ENSEMBLE MODELING OF ATMOSPHERIC POLLUTANTS: A CASE STUDY WITH WRF-CHEM AND LOTOS-EUROS IN ABURRÁ VALLEY, COLOMBIA

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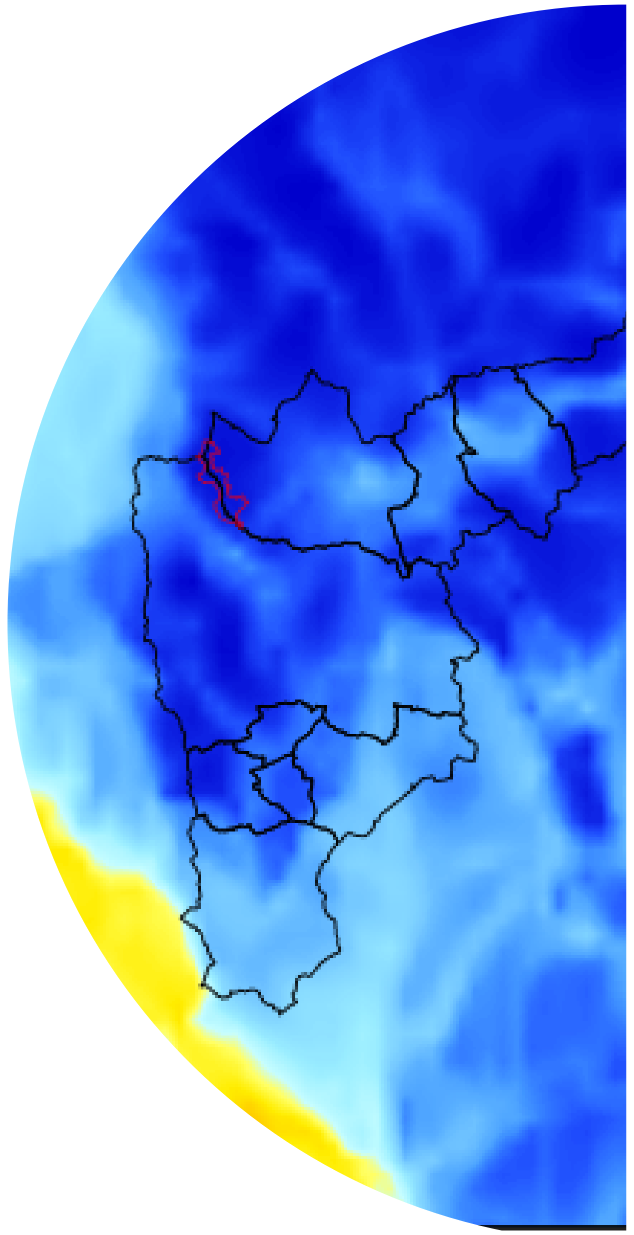
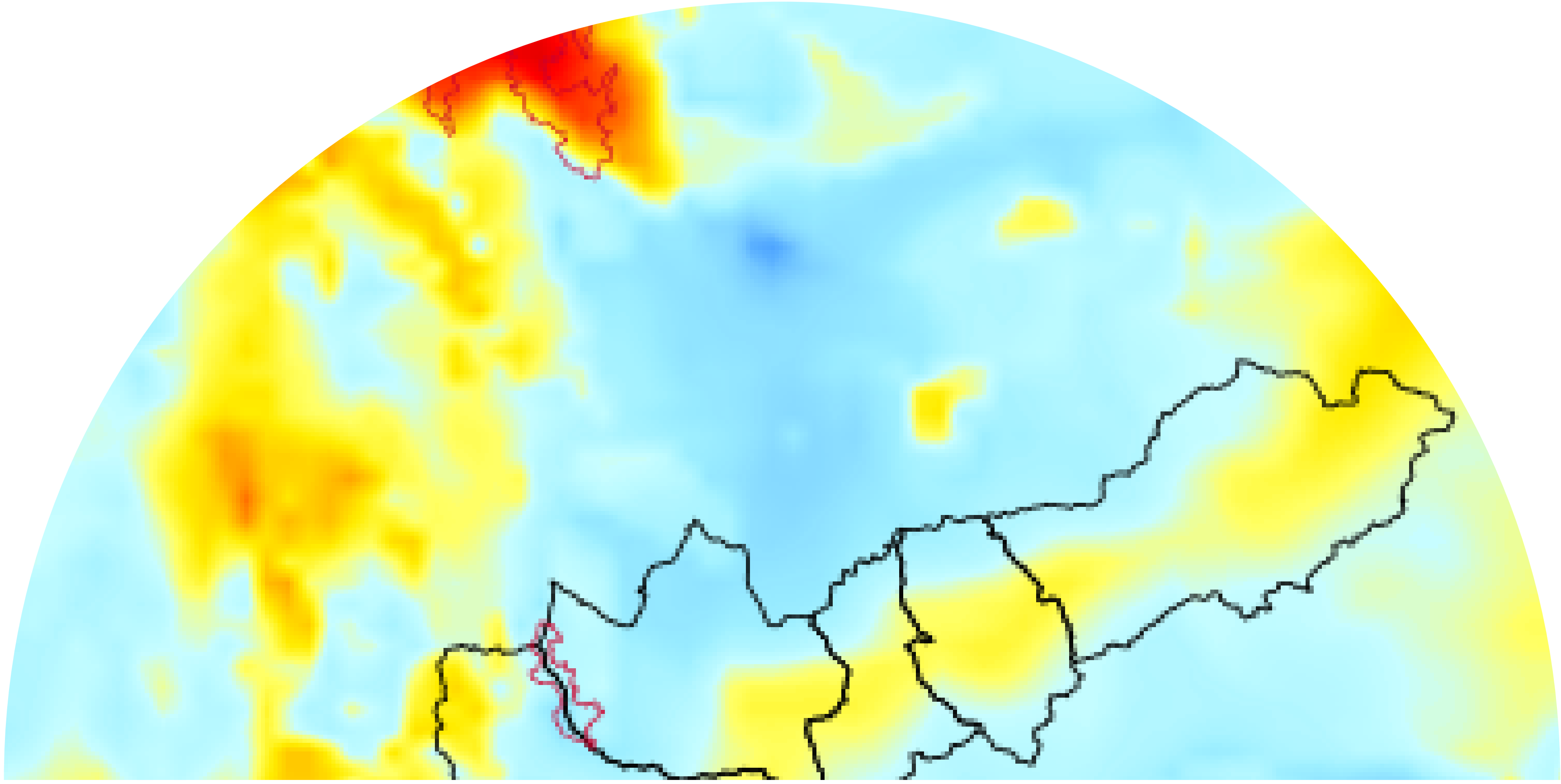


