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T1: Approaches to model evaluation and quality assurance

IMPACT OF BOUNDARY AND INITIAL CONDITIONS ON NOx, NO_2 AND O_3 CONCENTRATIONS IN WRF-CMAQ SIMULATIONS OVER THE METROPOLITAN AREA OF BUENOS AIRES, ARGENTINA

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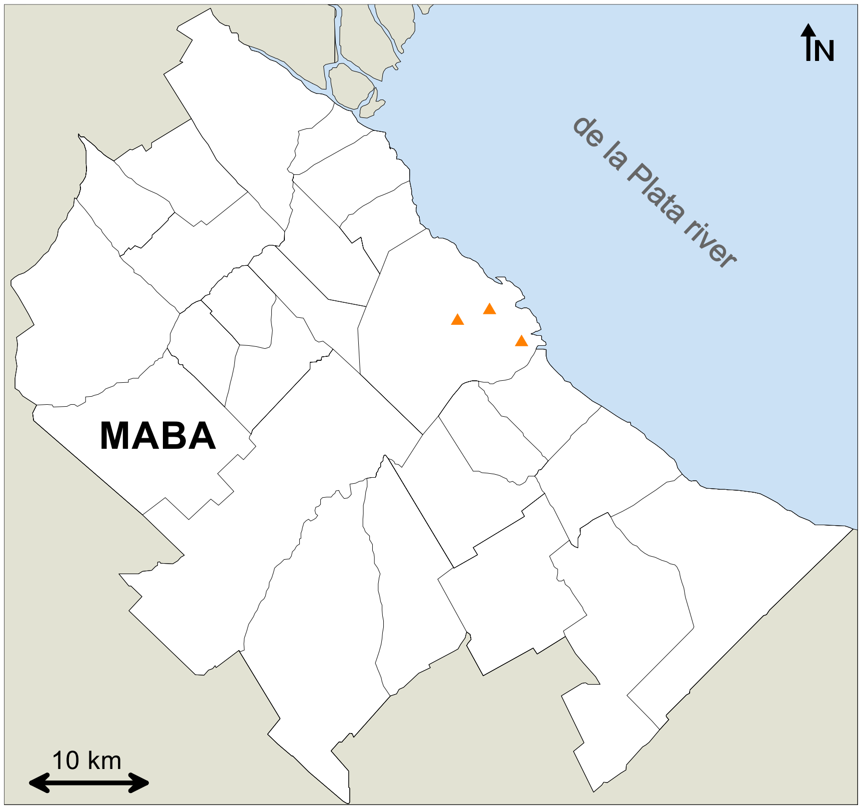
1. MOTIVATION AND OBJECTIVES

Metropolitan Area of Buenos Aires (MABA)



3,830 km², +15,000,000 inhab.

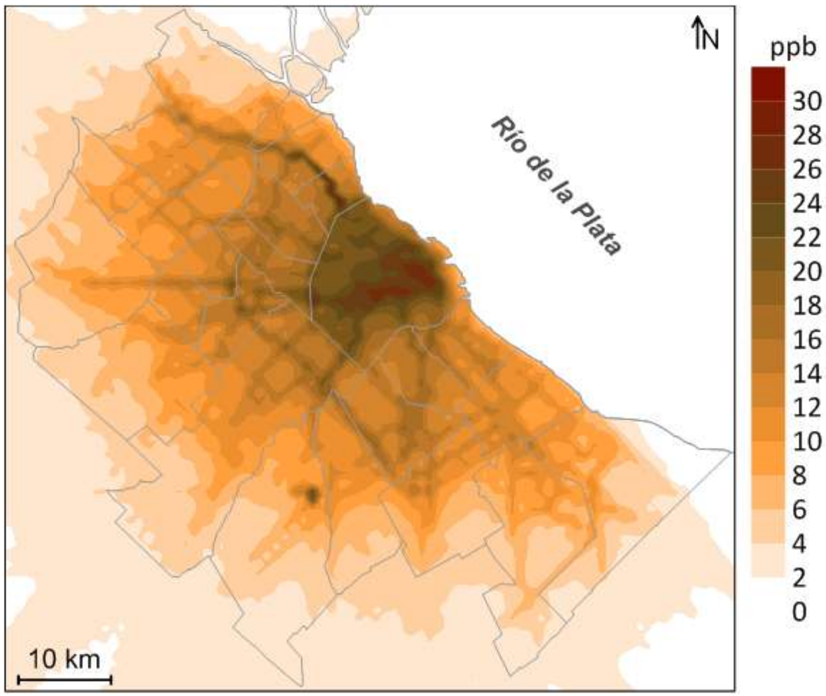
- MABA is the third mega city in Latin America.
- It is located on flat terrain and surrounded by non-urban areas.
- Few observational studies on AQ (e.g., Bogo et al., 2001; Mazzeo et al., 2005).
- Three AQ monitoring stations measuring CO, NO_2 and PM_{10} since 2009 (Pineda Rojas et al., 2020).

1. MOTIVATION AND OBJECTIVES

DAUMOD-GRS

(MODelo de Dispersión Atmosférica Urbana - Generic Reaction Set)

Annual mean concentration of NO_2

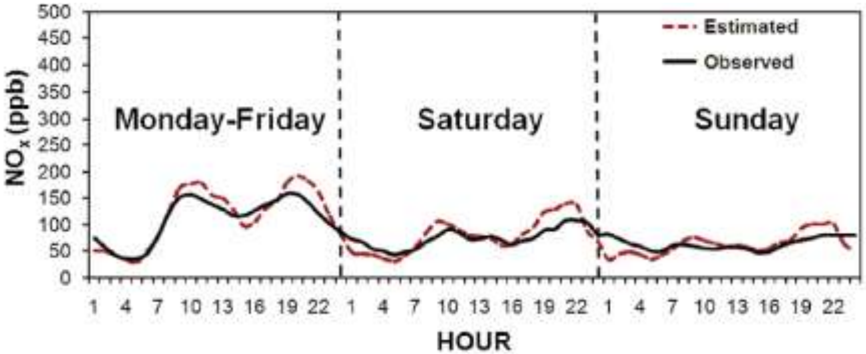


Pineda Rojas and Venegas, Atmos Res, 2013: https://doi.org/10.1016/j.atmosres.2012.08.010

SEUS

(Semi Empirical Urban Street model)

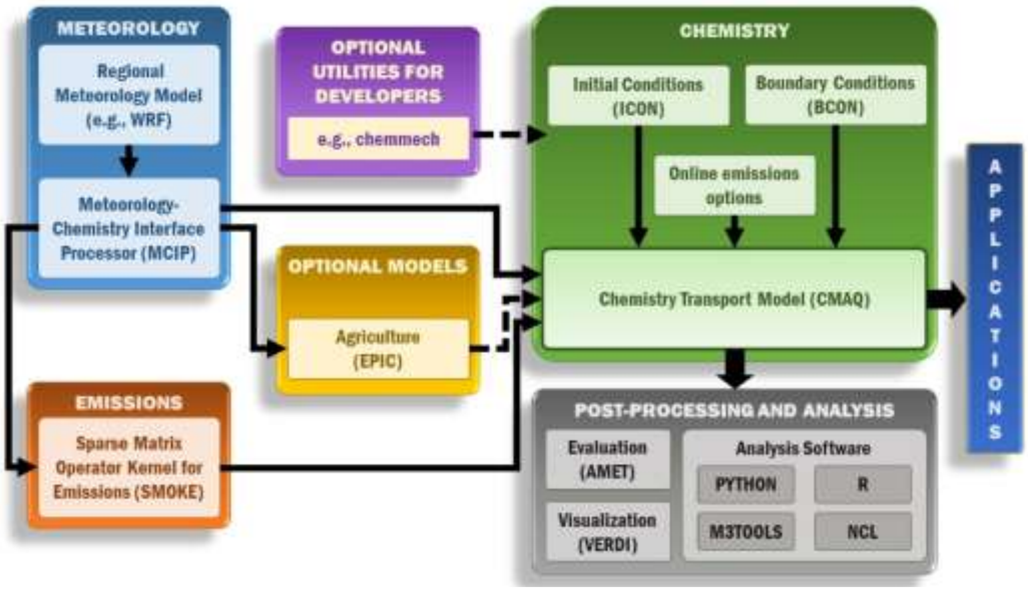
Averaged NOx concentration at COR



Venegas et al., Atmos Environ, 2014: https://doi.org/10.1016/j.atmosenv.2014.01.005

1. MOTIVATION AND OBJECTIVES

WRF-CMAQ



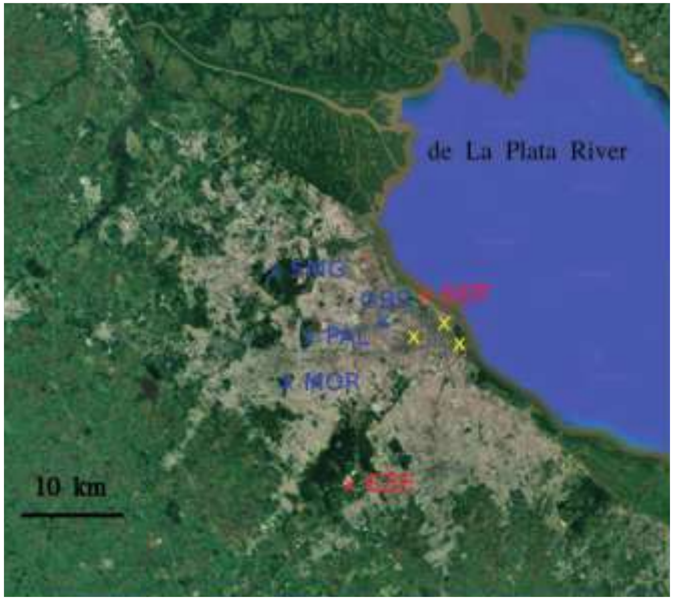
Source: https://www.epa.gov/cmaq/cmaqs-purpose

