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Chemical Speciation of PM2.5 in Bogotá, Colombia: Experimental Determination and Simulation with the Chemical Transport Model WRF-Chem

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Introduction

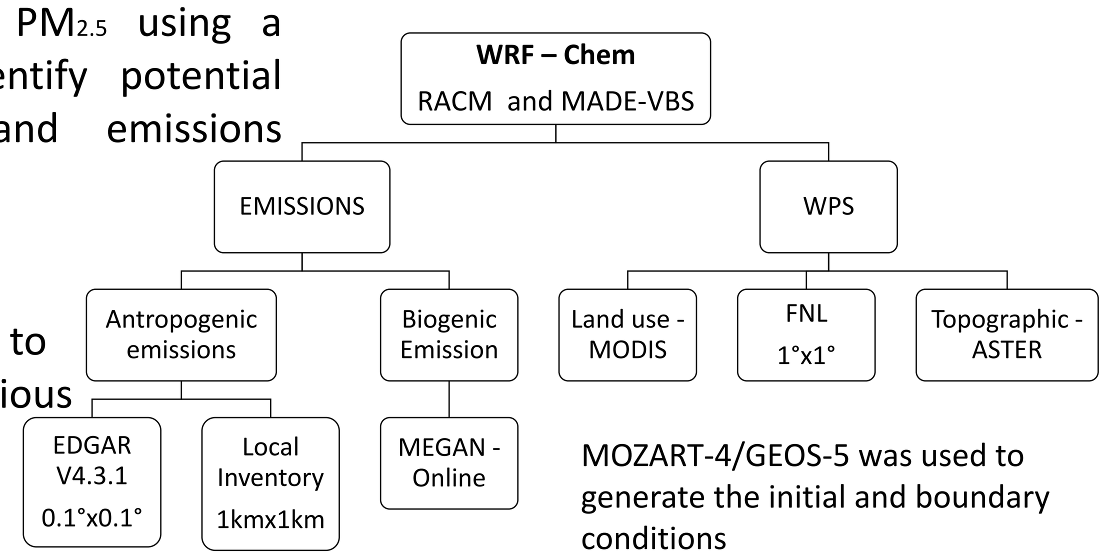
GOAL

To model the chemical speciation of $PM_{2.5}$ using a chemical transport model and to Identify potential weaknesses in emissions sources and emissions speciation.

MOTIVATION

- The scarcity of studies on the chemical composition of $PM_{2.5}$, has hindered efforts to properly attribute the contributions of various sources to particulate matter.
- SOA contribution to PM in Bogotá is poorly understood

FIGURE 1. Modelling process.

