicular counts disaggregated by type of fleet. (PTV, 2017).

The temporal disaggregation of emissions is based on scaling according to available vehicle counts in many parts of the city. Activity patterns are then used to compute emission rates. Point sources emissions inventories (industrial, commercial and gas facilities) constructed by local environmental agencies are used (SDA, 2014). Both inventories were speciated according to the requirements of the selected gas-phase chemical mechanism, RACM.

2. METHODS

2.1 Implementation of PTV VISUM traffic model

PTV VISUM was implemented using Bogotá's road network information and vehicle fleet data. Results were gridded to match WRF-Chem modelling grid, using equation (1).

$$AF_j = \sum_{(l=1)\in x}^{n\in x} Nf_j \times L_{l\in x} \quad (1)$$

where AF_j is the gridded activity factor per fleet, Nf_j is the traffic volume, and $L_{l\in x}$ the road length.

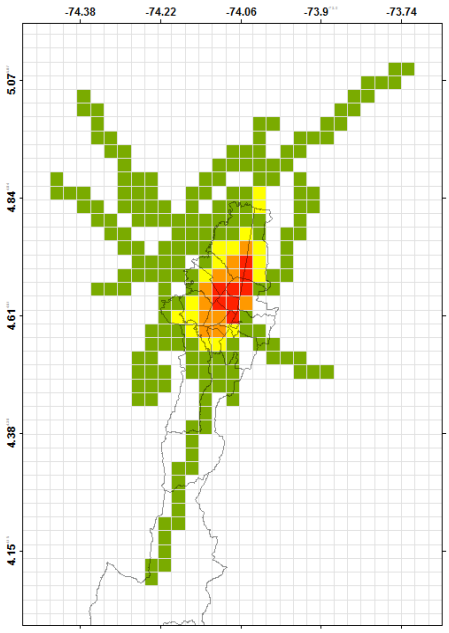

Figure 1 Spatial distribution of emissions from mobile sources

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Using the spatially distributed activity factors, emissions were calculated using emission factors from the International Vehicle Emissions (IVE) model as described by Giraldo & Behrentz (2005), as seeing in equation 2.

$$E_{(x,y,t)} = \sum EF_{i,j} \times AF_{j(x,y,t)} \quad (2)$$

where $EF_{i,j}$ is the emission factor per vehicle fleet, and $AF_{j(x,y,t)}$ is the activity factor. A spatial distribution of the obtained emissions is shown in Figure 1.

2.2 WRF-Chem model configuration and experimental design

2.2.1 Model Configuration

WRF-Chem v3.9 was used to carry the simulations. The model was configured for three nested domains centered in Bogotá. The outermost domain d01 with a resolution of 27km (100x100), d02 domain with a resolution of 9km (86x86) and d03 domain with a resolution of 3km (76x76). Meteorological parameterizations and static field data, were selected based on previous studies performed in the city (Arango & Ruiz, 2011; Nedbor-Gross et al., 2017). The vertical resolution was 30 layers as the default configuration.

Modelling period was selected based on meteorological conditions and $PM_{2.5}$ and CO concentrations observed at air quality monitoring stations. The selection criteria had two components: a) The period should have 10 consecutive days with high PM concentration (greater than the 75th percentile). b) Should have 10 consecutive dry days (with an average precipitation less than 2mm). Observations from January 2014 to June 2017 were screened in search for an appropriate period. The selected simulation period starts in January 10th, 2016 and only seven days were used to run the model. A 24 hour spin-up time was used to allow model stabilization.

Final Operational Global Analysis FNL data (1°x1°) (UCAR, 2016) was used as meteorological boundary conditions. Chemical initial and boundary conditions were gridded from MOZART-GEOS5 for the outermost domain d01. One-way nested simulations were performed using EDGAR-HTAP 2010 global anthropogenic emissions inventories for d01 and d02. For d03 EDGAR-HTAP was given a diurnal behavior, based on activity in Bogotá. The global emissions inventory was merged with locally developed emissions. As for biogenic emissions, online MEGAN calculations for all domains was used.

2.2.2 Experimental design

To evaluate the influence of mobile sources on SOA formation, four modelling simulations were tested. A base case was set to perform comparisons using all VOC's emissions, the gas-phase chemical mechanism RACM and the MADE/SORGAM aerosol option. Three sets of experiments were designed.

Two changes were made amongst modeled scenarios: VOC's from mobile sources were removed and the organic aerosol scheme was modified to MADE/VBS. A summary of the experiments is shown in Table 1.

Table 1. Summary of experiments and features tested.

Exp.	Gas-phase chem. mech	Aerosol scheme	Emissions
BsC	RACM	MADE/SORGAM	All emissions
SC1	RACM	MADE/SORGAM	No mobile VOC
SC2	RACM (AQ)	MADE/VBS	All emissions
SC3	RACM (AQ)	MADE/VBS	No mobile VOC

3. RESULTS

3.1 Base case meteorology results and PM estimates

Estimated meteorological variables were compared against observations at air quality monitoring stations. Good agreement was observed for variables such as temperature and wind speed. Wind direction was found not to be well represented by the model (see Figure 2).

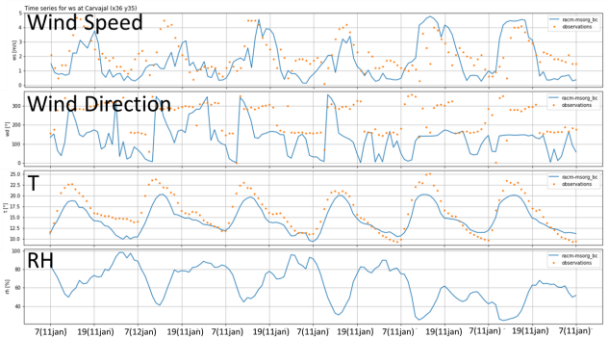

Figure 2 Time series of meteorological Variables at *Carvajal* AQ monitoring station. Dots: Observations. Line: Model estimates.