- Its implementation in the MABA can contribute to study:
  - Interactions that cannot be addressed by simple models (e.g., CC-AQ)
  - The role of sources not previously considered (e.g., remote)

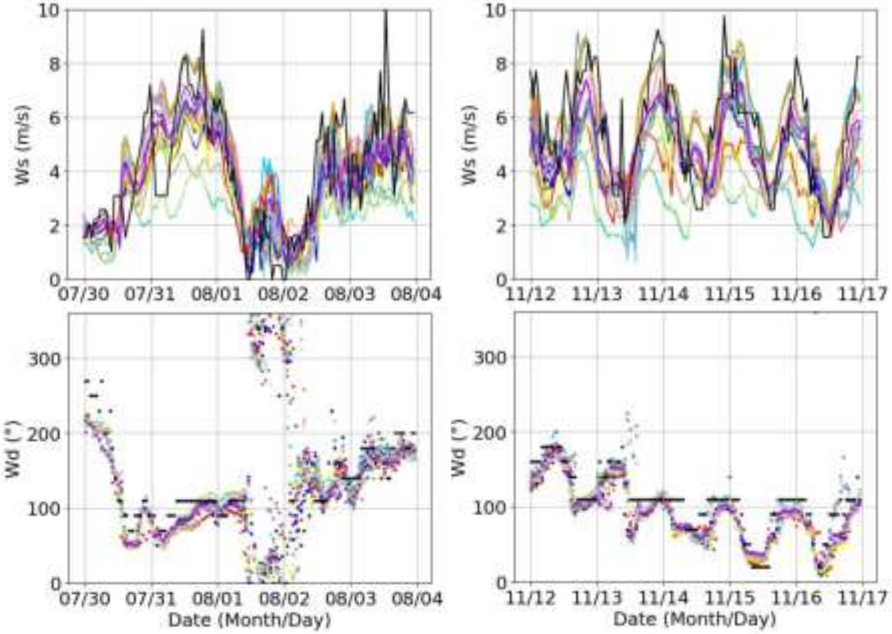
- A limitation in low and middle income countries:
  - Scarce AQ monitoring
  - Lack of detailed input data

1. MOTIVATION AND OBJECTIVES

✓ *WRF sensitivity study in the MABA*



WS and WD at AEP station



Luque et al., Atmósfera, 2024: https://doi.org/10.20937/ATM.53255

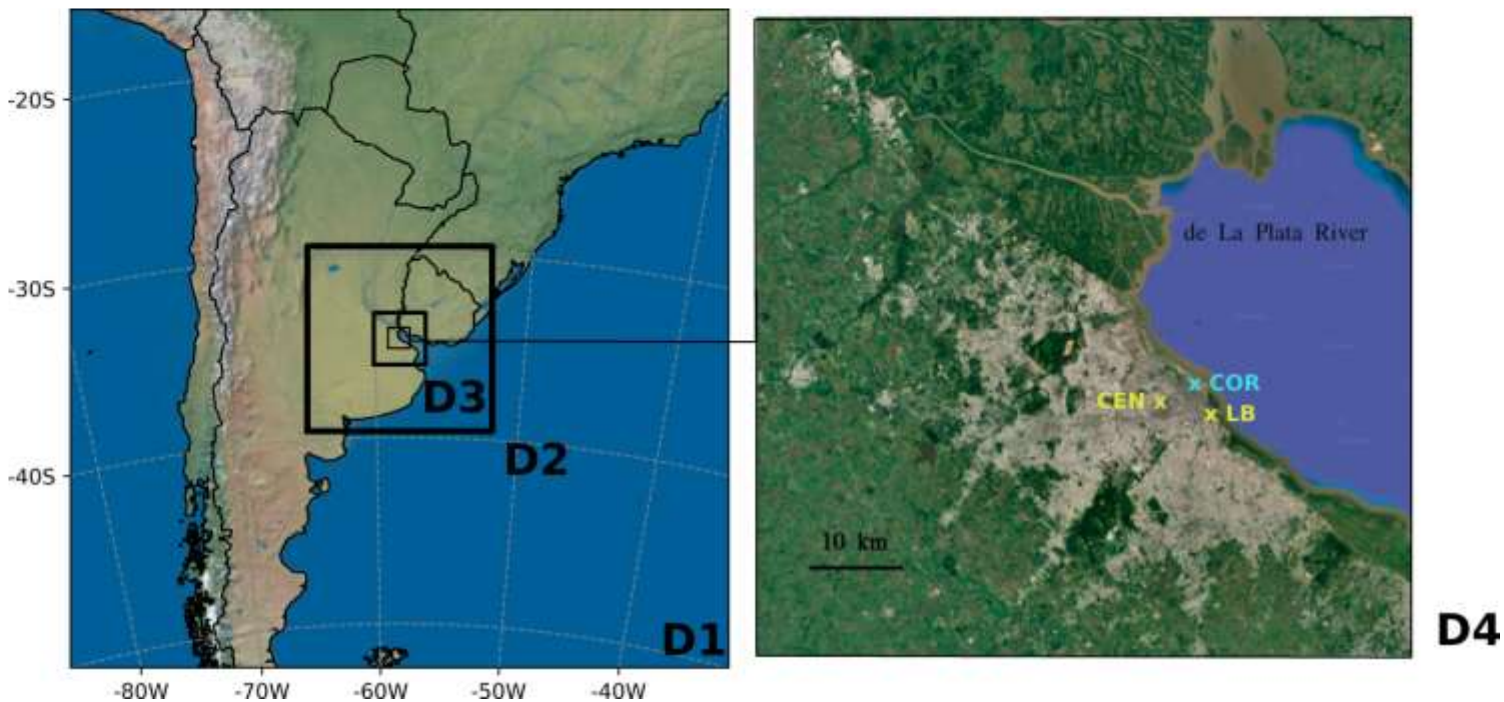
✓ *Implementation of WRF-CMAQ*

Objectives:

- ➢ Perform a sensitivity analysis to domain configuration and background O_3.
- ➢ Compare modelled and observed NOx and NO_2 concentrations at two AQ sites.

2. INPUT DATA AND CONFIGURATIONS

- Up to 4 nested domains w/ resolutions 1 km, 3 km, 15 km and 45 km

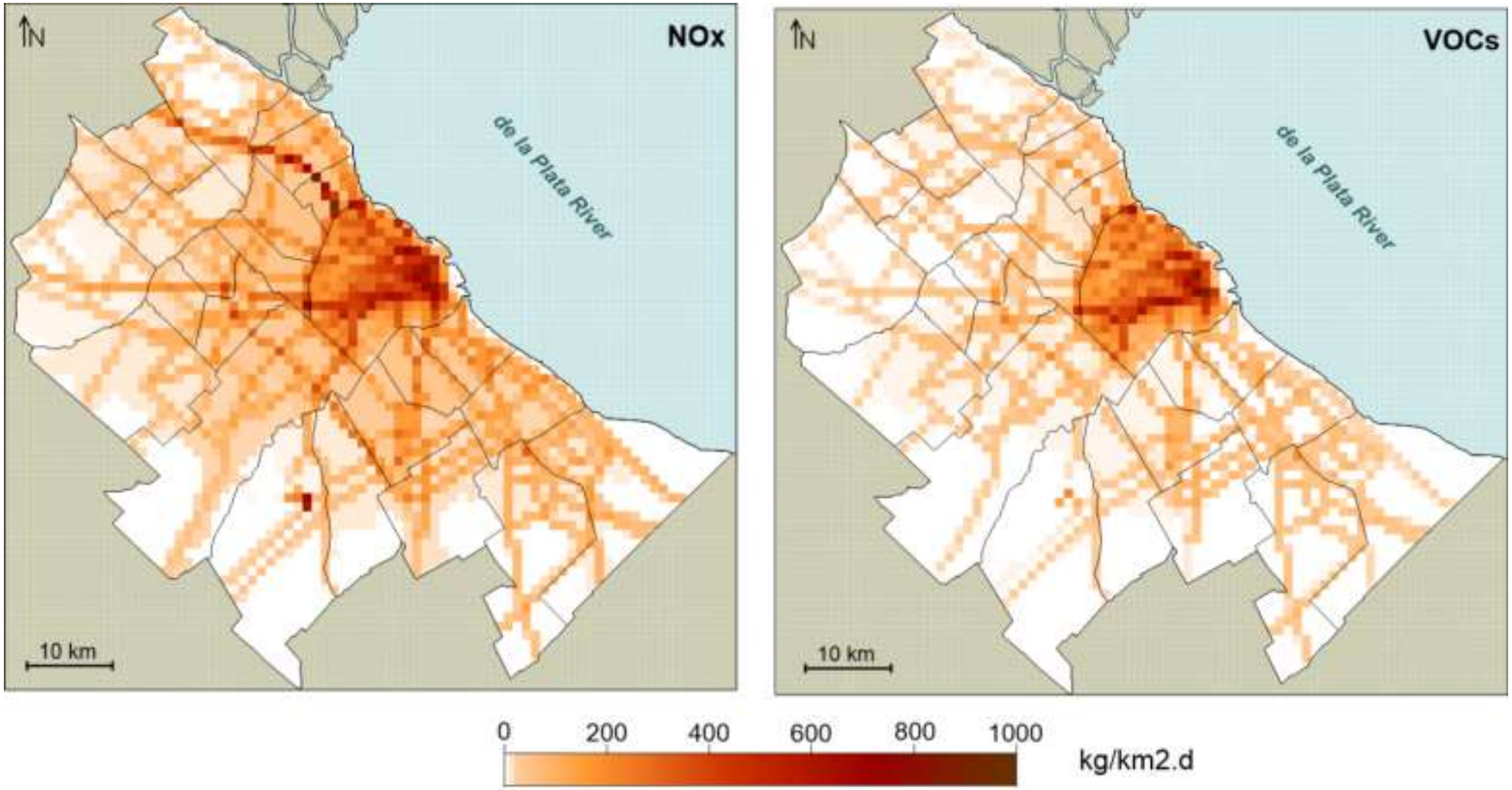


- Two background O_3 concentrations:
  - 20 ppb (Mazzeo et al., 2005)
  - 30 ppb (default surface level in CMAQ)

- Domains D1-D3: NOx and VOCs emissions from EDGAR HTAPv2 inventory (Janssens-Maenhout et al., 2015) for year 2010, processed with HERMES: transport, energy, industry, residential, ships and agriculture

2. INPUT DATA AND CONFIGURATIONS

➢ Domain D4: Area source emission inventory developed by Venegas et al. (2011), including: road transport, aircraft operations, residential, commercial and small industry activities.