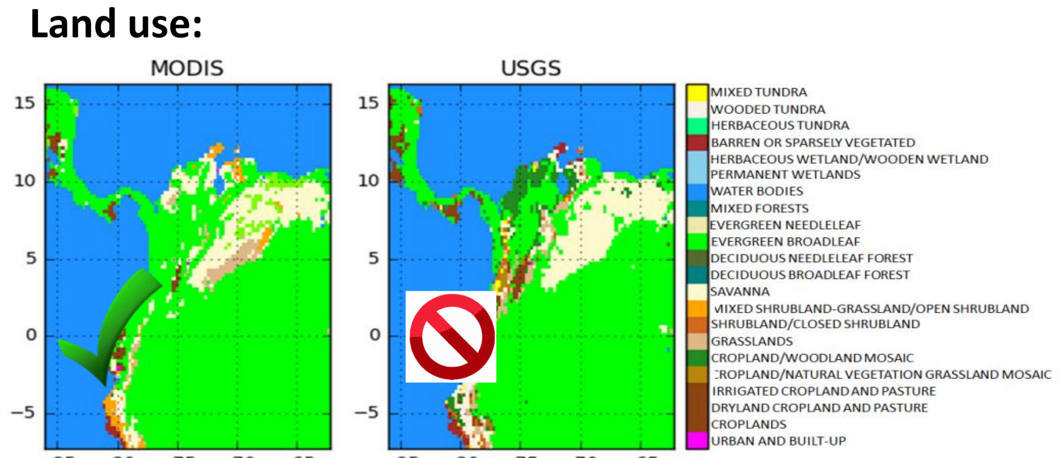


Methods

Previous Work: WRF-CHEM -UniAndes Research Group – Maria P. Perez

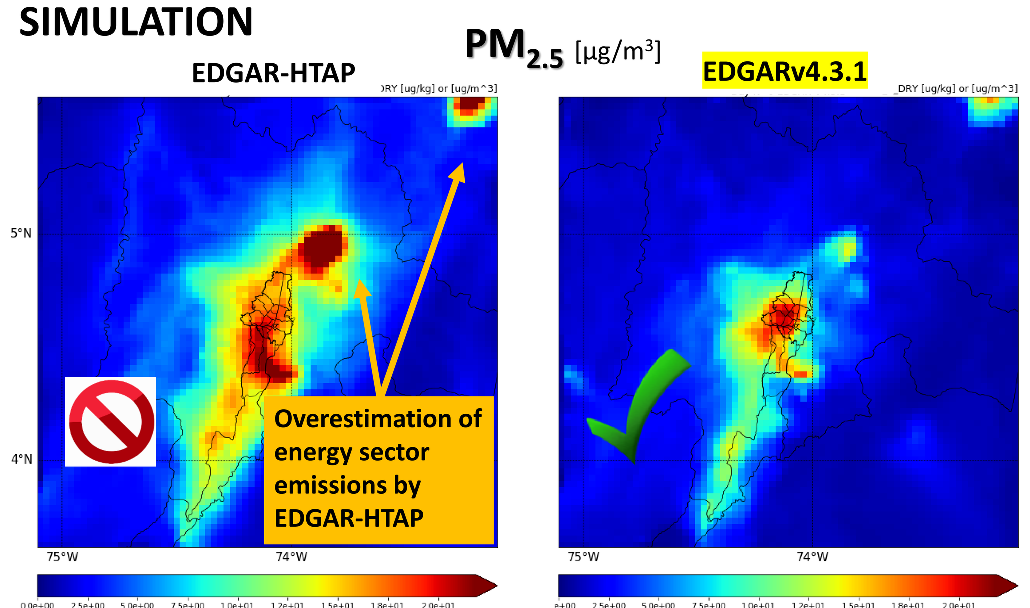
STATIC FIELDS

Land use:



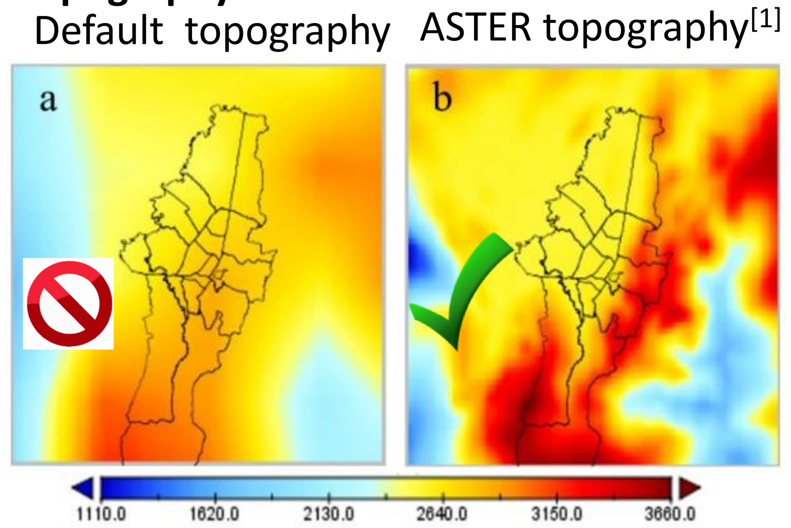
SIMULATION

$PM_{2.5}$ [μg/m³]



Topography:

Default topography ASTER topography[1]



We included emissions from local, 1x1 km, emission inventory of Bogotá [2], and merged them with EDGAR 4.3.1 anthropogenic emissions

We compared modeled $PM_{2.5}$ chemical composition of with observed chemical speciation in Bogota.