From the perspective of atmospheric modeling, physico-chemical processes affecting a narrow valley have been interesting due to the geography and human activities on climate behavior and pollutant dynamics [1,2].

GEOGRAPHY

NARROW VALLEY

The Aburrá Valley in the second largest metropolitan Area in Colombia, It is situated in an Intertropical Andean Zone with high population and industrital activities. Also it experiences a diverse climate due to the variations in the elevation of the mountains (1500 masl to 2500 masl). Additionally it is surrounded by vulnerable and particular ecosystems such as Páramos and High Andean Forests [3-8].



CHEMICAL TRANSPORT MODELS (CTM)

ATMOSPHERIC MODELLING TO UNDERSTAND THE AIR POLLUTION BEHAVIOUR

LOTOS EUROS

- Long Term Ozone Simulation - European Operational Smog Model, was developed in 2004.
- It was coupled with WRF (Weather Research and Forecasting) as NWPM (Numerical Weather Prediction Model).
- LOTOS EUROS has been in use in Colombia since 2017, and its implementation allowed to develop MAUI (Medellín Air Quailty Iniciative), and the National Scientific Iniciative 4DAir.

WRF-CHEMISTRY

- Weather Research and Forecasting (WRF) model coupled with Chemistry.
- Its first implementation in Colombia was in 2016, for PM10 in the city og Bogotá, with data assimilation.
- It is automatically coupled with WRF as NWPN.
- WRF Chem now is available at EAFIT university in HPC, Apolo EAFIT.

CTM SET UP

LOTOS EUROS SET UP

Preliminary comparison periods	January 9th of 2019
Metereology	WRF; Temp.res: 6h; Spat.res: 0.07° x0.07°
Initial and boundary conditions	LOTOS-EUROS (D1). Temp.res: 1h. Spat.res: 0.09° x0.09°
Anthropogenic emissions	EDGAR v4.3.2 Spat.res: 10km x10km
Biogenic emissions	MEGAN Spat.res: 10km x10km
Fire emissions	MACC/CAMS GAFS Spat.red: 10km x10km
Landuse	CCLI. Spat.res: 1km x1km
Topography	GMTED2010. Spat.res: 0.002° x0.002°
Domain 1 (D1) Lat x Lon	[-8.5°, 18°] x [-84°, -60°]
Domain Colombia (DCol) Lat x Lon	[-4.55°, 13.27°] x [-79.80°, -65.94°]