Pineda Rojas, Env Model Softw, 2014: https://doi.org/10.1016/j.envsoft.2014.05.016

2. INPUT DATA AND CONFIGURATIONS

WRFv4.2.1 (Luque et al., 2024):

- BouLac (planetary boundary layer)
- MM5 (surface layer)
- Noah (land surface)
- Thomson (microphysics)
- RRTMG (radiation)
- SLUCM (urban)

CMAQv5.4:

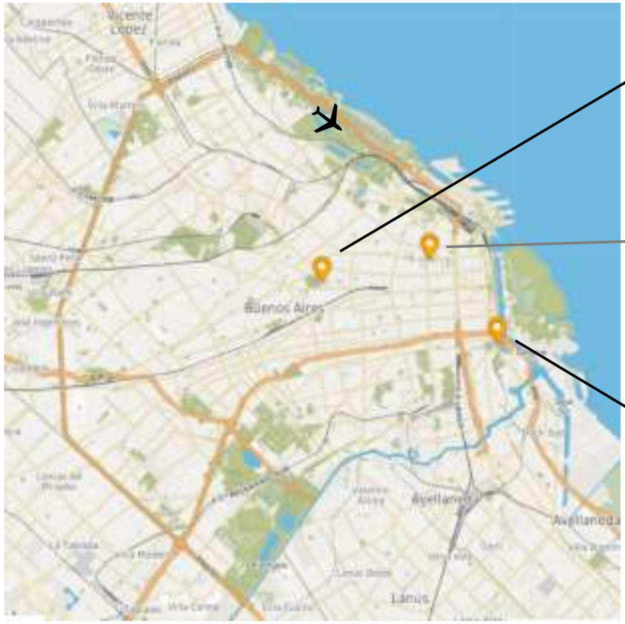
- CB6r3_ae7_aq
- 80 vertical levels (8 within the first kilometre)
- No bVOCs emissions
- No deposition processes

Simulation periods:

- A winter week (Jul 28 - Aug 4 2012)
- A spring week (Nov 10 - 17 2012)
- 2 days for spin-up

2. INPUT DATA AND CONFIGURATIONS

City of Buenos Aires



- <u>Comparison with observations</u>: NOx and NO_2 at CEN and LB
- <u>Sensitivity analysis to six configurations</u>: NOx, NO_2 and O_3 at the two sites and across the MABA

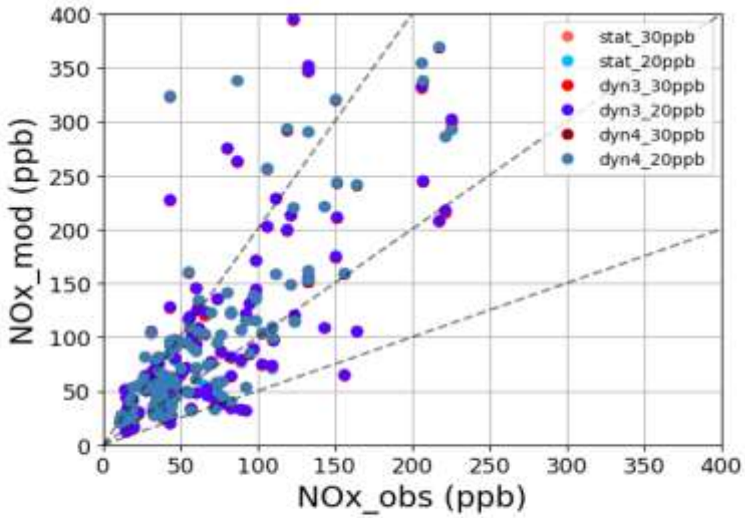
WRF-CMAQ sensitivity simulations

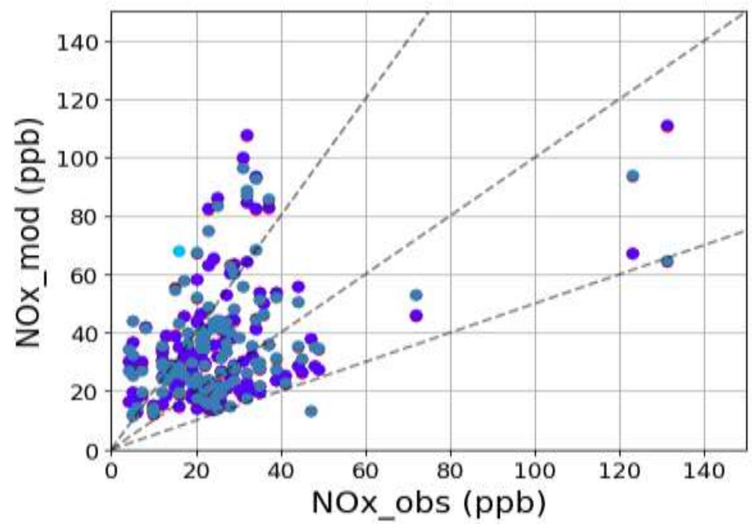
Configuration label	# of domains	Domains	$[O_3]_b$
stat_20ppb	1	D4	20 ppb
dyn3_20ppb	3	D2-D4	
dyn4_20ppb	4	D1-D4	
stat_30ppb	1	D4	30 ppb
dyn3_30ppb	3	D2-D4	
dyn4_30ppb	4	D1-D4	