2.1 WRF-Chem model configuration

Simulation

- WRF-Chem V3.9.1
- 3 Nested domains

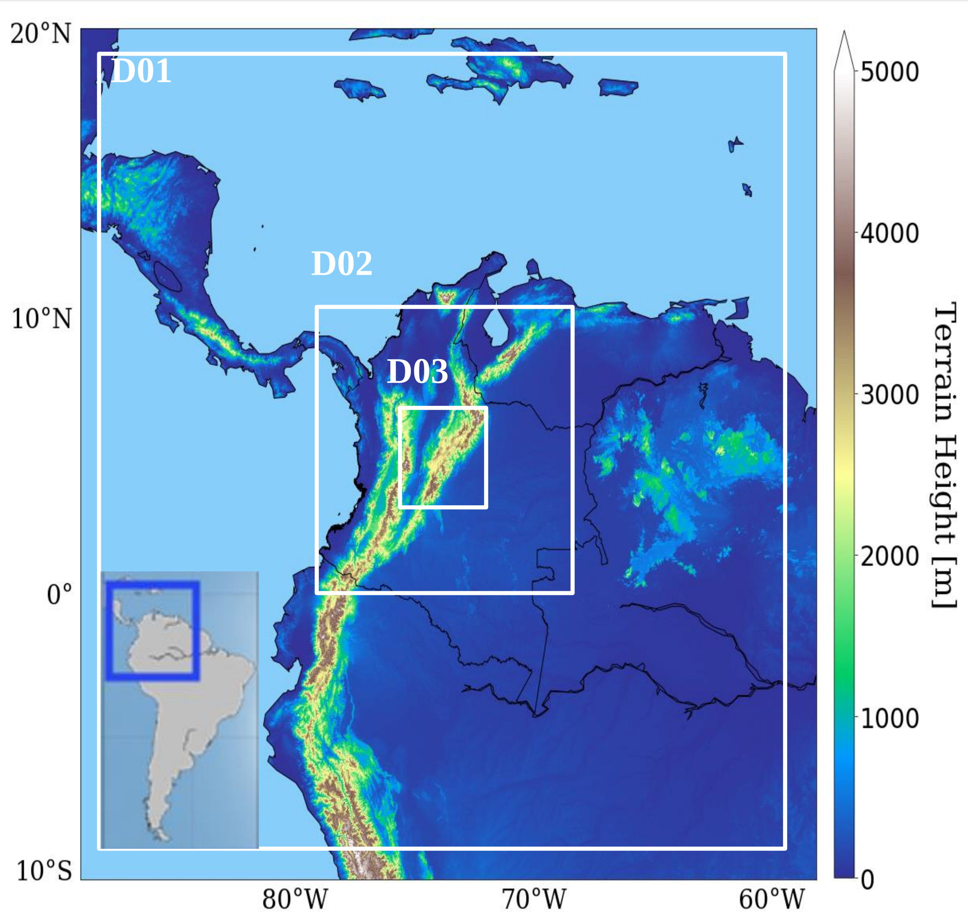
D01: 121 x 121 grid
Resolution: 27 x 27km