WRF CHEM SET UP

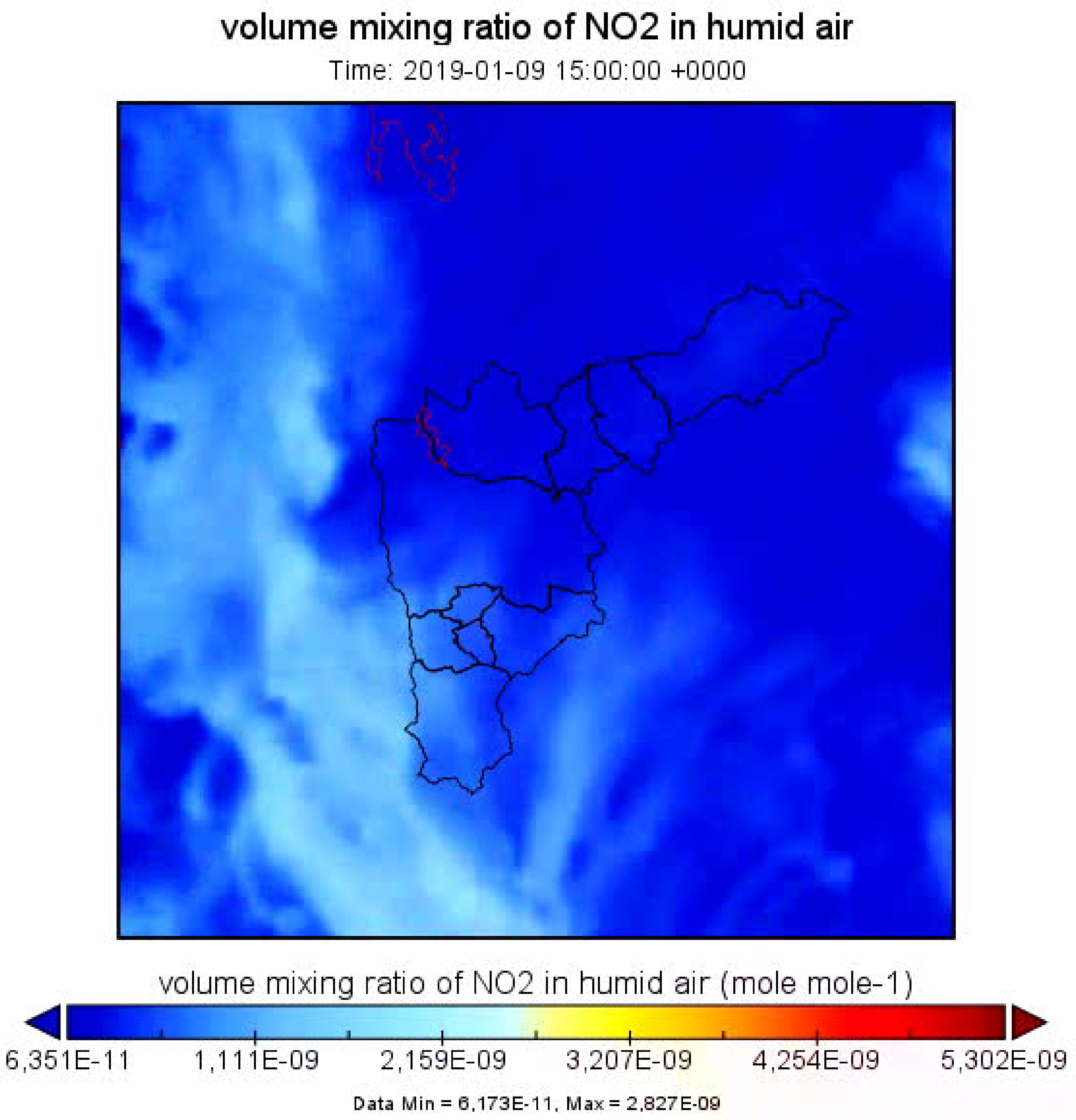
Preliminary comparison periods	January 9th of 2019
Metereology	WRF; Temp.res: 6h; Spat.res: 0.07° x0.07°
Initial and boundary conditions	Idealized profile. Temp.res: 1h. Spat.res: 0.09° x0.09°
Anthropogenic emissions	N/A (Idealized model conditions)
Biogenic emissions	N/A (Idealized model conditions)
Fire emissions	N/A (Idealized model conditions)
Landuse	MODIS. Spat.res: 1km x1km
Topography	GMTED2010. Spat.res: 0.002° x0.002°
Domain 1 (D1) Lat x Lon	[-10°, 8.8°] x [20°, -56°]
Domain Colombia (DCol) Lat x Lon	[-4.55°, 13.27°] x [-79.80°, -65.94°]

It takes into account the time simulation plus the spin up time.