3. RESULTS: Modelled vs observed hourly concentrations **CEN (UB)**

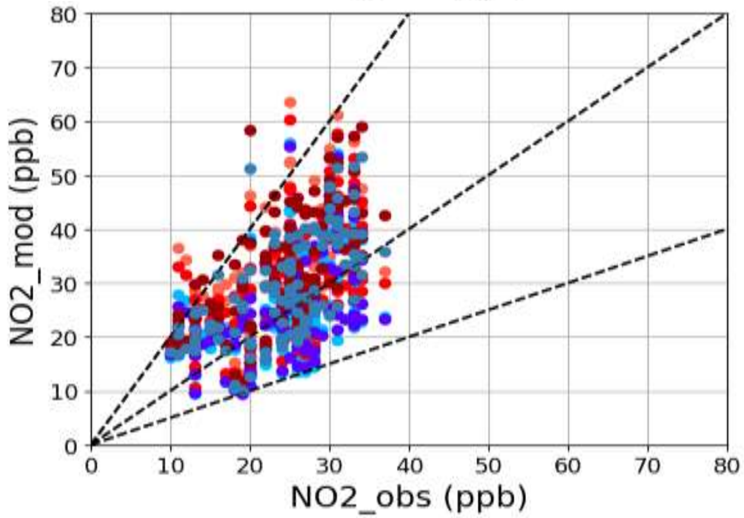
WINTER | SPRING

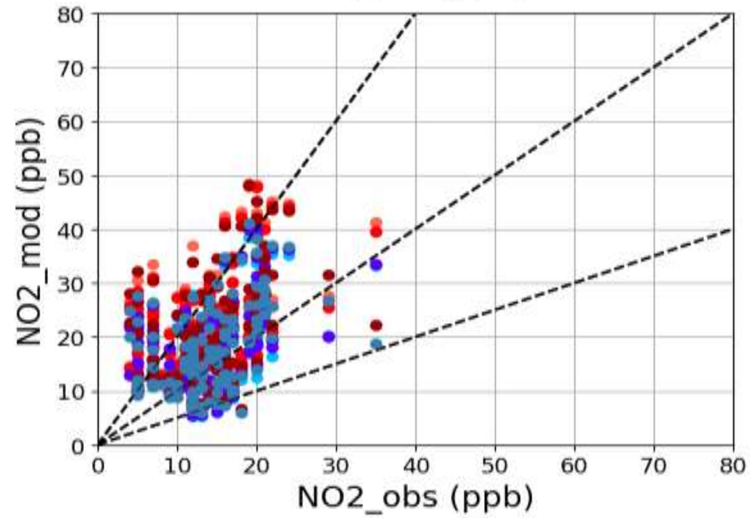
NOx





NO_2

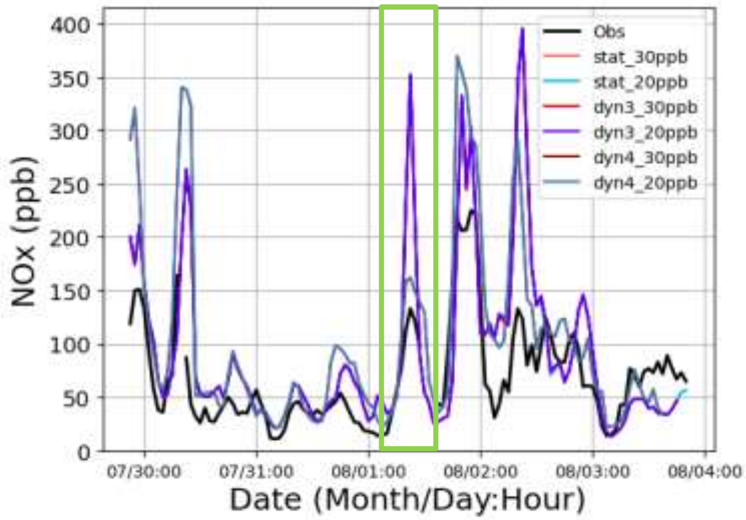


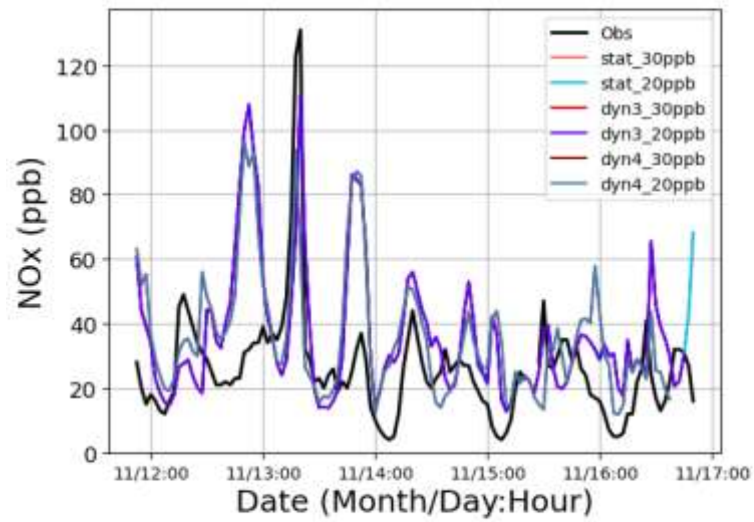


3. RESULTS: NOx and NO_2 hourly variations **CEN (UB)**

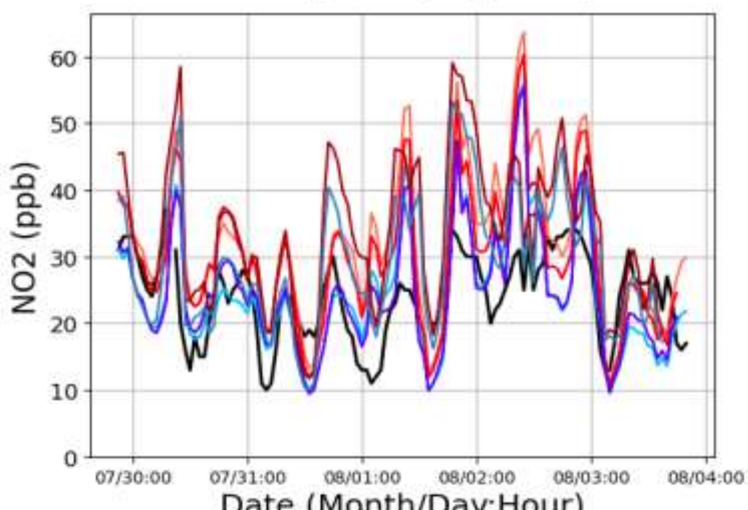
WINTER SPRING

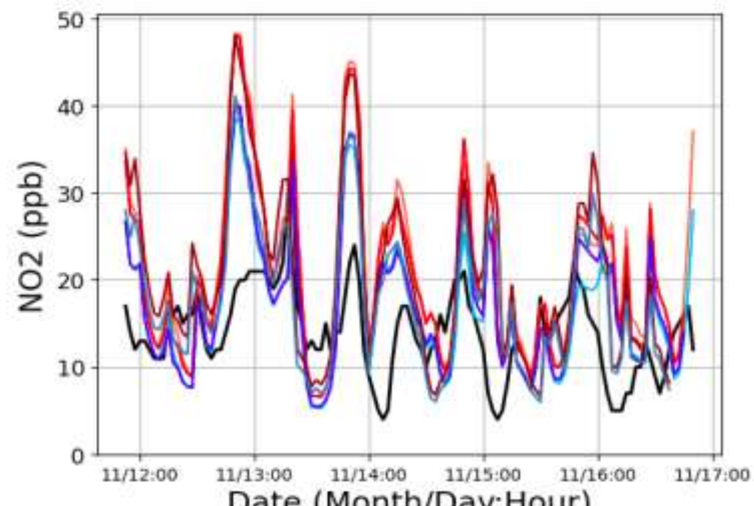
NOx



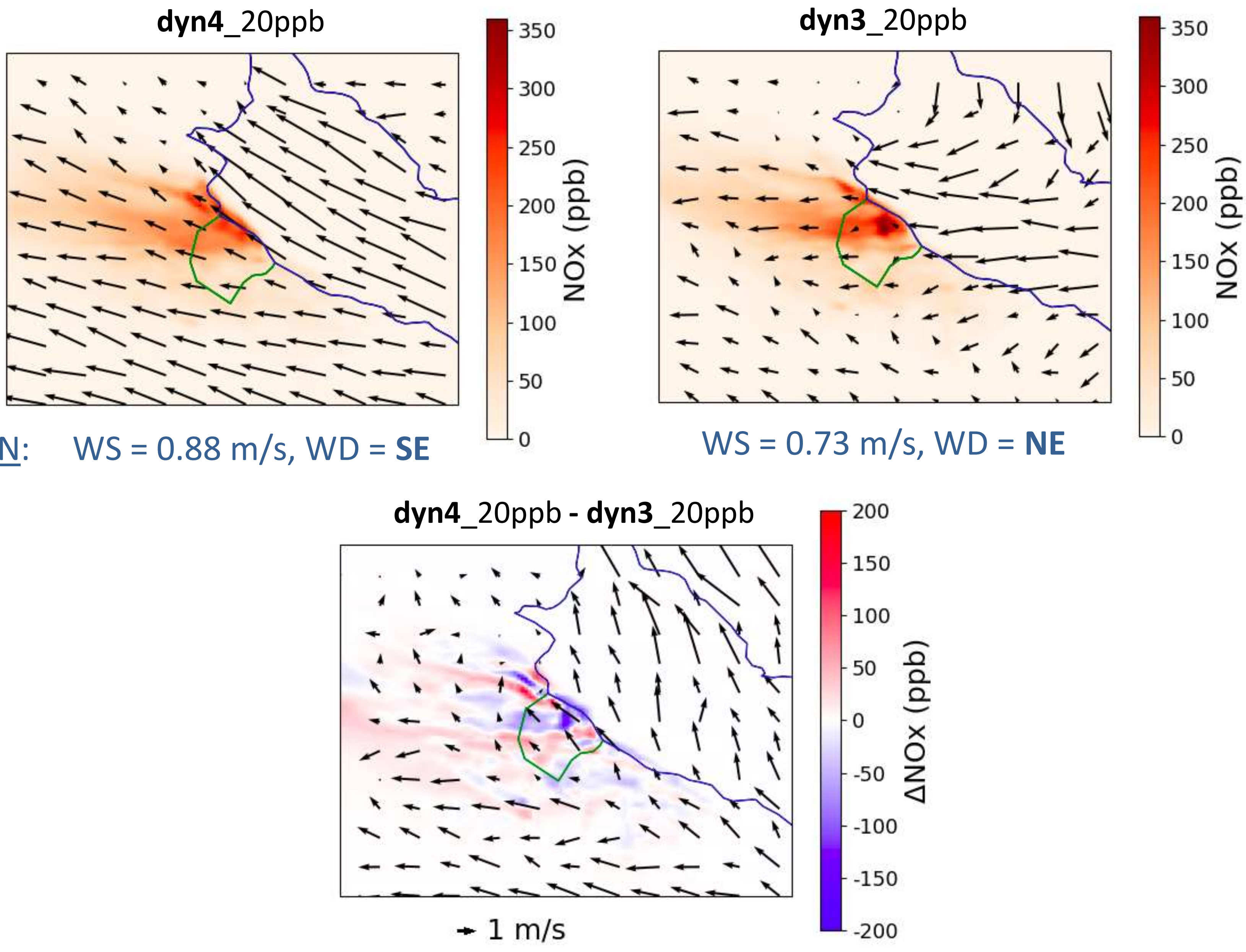


NO_2





3. RESULTS: Wind fields at the time of the largest NOx difference



At CEN: WS = 0.88 m/s, WD = **SE** — WS = 0.73 m/s, WD = **NE**

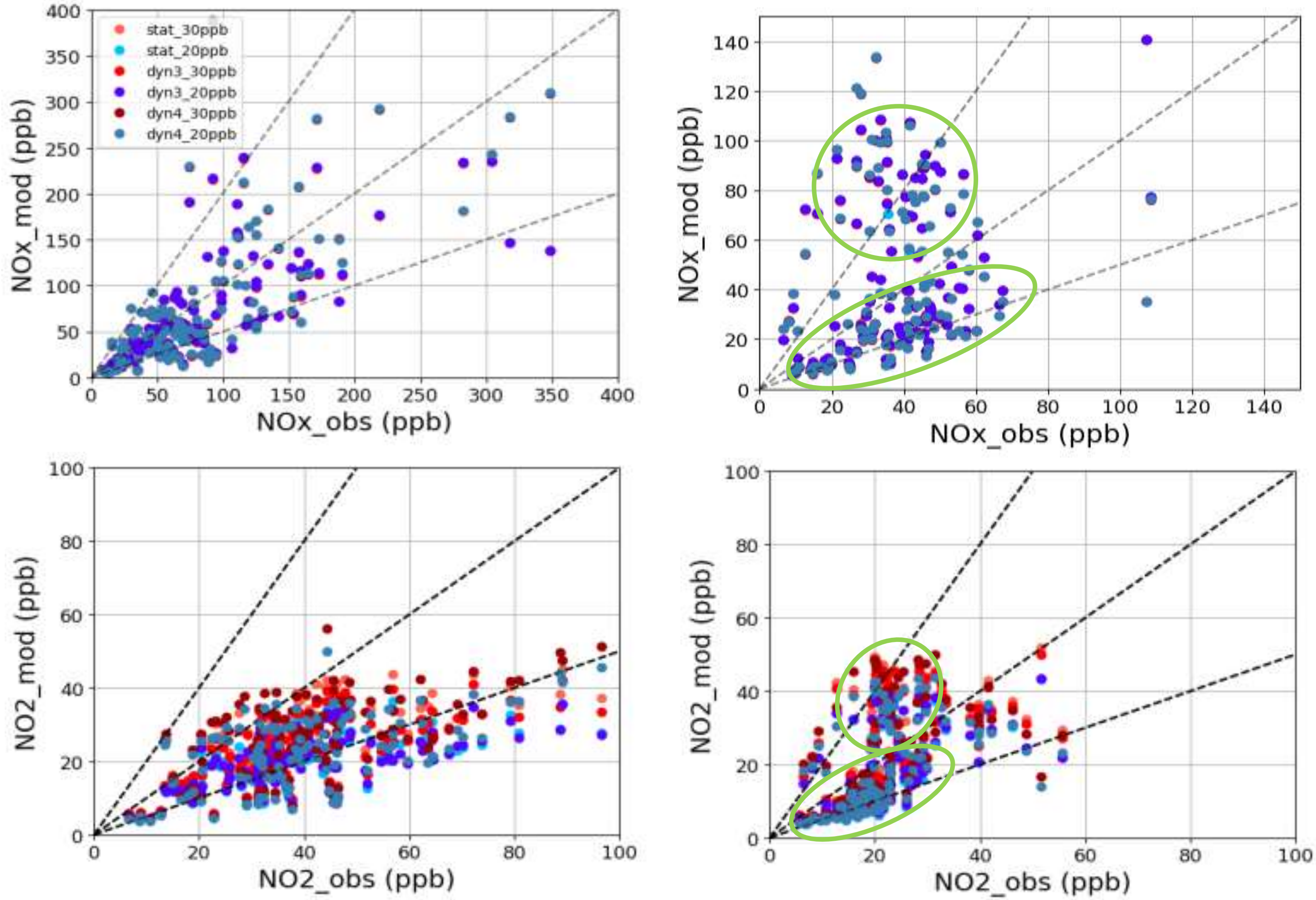
3. RESULTS: Modelled vs observed concentrations

LB (RI)