D02: 127 x 127 grid
Resolution: 9 x 9km

D03: 133 x 133 grid
Resolution: 3 x 3

- 41 vertical levels

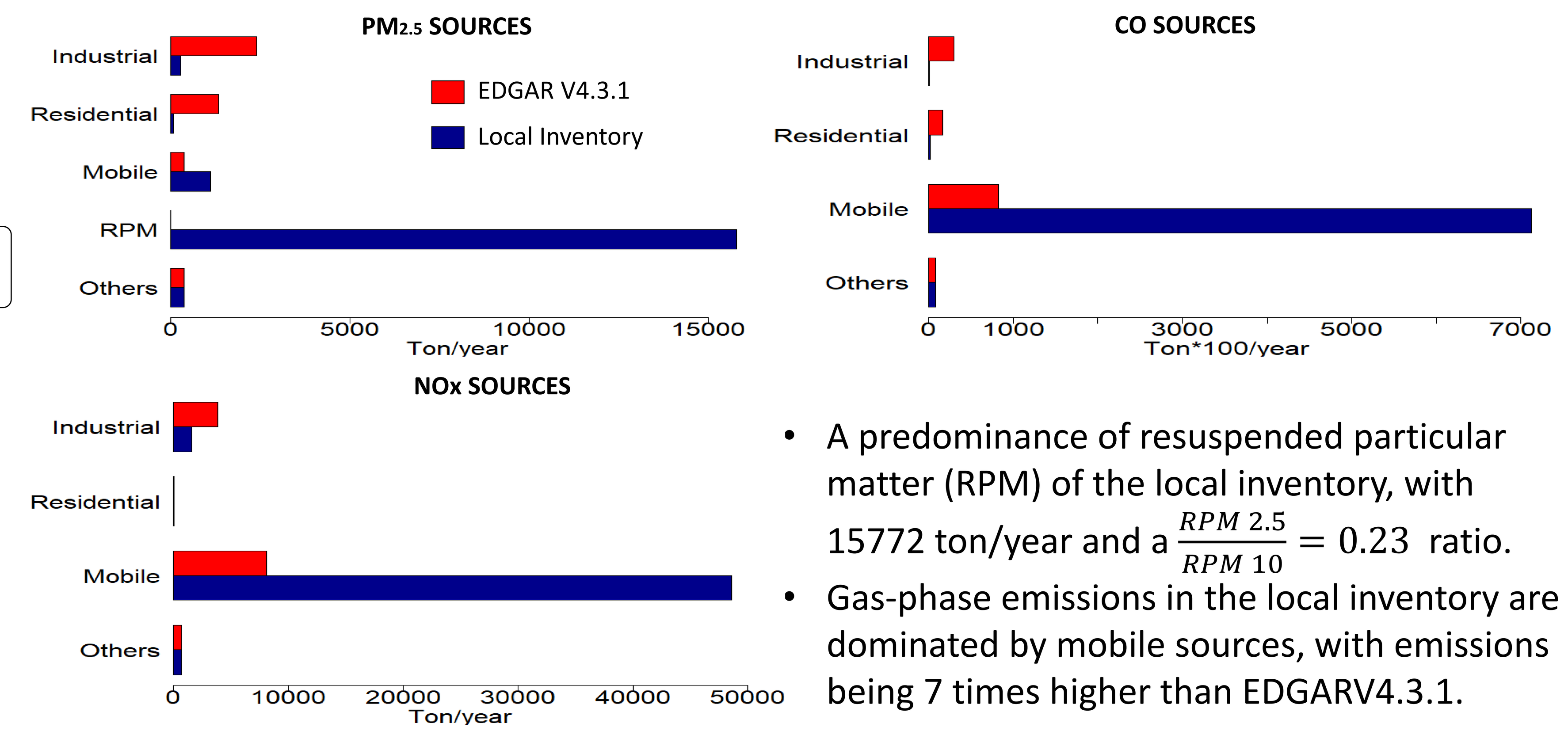
Simulation date
Sep 2018



Processes	Scheme
Microphysics	Lin microphysics scheme
Surface layer	Monin-Obukhov Similarity scheme
Land surface	Noah land-surface model
Planet boundary layer	YSU scheme
Cumulus	Grell-Devenyi ensemble scheme
Gas-phase chemical mechanism	RACM
Aerosol module	MADE-VBS
Biogenic emissions	Calculate on-line using MEGAN