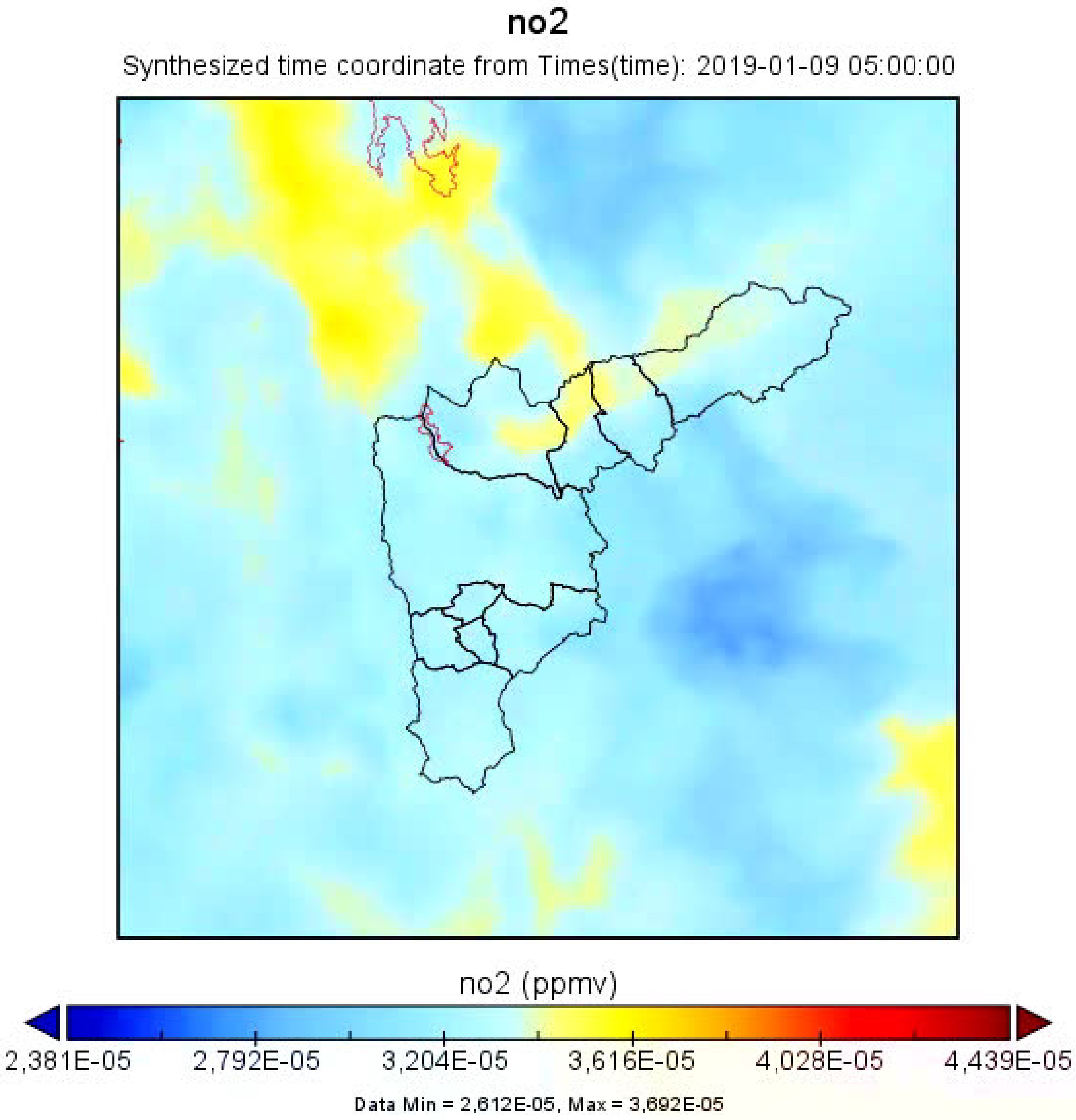
NO2

OUR INTEREST DUE TO THEIR IMPACTS ON NATURAL AND VULNERABLE ECOSYSTEMS

LE SIMULATION



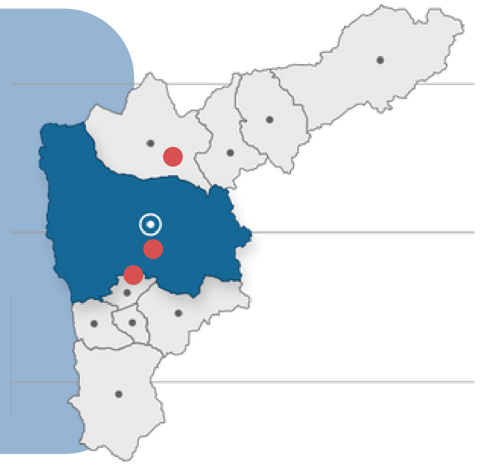
WRF-C SIMULATION



IN SITU DATA

SIATA STATIONS

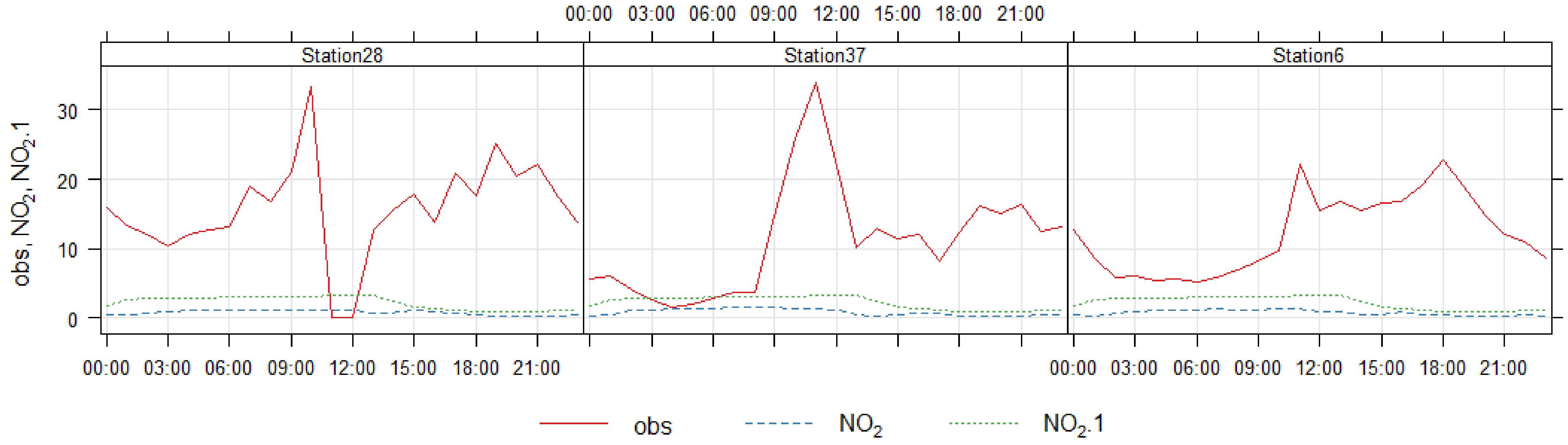
(Aburrá Valley Early Warning System).
Local network for air quality monitoring with more than 60 surface stations.



LOCATION

Numeration	Local Air Quality Station Name	Longitude	Latitude
6	Politécnico Jaime Isaza Cadavid	6.20897	-75.57777
28	Casa de Justicia Itaguí	6.18567	-75.59721
37	Universidad San Buenaventura	6.33070	-75.56867