WINTER | SPRING

NOx

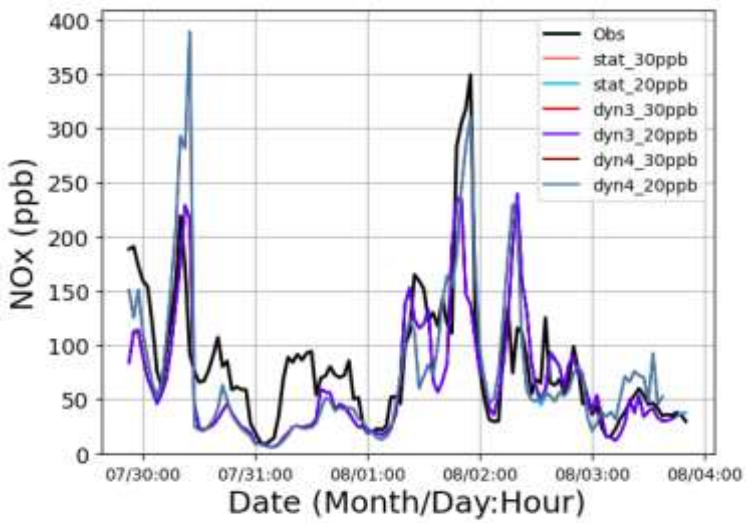
NO_2

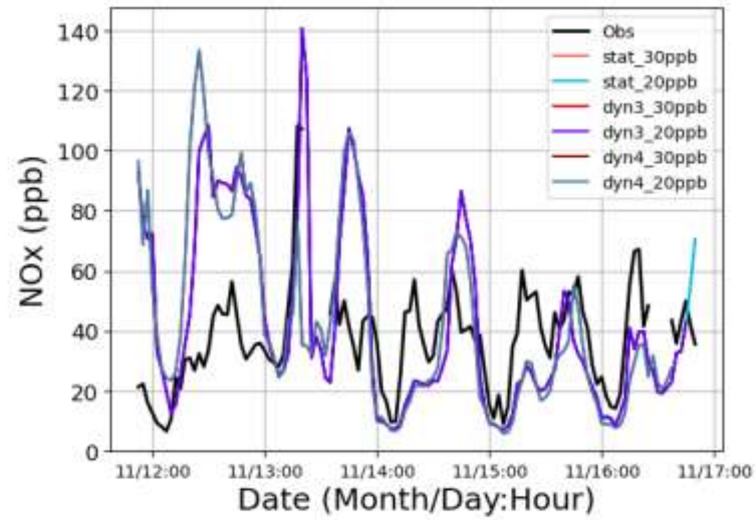


3. RESULTS: NOx and NO_2 hourly variations **LB (RI)**

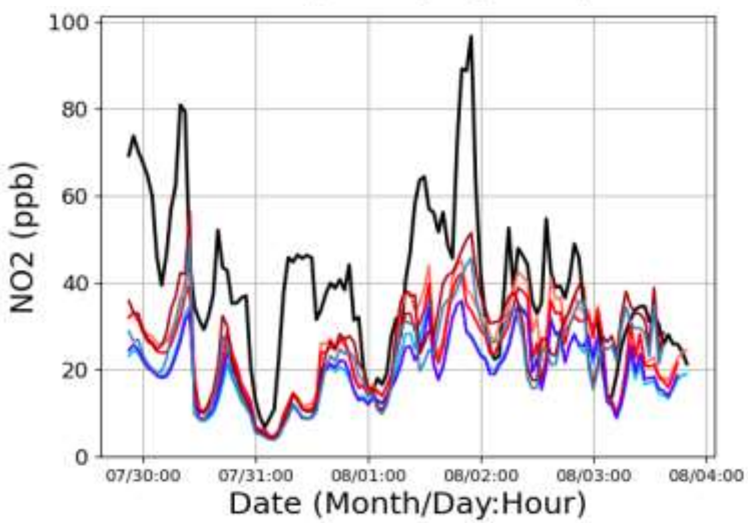
WINTER SPRING

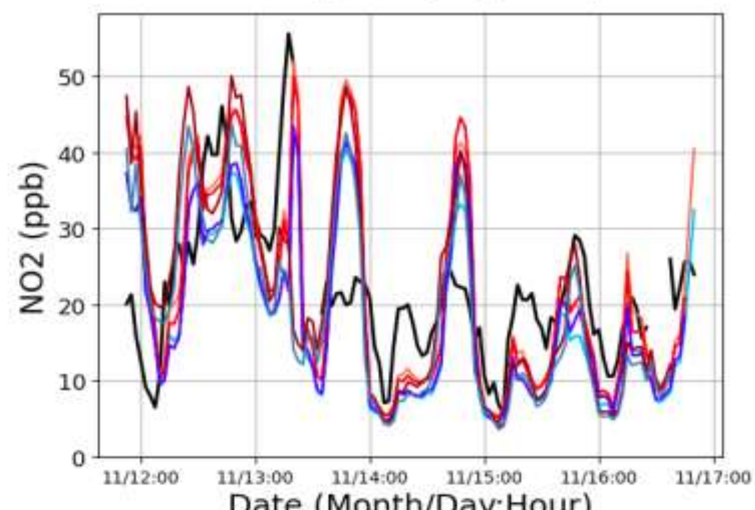
NOx





NO_2



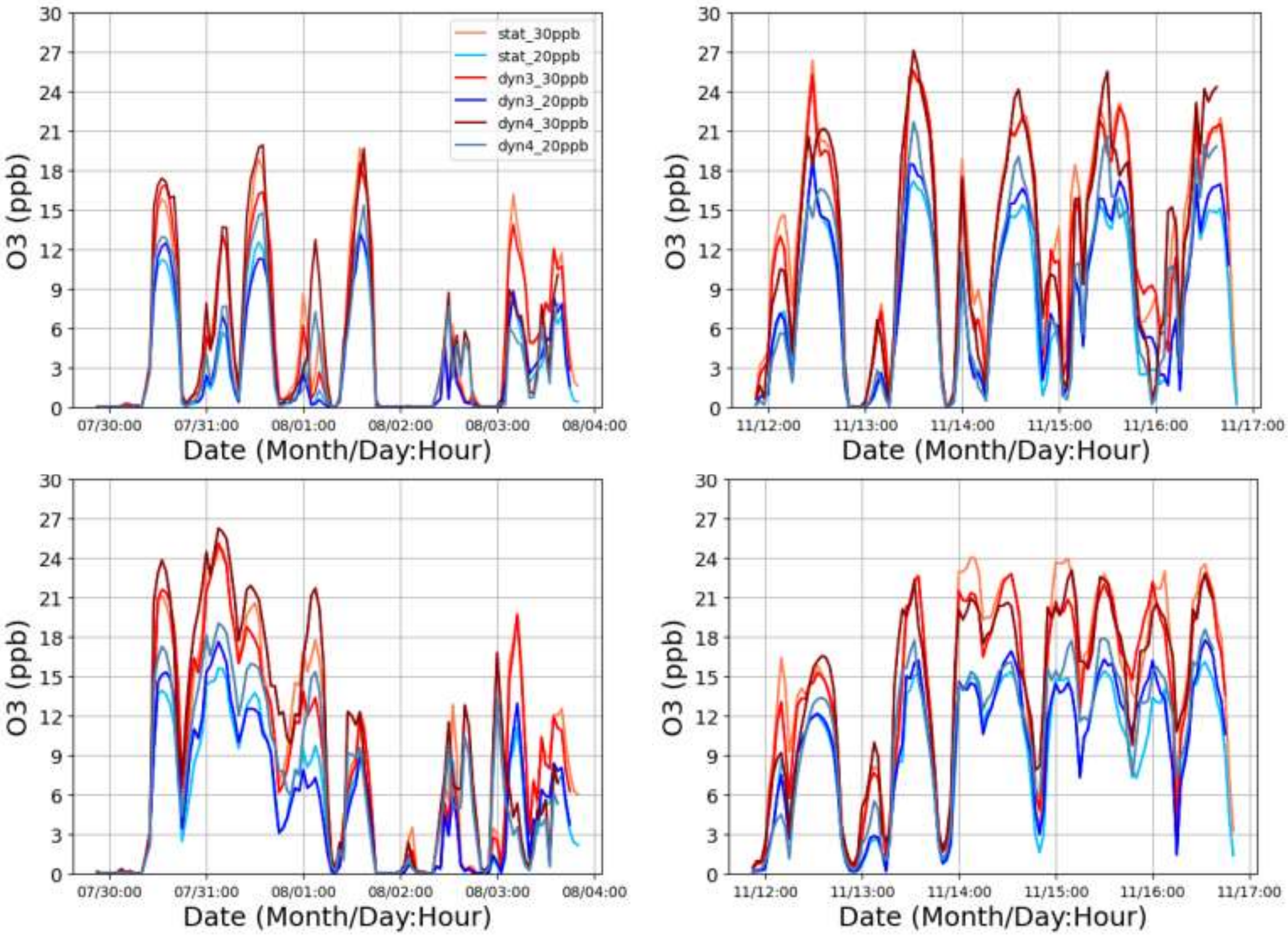


3. RESULTS: O_3 hourly variations

WINTER SPRING

CEN

LB



3. RESULTS: Model performance of different configurations

✓ There is no single configuration that performs best for all cases (pollutants, sites and weeks).