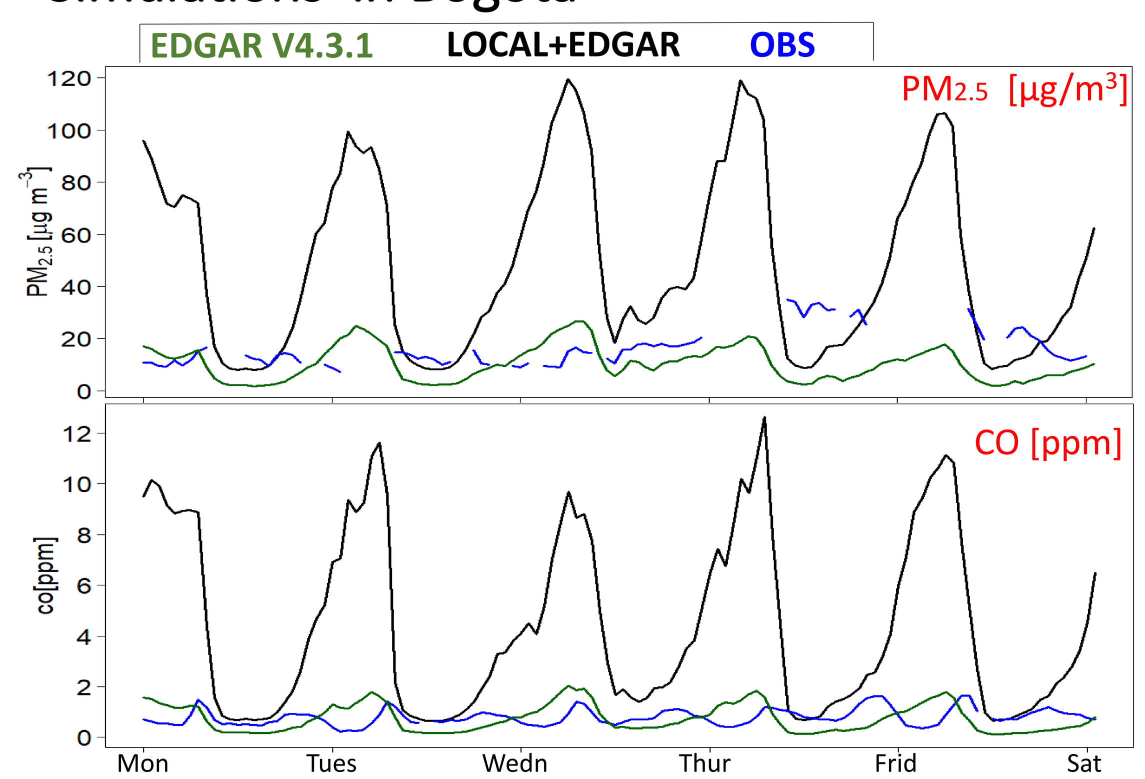
Results

3.1 EDGAR V4.3.1 VS Local Inventory in Bogotá



- A predominance of resuspended particular matter (RPM) of the local inventory, with 15772 ton/year and a $\frac{RPM\ 2.5}{RPM\ 10} = 0.23$ ratio.
- Gas-phase emissions in the local inventory are dominated by mobile sources, with emissions being 7 times higher than EDGARV4.3.1.

Simulations in Bogotá



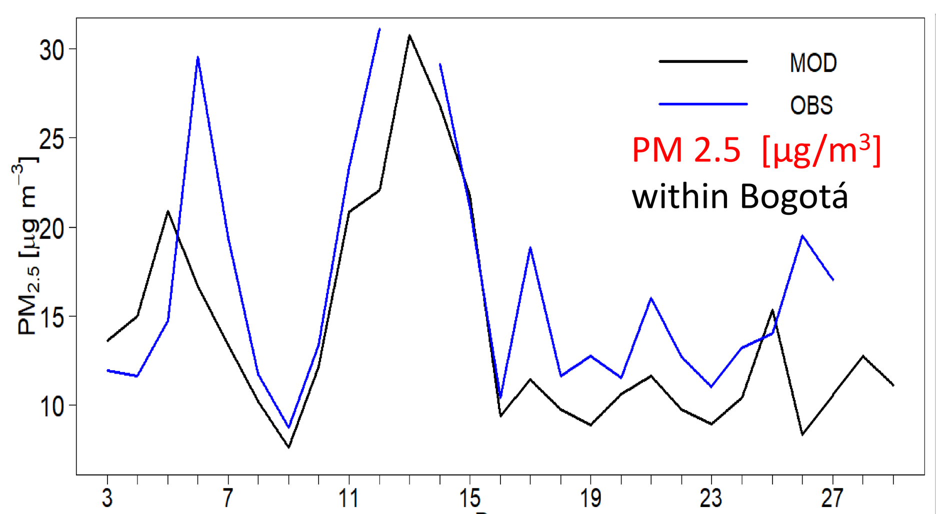
Sep 3-7 /2018

- Simulations with the local inventory overestimate particles and gas-phase species.
- When only EDGAR V4.3.1 is used aerosol concentrations are underestimated
- Gas phase species were in good agreement with observations on average in EDGAR V4.3.1

3.2 Base case

Particles from local emission with 40% RPM and $\frac{RPM\ 2.5}{RPM\ 10} = 0.1$[3] + EDGAR gas-phase emissions + spatial distribution from Local Inventory = Base Case