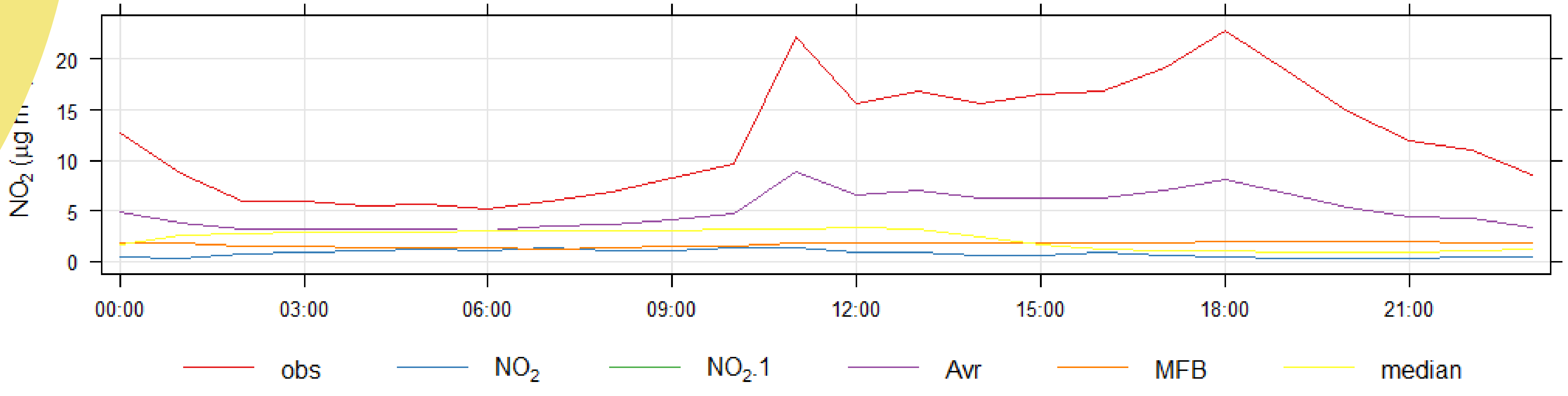
DATA COLLECTED

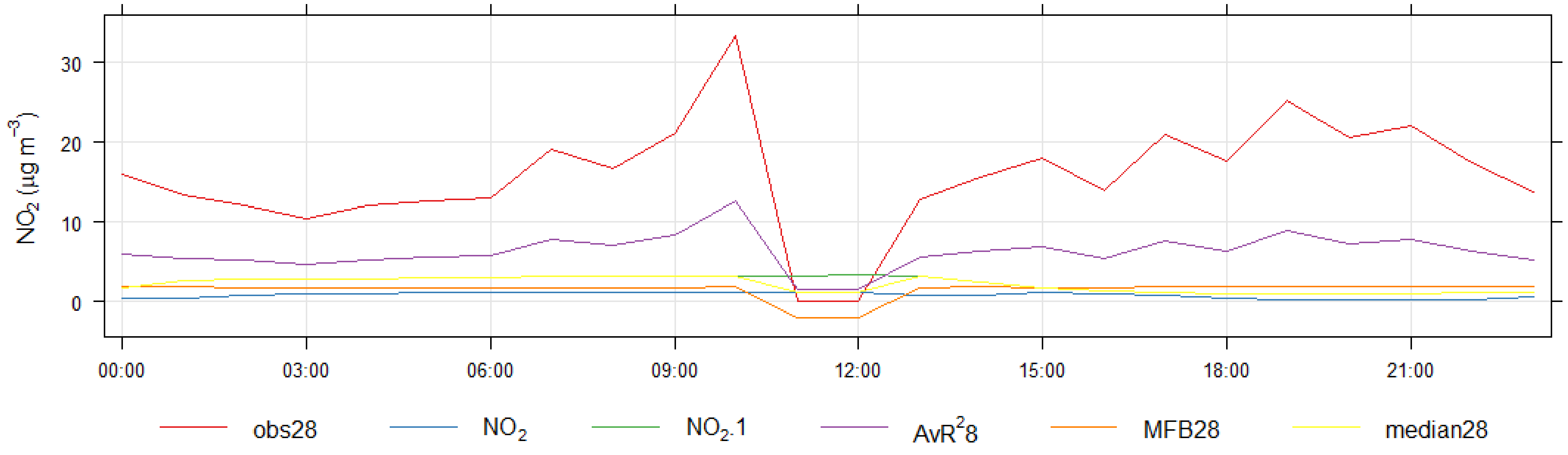


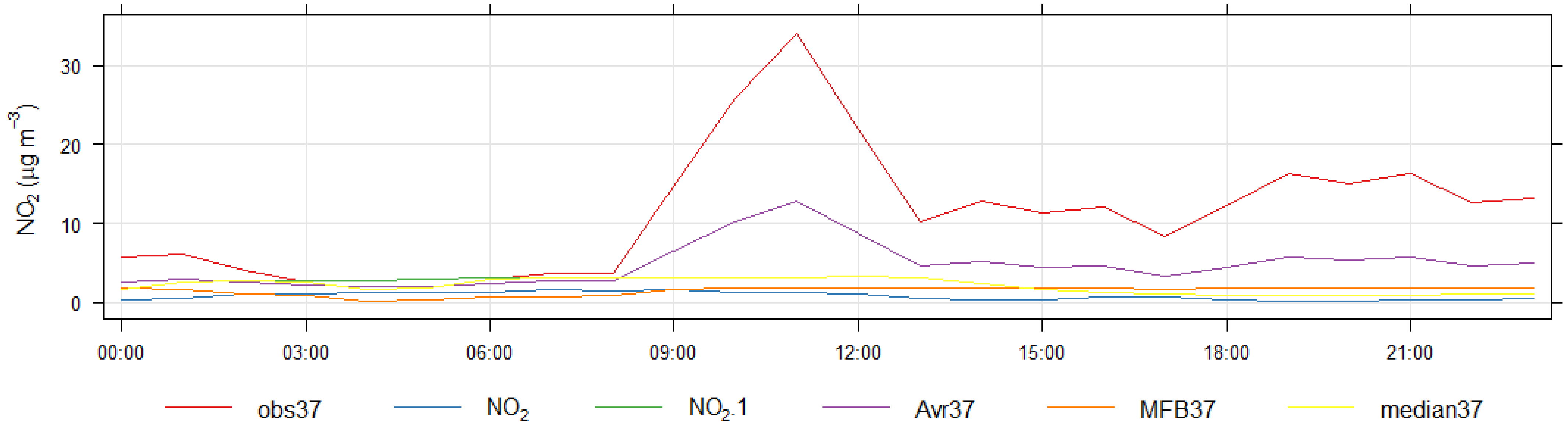
ENSEMBLE

STATISTICAL ANALYSIS

COMPARISON







Time series for obs (SIATA observations), no2 (LOTOS EUROS output) and no2.1 (WRFChem output) and statistics such as the average, mean fractional bias and median of the observation and the two outputs from the models for each station

METHODOLOGY

$$\mathrm{MFB} = \frac{2}{M}\sum_{i=1}^{M}\frac{\left(y^{Mod}\right)_i - y_i^{obs}}{\left(y^{Mod}\right)_i + y_i^{obs}}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{M}\sum_{i=1}^{M}\left(\left(y^{Mod}\right)_i - y_i^{obs}\right)^2}$$

$$\mathrm{Corr} = \frac{\Sigma_{i=1}^{M}\left(\left(y^{Mod}\right)_i - \overline{\left(y^{Mod}\right)}\left(y_i^{obs} - \overline{y^{obs}}\right)\right)}{\sqrt{\Sigma_{i=1}^{M}\left(\left(y^{Mod}\right)_i - \overline{\left(y^{Mod}\right)}\right)^2}\sqrt{\Sigma_{i=1}^{M}\left(y_i^{obs} - \overline{y^{obs}}\right)^2}}$$