✓ Configurations with 'dyn4' are expected to better capture the variability of regional O_3 in general.

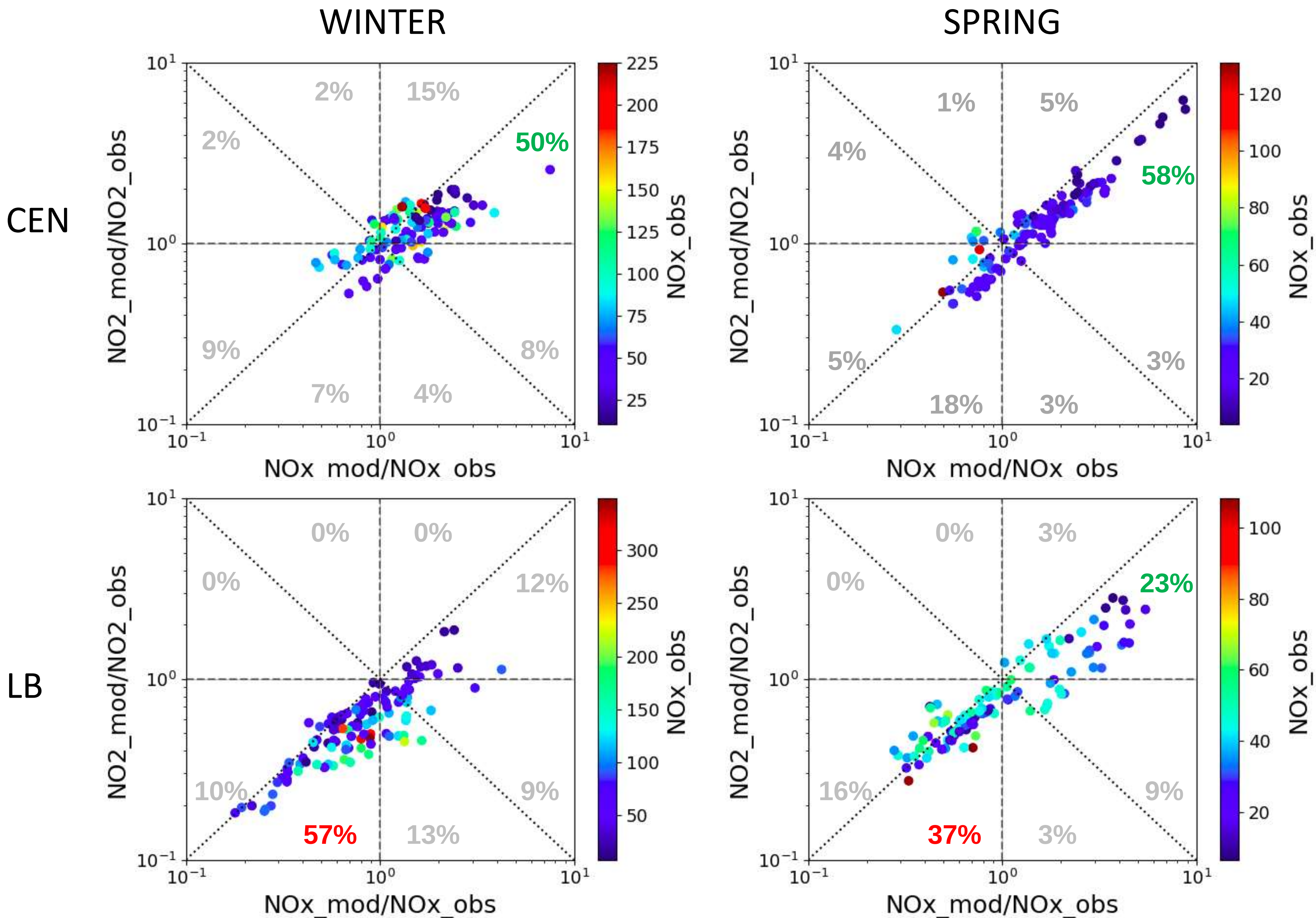
✓ Simulations with '20 ppb' perform better at CEN (UB), consistent with previous studies (e.g. Mazzeo et al., 2005).

Model performance metrics for configuration dyn4_20ppb

NOx	CEN		LB	
	WIN	SPR	WIN	SPR
r	0.8	0.4	0.7	0.2
FA2	0.8	0.7	0.7	0.4
FB	0.4	0.3	-0.1	0.1

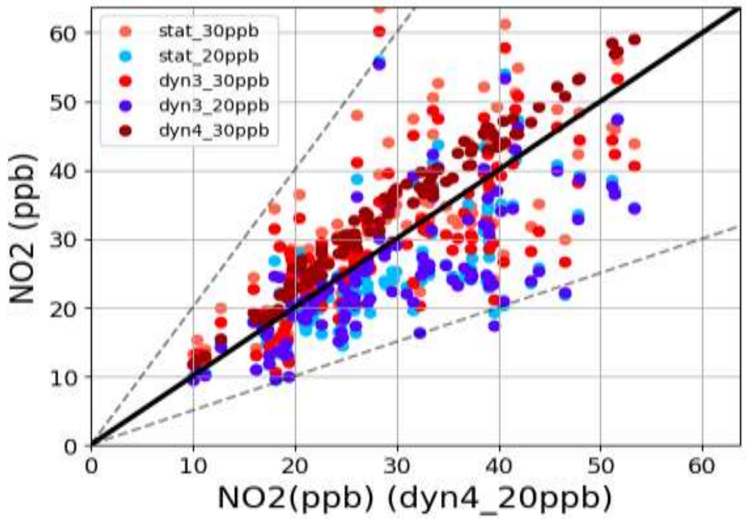
NO_2	CEN		LB	
	WIN	SPR	WIN	SPR
r	0.6	0.4	0.6	0.5
FA2	0.9	0.8	0.6	0.7
FB	0.2	0.2	-0.5	0.2

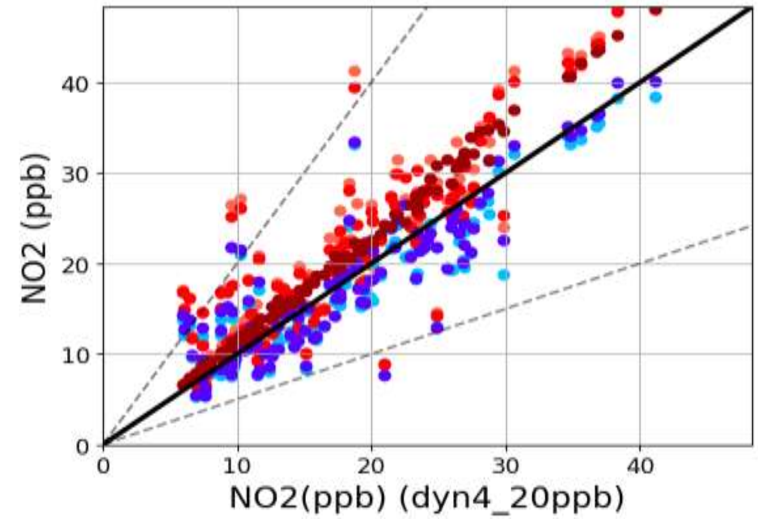
3. RESULTS: NO_2 vs. NOx errors (dyn4_20ppb)