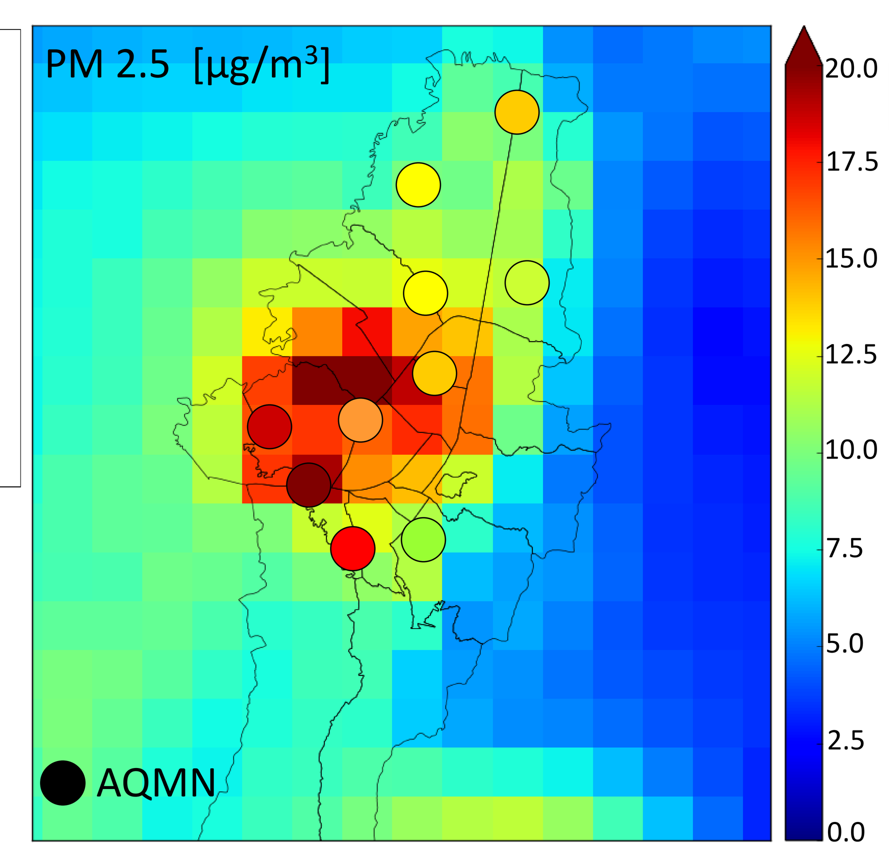
We included different emissions for weekdays and weekends, and diurnal variations in emissions.