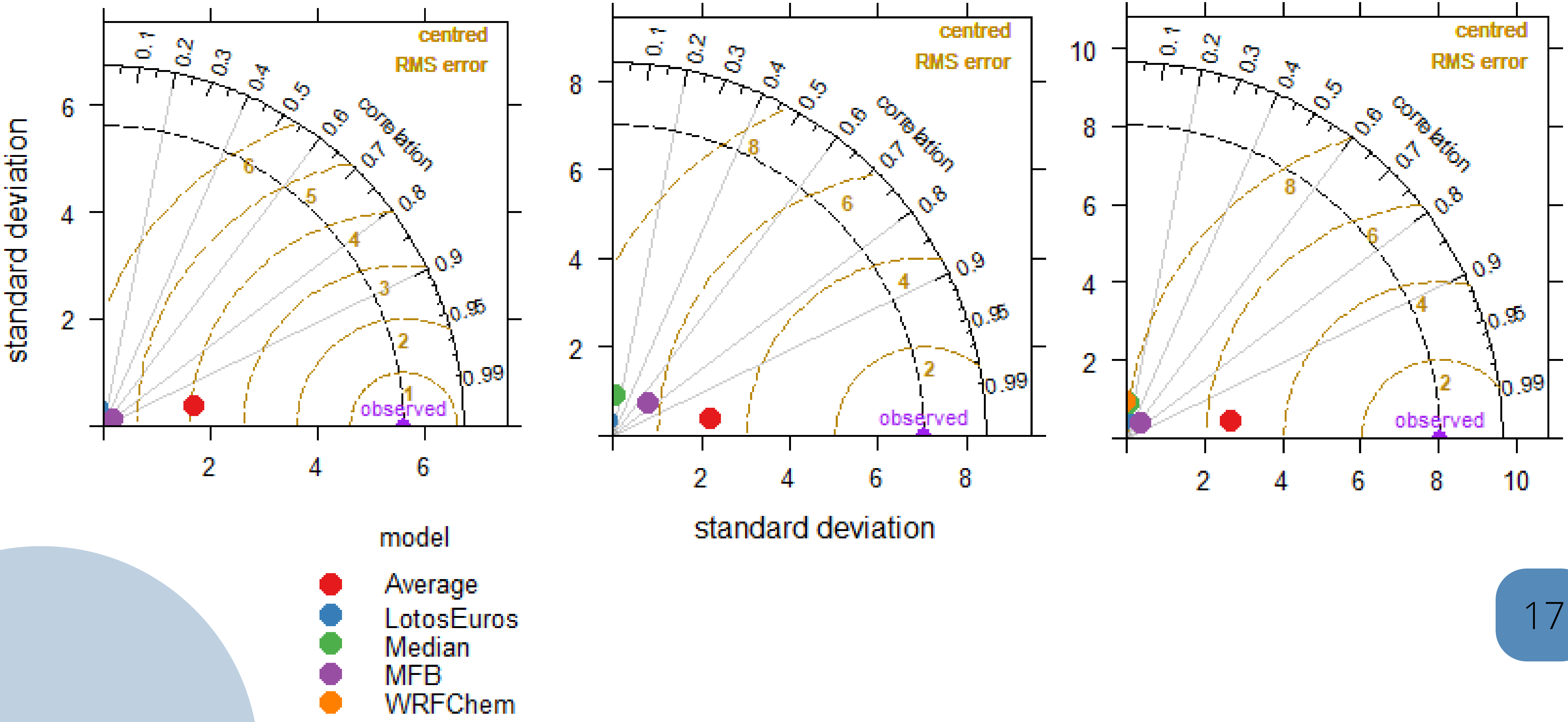
The ensemble includes calculations of the average, median, and mean fractional bias of observations, along with models results. The comparison is made using three metrics widely employed in atmospheric sciences: the mean fractional bias (MFB), root mean square error (RMSE), and correlation factor (CF).

SAMPLE

	date	obs	no2	no2.1	Avr	MFB	median
1	2019-01-09 00:00:00	12.7080	0.4337429	1.7021852	4.947976	1.867980	1.7021852
2	2019-01-09 01:00:00	8.7448	0.3387610	2.5794547	3.887672	1.850825	2.5794547
3	2019-01-09 02:00:00	5.9372	0.8127504	2.7823813	3.177444	1.518367	2.7823813
4	2019-01-09 03:00:00	5.9924	0.9416937	2.8323740	3.255489	1.456775	2.8323740
5	2019-01-09 04:00:00	5.5295	1.0772226	2.8664073	3.157710	1.347802	2.8664073
6	2019-01-09 05:00:00	5.6714	1.1471981	2.9737050	3.264101	1.327018	2.9737050
7	2019-01-09 06:00:00	5.2249	1.0488513	3.0606120	3.111454	1.331276	3.0606120
8	2019-01-09 07:00:00	5.9030	1.3389699	3.1048516	3.448940	1.260439	3.1048516
9	2019-01-09 08:00:00	6.8486	1.1110172	3.1345688	3.698062	1.441673	3.1345688
10	2019-01-09 09:00:00	8.2774	1.0588263	3.1335072	4.156578	1.546358	3.1335072
11	2019-01-09 10:00:00	9.6959	1.3799842	3.1701573	4.748680	1.501626	3.1701573
12	2019-01-09 11:00:00	22.1774	1.4282492	3.2327345	8.946128	1.757982	3.2327345