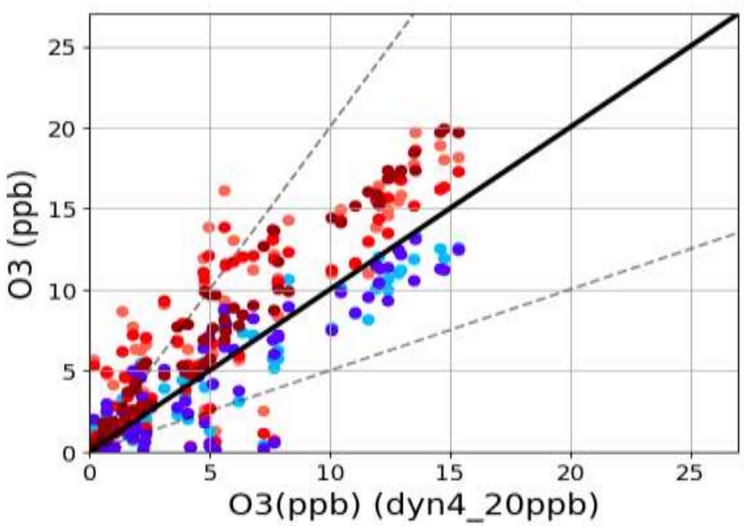
WINTER SPRING

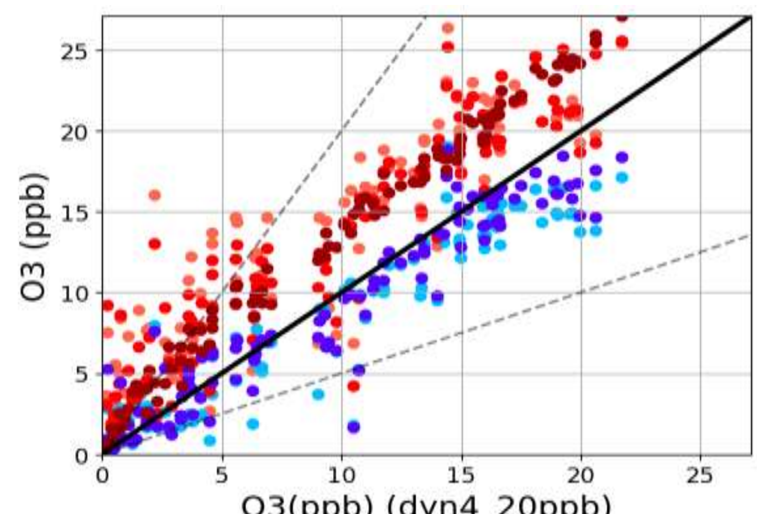
NO_2





O_3



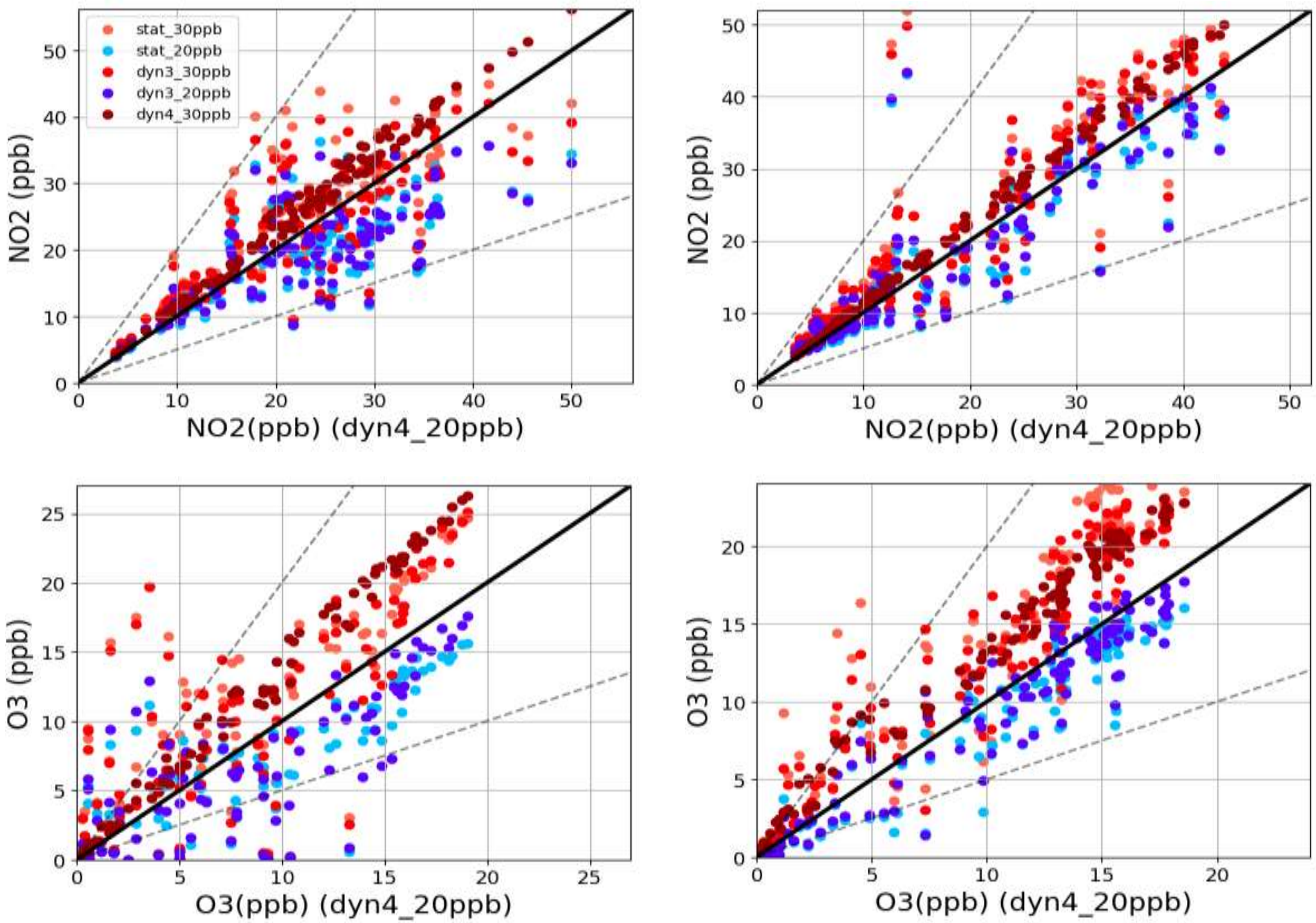


3. RESULTS: dyn4_20ppb vs other configurations **LB (RI)**

WINTER SPRING

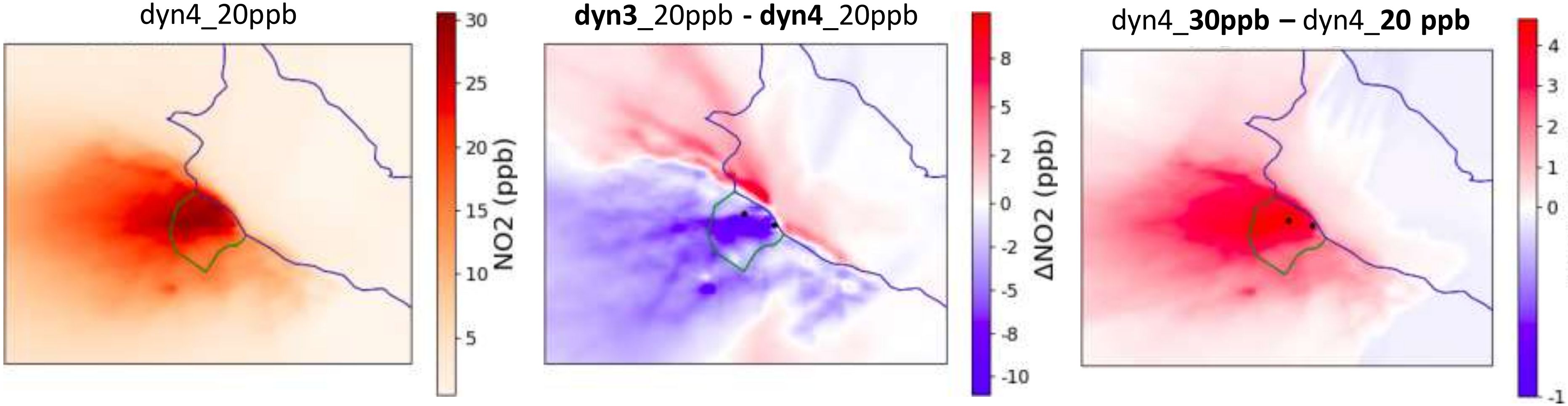
NO_2

O_3

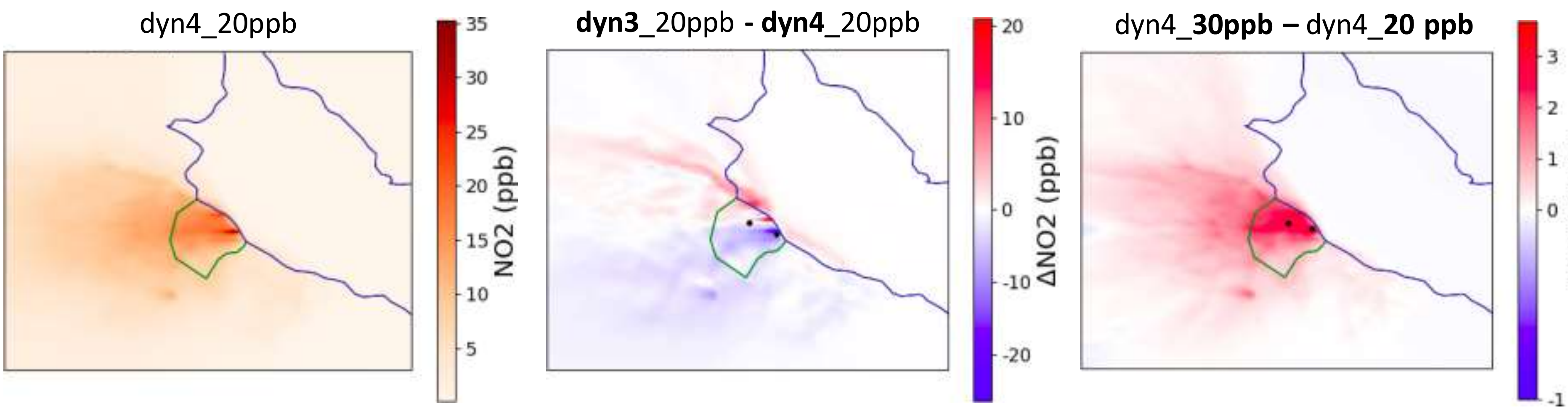


3. RESULTS: Mean NO_2 concentration

Winter wk

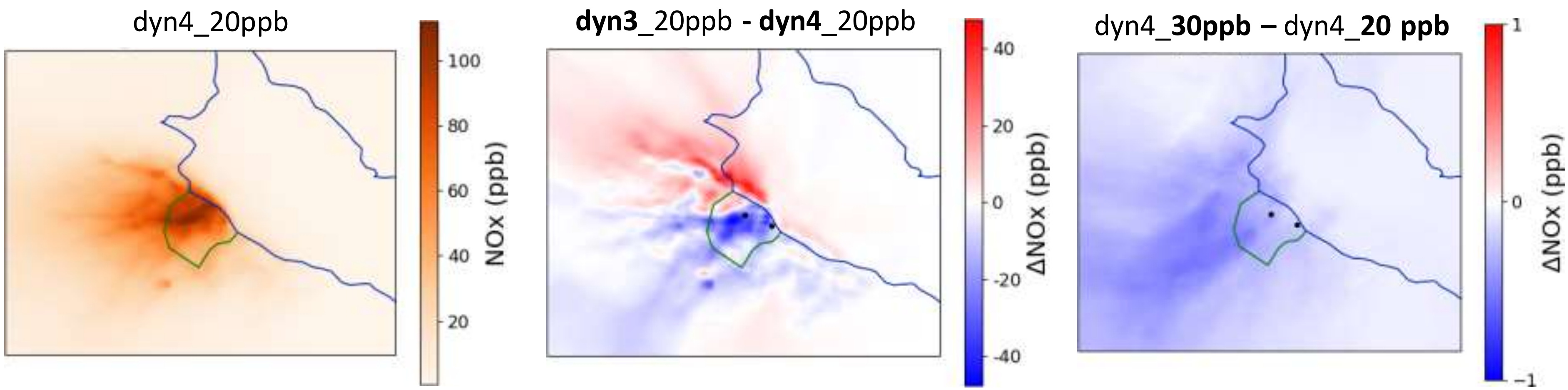


Spring wk

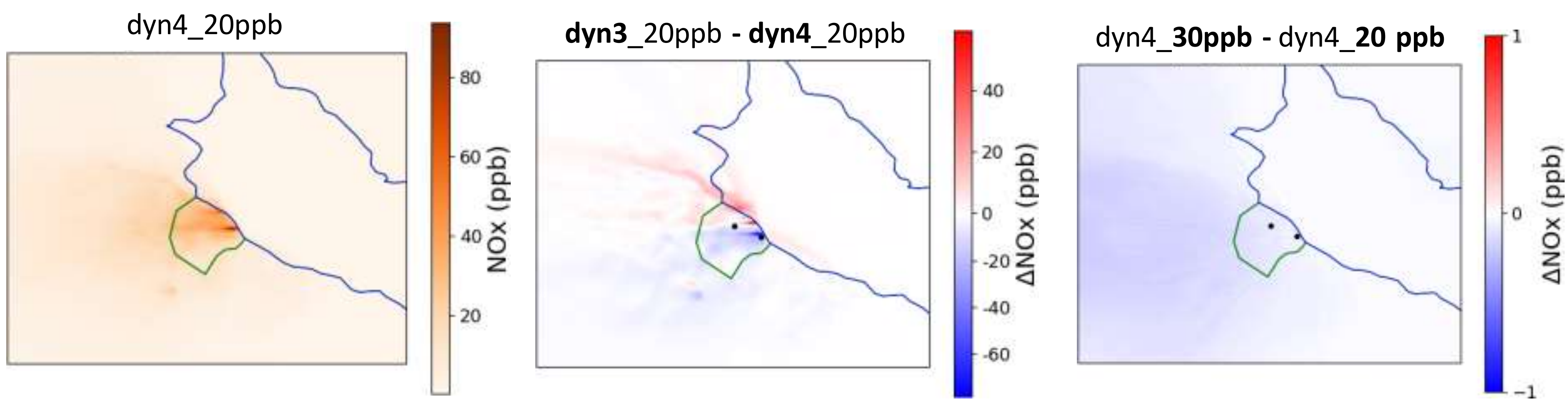


3. RESULTS: Mean NO_x concentration

Winter wk

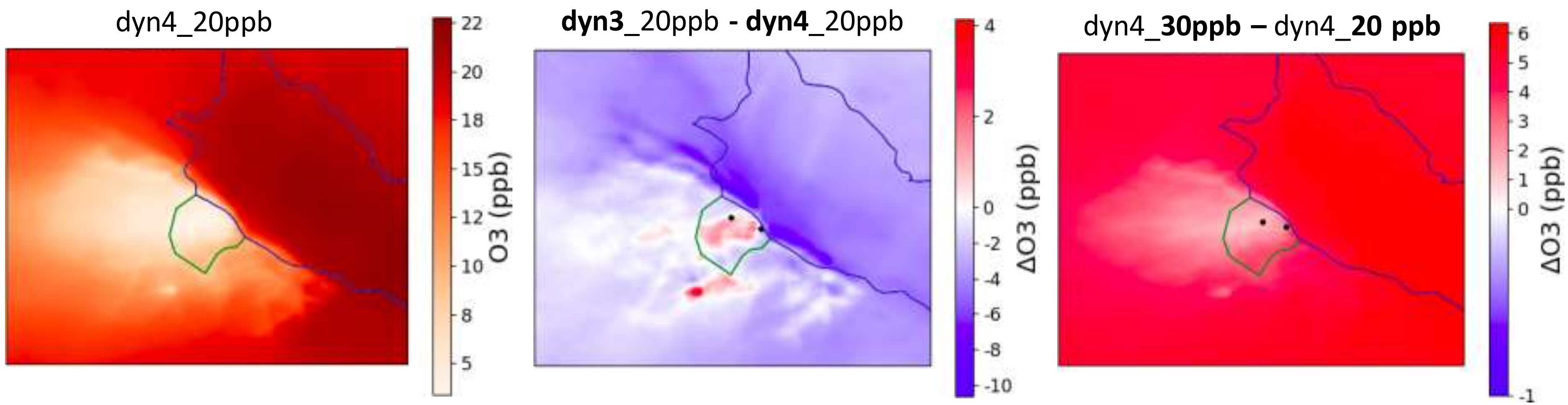


Spring wk

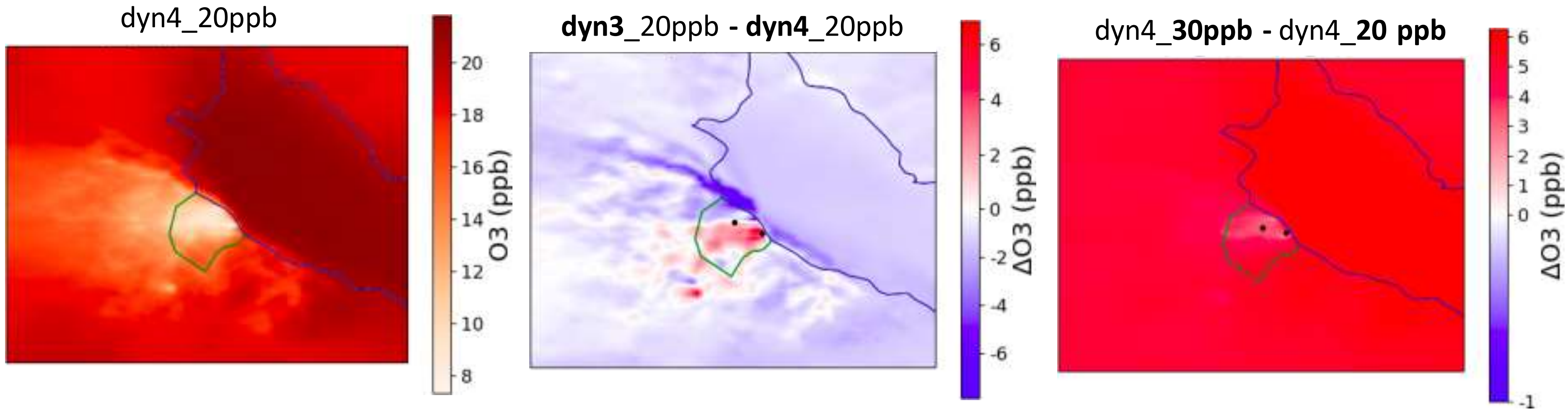


3. RESULTS: Mean O_3 concentration

Winter wk



Spring wk



4. CONCLUSIONS

Main remarks

✓ First implementation of WRF-CMAQ to estimate NO_2 and O_3 in MABA

✓ Peak hourly concentrations of these pollutants are sensitive to both the background O_3 level and the domain configuration.

✓ Errors in NO_2 are mainly caused by those in NOx, with some contribution from background O_3.

✓ The dyn4_20ppb configuration seems to be appropriate for the MABA.

Next steps

➢ Assess the sensitivity of the simulations to the height of the lower layer.

➢ Evaluate the performance of the model considering longer runs (two months) to have more robust metrics.

Thank you