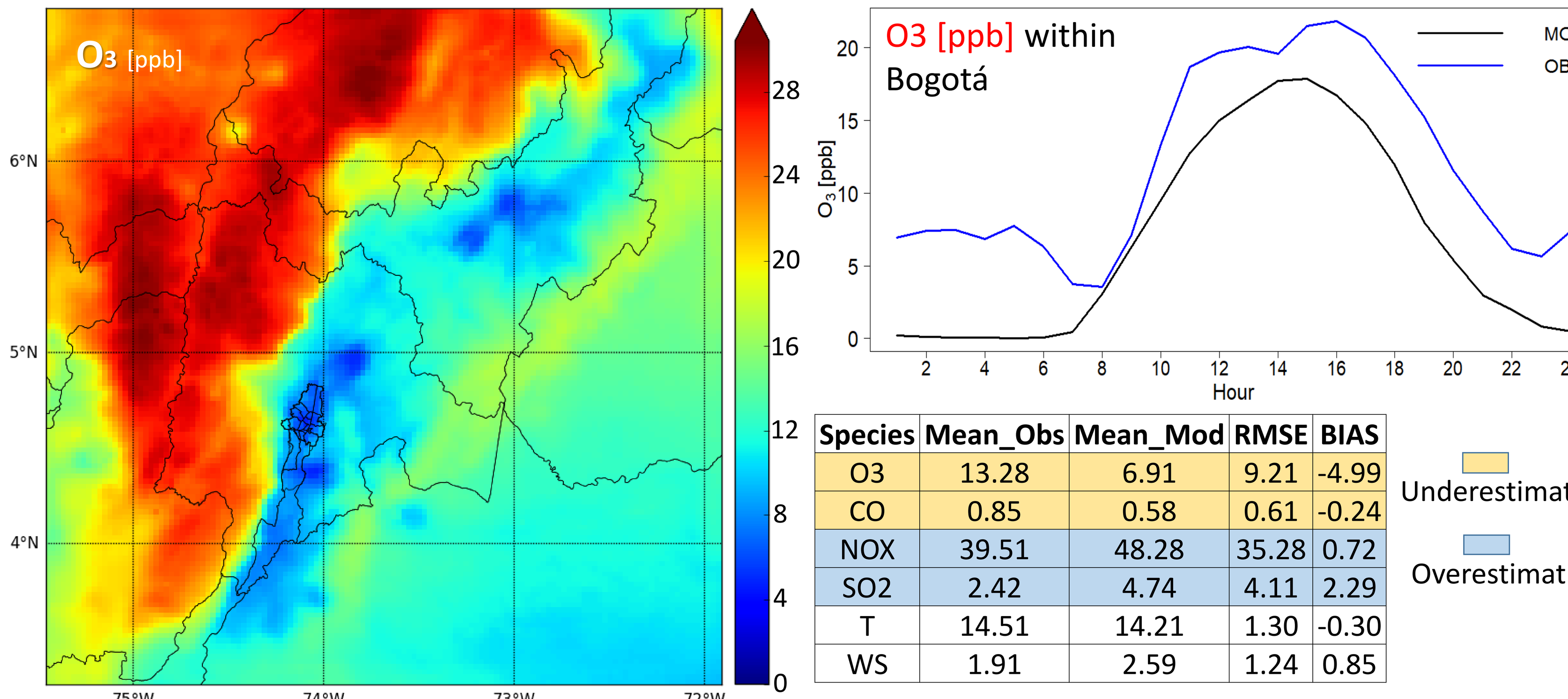
Sep 3-29 /2018

Mean_Obs (μg/m³)	Mean_Mod (μg/m³)
16.40	14.10

Species	RMSE	BIAS
PM2.5	11.58	-2.58



3.2 Base case

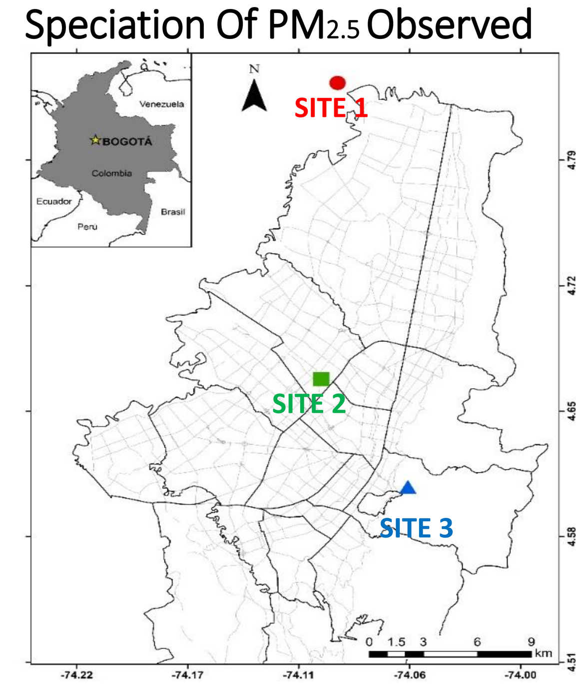


Species	Mean_Obs	Mean_Mod	RMSE	BIAS
O3	13.28	6.91	9.21	-4.99
CO	0.85	0.58	0.61	-0.24
NOX	39.51	48.28	35.28	0.72
SO2	2.42	4.74	4.11	2.29
T	14.51	14.21	1.30	-0.30
WS	1.91	2.59	1.24	0.85

Underestimation
Overestimation

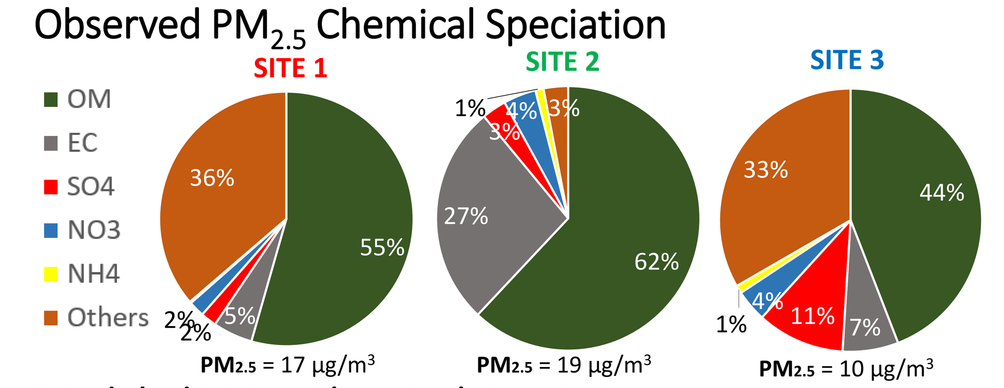
3.3 Chemical Speciation – Observation vs simulation