A comparison of PBL height was also conducted. Observed PBL height was determined

using the morning radio sound data available in the city. The model captures the growth and collapse of the boundary layer, although it underestimates the height after the sixth day of simulation (see Figure 3).

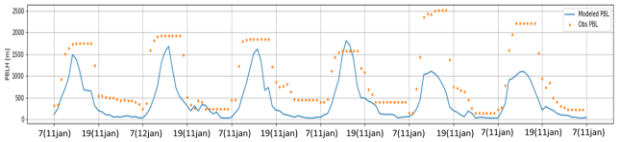

Figure 3 Time series of planet boundary layer height. Dots: Observations. Line: Model estimates.

Additionally, comparisons of PM_{10} estimates with observations show that the model is over predicting particulate matter. Diurnal behavior is highly influenced by PBL height (see Figure 4).

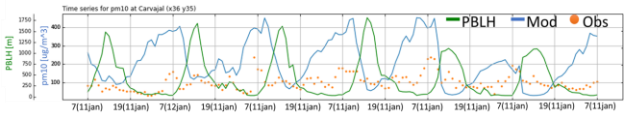

Figure 4 Time series of PM_{10} at *Carvajal* AQ monitoring station. Dots: Observations. Blue line: Model estimates. Green line: PBL height model estimates

3.2 Base case comparison with experiments

Base case modelling results were compared with the different scenarios. Spatial average differences in anthropogenic secondary organic aerosol -ASOA- (Figure 5 and Figure 6), show the importance of mobile VOC's on SOA formation in the city. The organic aerosol scheme combination of MADE/SORGAM estimated more SOA than MADE/VBS (Figure 6).

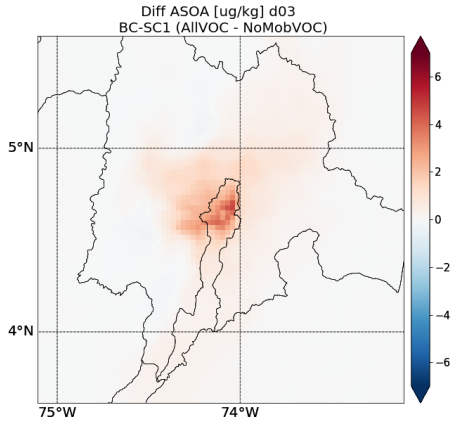

Figure 5 Average spatial difference of ASOA for Base case minus Scenario 1 (With and without VOC's) for RACM and MADE/SORGAM

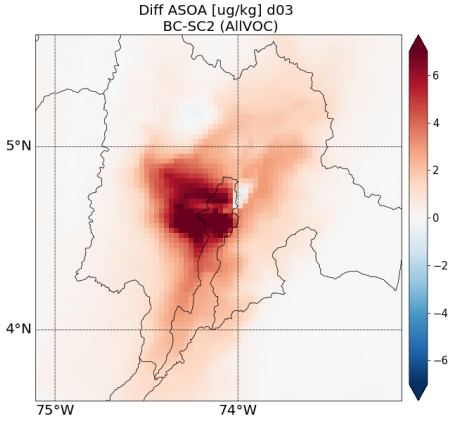

Figure 6 Average spatial difference of ASOA for Base case minus Scenario 2 (all VOC), RACM and MADE/SORGAM minus RACM and MADE/VBS

3.3 Composition of $PM_{2.5}$

$PM_{2.5}$ composition, within city boundaries, when using RACM with MADE/SORGAM (Figure 7), shows an important contribution of Anthropogenic SOA (bright green). Primary components of particles are non-speciated $PM_{2.5}$ (orange), followed by sulfate (red) and ASOA. Biogenic SOA -BSOA- (dark green) does not have an important contribution to particle composition. Elemental carbon (black) seems to be unrepresented, this considering the important diesel vehicle fleet present in Bogotá.

Figure 7 Average composition of $PM_{2.5}$ for base case. Orange: NSP $PM_{2.5}$. Red: SO_4. Yellow: NH_4. Bright green: ASOA. Dark green: BSOA. Black: EC. Gray: POA. Blue: NO_3.

6. CONCLUSIONS

WRF-Chem was implemented over Colombia, with a domain centered in Bogotá using global emissions inventory EDGAR-HTAP 2010 for d01 and d02. Local emissions inventories combined with varying EDGAR-HTAP emissions were provided for inner most domain d03.

The photochemical model is able to reproduce diurnal meteorological behavior for variables such

as wind speed and temperature. Wind direction is not well represented by the model, this might be due to the complex topography of Bogotá, which has a chain of mountains at the east of the city.

When comparing modeled PBL height with observations, the model displays an important underestimation after day 5, perhaps becoming unstable. New runs need to be conducted changing the spin-up methodology.

Simulated pollutant diurnal pattern was shown to be highly sensitive to modeled PBL height. The over estimation of concentrations, appears to be related to the fact that the model is not successfully representing vertical transport, with resulting accumulation in the first model layer. Further evaluations are required to determine the cause of such lack of vertical transport.

Mobile emissions are a significant source of SOA precursors in Bogotá. Modeled experiments show a difference on average of 5ug/kg ASOA when mobile VOC's are removed. The composition of $PM_{2.5}$, indicates a possible misrepresentation of black carbon in emissions inventories, which needs to be assessed.

RACM gas-phase chemical mechanism coupled with MADE/SORGAM model configuration estimated more SOA than RACM coupled with MADE/VBS.

ACKNOWLEDGMENTS

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