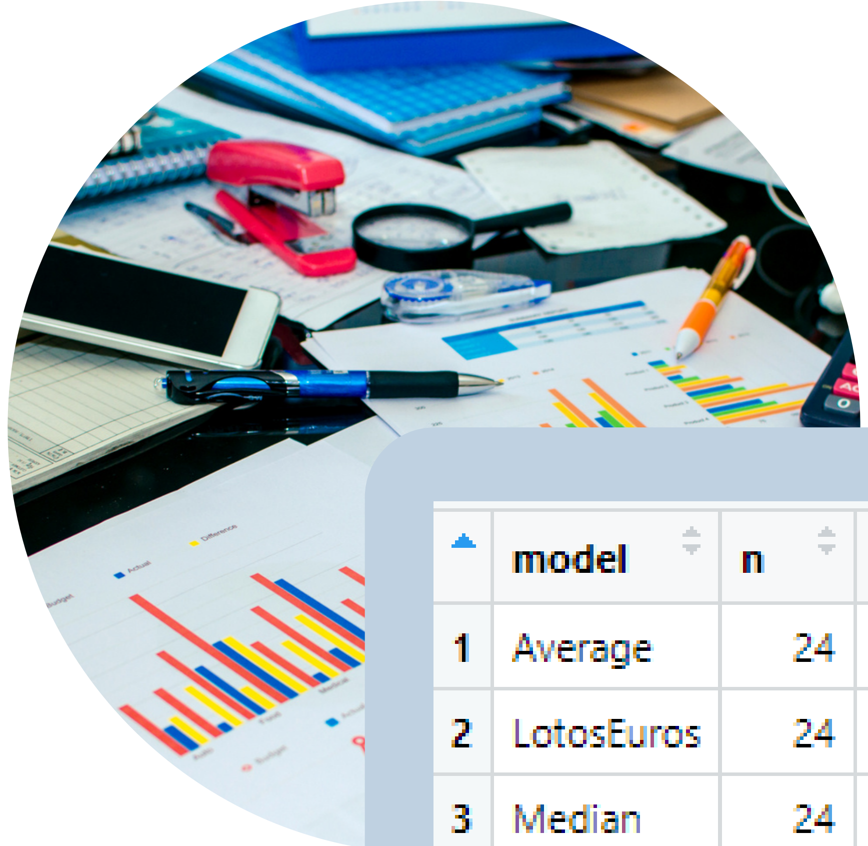
STATION 6

TAYLOR DIAGRAMS



STATISTICAL RESULTS

ENSEMBLE DONE (6)



	model	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r	P	COE	IOA
1	Average	24	0.3333333	-7.092642	7.092642	-0.5839253	0.5839253	8.076301	0.9750931	7.027571e-16	-0.4590977	0.27045116
2	LotosEuros	24	0.0000000	-11.367400	11.367400	-0.9358590	0.9358590	12.682890	-0.3084640	1.425050e-01	-1.3385006	-0.14475112
3	Median	24	0.1666667	-9.910525	9.910525	-0.8159170	0.8159170	11.573494	-0.4502965	2.724012e-02	-1.0387924	-0.01902716
4	MFB	24	0.0000000	-10.456429	10.456429	-0.8608603	0.8608603	11.735975	0.7701175	1.076798e-05	-1.1510957	-0.07024129
5	WRFChem	24	0.1666667	-9.910525	9.910525	-0.8159170	0.8159170	11.573494	-0.4502965	2.724012e-02	-1.0387924	-0.01902716

- n: number of samples
- FAC2: fraction of predictions within a factor of two
- *MB:* the mean bias
- *MGE:* the mean gross error.
- *NMB:* the normalised mean bias.

- NMGE: the normalised mean gross error.
- RMSE: the root mean squared error
- r: the Pearson correlation coefficient
- COE: the Coefficient of Efficiency

DISCUSSION

FACT 1

Colombia faces a lack of remote sensing devices or data collecting activities to improve the results of the atmospheric modelling.

FACT 2

Comparing the results of various models and evaluating which performs best for a specific spatial domain, for certain chemical species posing high risks to health and ecosystems, can facilitate decision-making.

FACT 3

Offline models runs, such as LOTOS EUROS, WRF CHEM, and CMAQ, have been conducted throughout Colombia to understand dynamics in major cities like Medellín, Bogotá, and Cali

FACT 4

An ensemble of models with real-time statistical analysis should be performed.

CONCLUSION

- From the simulations and visualizations of the models, it is possible to identify the relationship between nitrogen compounds and exposure to solar radiation.
- Through this ensemble, WRF Chem shows a better performance for the analysis of NO2 in the timeframe, however, both models are quite far from the observations.

CONCLUSION

- We suggest inaccuracies in the predictions due to model configurations, low precision of the models, or difficulties in generalizing the data. Geography also has an impact.

- LOTOS-EUROS has been in use in Colombia since 2017, and now WRFChem is available to simulate the atmospheric composition in the country, with this the ensemble perspective can begin to be approached with the statistical advantages this promotes.

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¡MUCHAS GRACIAS!

THANK YOU

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