Speciation Of $PM_{2.5}$ Observed

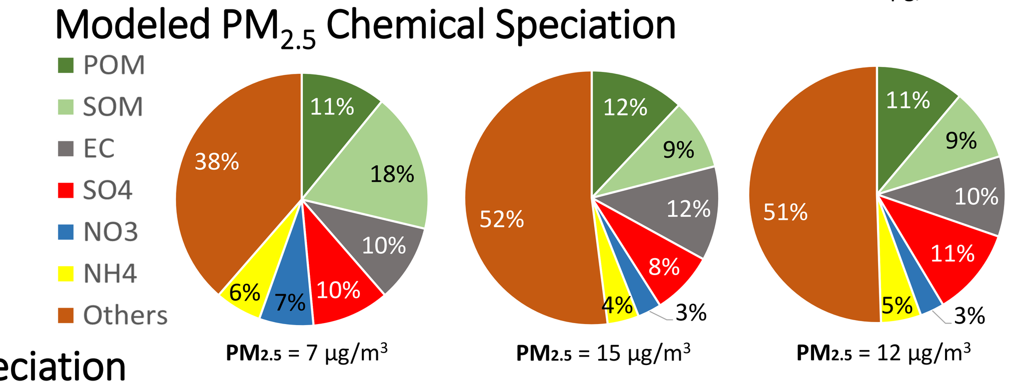


JUL-AGOS-SEP 2018

Observed $PM_{2.5}$ Chemical Speciation



Modeled $PM_{2.5}$ Chemical Speciation

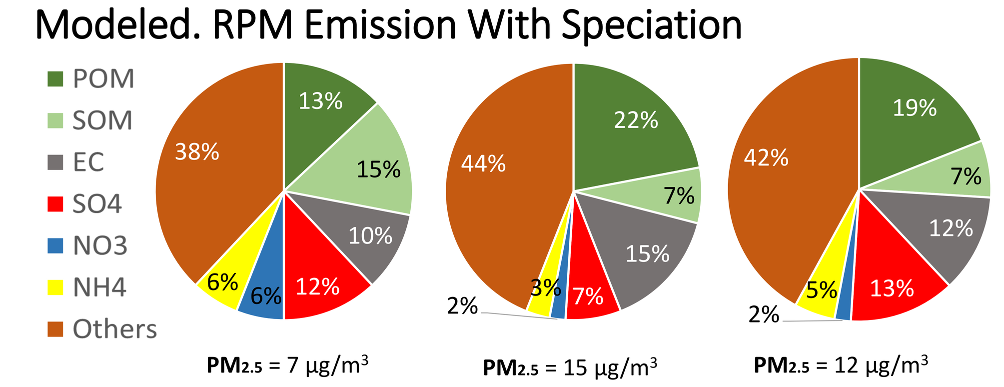


Modeled. RPM Emission With Speciation

RPM10 EMISSION [4]	
SPECIES	%PERCENTAGE
OC	13-29
EC	0.2-1.9
Soluble Ions	1.4-3.8
Others	61.2-96.5

We adapted observed RPM_{10} speciation to $RPM_{2.5}$ emissions

Modeled. RPM Emission With Speciation



Concluding remarks

- According to our simulations, the current local emission inventory seems to overestimate gas-phase emissions from mobile sources and to overestimate the contribution of RPM to primary particles emissions. EDGARV 4.3.1 shows a underestimation in primary particle emissions.
- Organic aerosols are not well represented in the simulations even with high concentration of SOA precursors and when POM is included in RPM fine speciation.
- There is significant uncertainty in the emissions speciation, and a large fraction of un-speciated emissions from **Mobile**, Residential, Industrial and fine RPM sectors. This can explain the underestimation of OM.
- The SO_4^{-2} is not well represented, it´s overestimated. This can be explained for the overestimation in SO_2 concentrations and the SA formation.

References

[1]Nedbor-Gross, R., B.H. Henderson, J.R. Davis, J.E. Pachon, A. Rincon, O.J. Guerrero, & F. Grajales (2016). "Comparing Standard to Feature-Based Meteorological Model Evaluation Techniques in Bogotá, Colombia." Journal of Applied Meteorology and Climatology, (In press) DOI:10.1175/JAMC-D-16-0058.1
[2] Local inventory developed by the Universidad de La Salle and the Secretaria Distrital de Ambiente
[3]EPA, (2005), Examination of the Multiplier Used to Estimate PM2.5 Fugitive Dust Emissions from PM10, Research. Retrieved July, 2019, from https://www3.epa.gov/ttnchie1/conference/ei14/session5/pace.pdf
[4] Omar Ramírez, Ana M. Sánchez de la Campa, Fulvio Amato, Teresa Moreno, Luis F. Silva, Jesús D. de la Rosa. (2019). "Physicochemical characterization and sources of the thoracic fraction of road dust in a Latin American megacity". Journal Science of the Total Environment 652 (2019) 434–446