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Evaluating simple and complex models for urban NO_2 concentrations: DAUMOD-GRS and WRF-CMAQ in Buenos Aires

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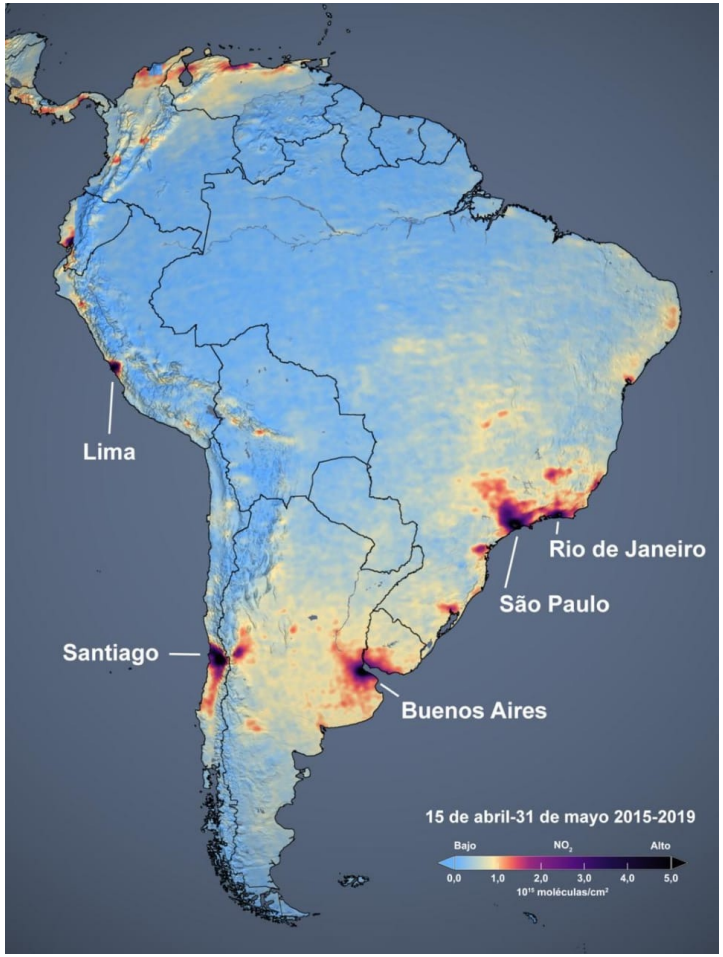
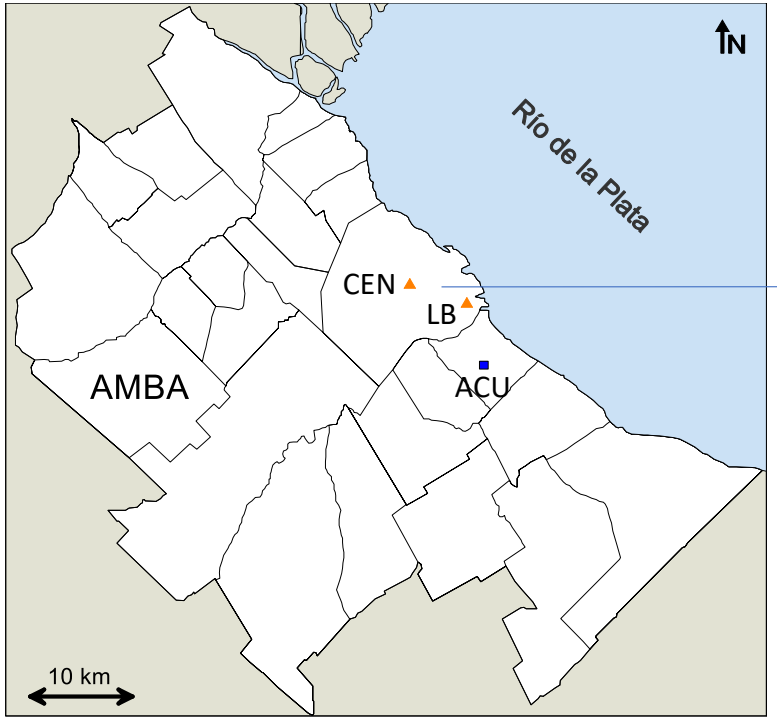
Motivation: monitoring limitations in Buenos Aires

NO_2 column in South America 2015-2019



Source: NASA, https://svs.gsfc.nasa.gov/4835/

Metropolitan Area of Buenos Aires (MABA)



NO, NO_2, CO, PM_{10} since 2009

DAUMOD-GRS

DAUMOD

Urban scale atmospheric dispersion model developed for area sources (Q_i)

$$C(z=0) = a\,[\,Q_0\,x^b + \sum_{i=1}^{N}(Q_i - Q_{i-1})(x - x_i)^b\,]\,/\,(|A_1|\,k\,z_0^b\,u_*)$$

GRS

NOx-VOCs-O_3 interaction

ROC + *hv* → ROC + RP
RP + NO → NO_2
NO_2 + *hv* → NO + O_3
NO + O_3 → NO_2
RP + RP → RP
NO_2 + RP → SGN
NO_2 + RP → SNGN

ROC: all VOC species
RP: radicals
SGN: stable gaseous nitrogen
SNGN: stable non-gaseous nitrogen

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

Simple vs complex models

Aspect	Air Quality Models	
	Simple	**Complex**
Approach & processes	Semi-empirical expressions to represent **T&D**	Numerical representation of **multiple processes**
Input data	Few	Detailed
Computing cost	Low	High
HR simulations	Long (several years)	Short (days to weeks)

WRF-CMAQ & objectives

WRF-CMAQ modelling system

- ✓ Chemical transport model developed by US EPA
- ✓ Extensively applied worldwide at regional and urban scales
- ✓ Provides a suitable reference against which to compare DAUMOD

Objectives:

1) To evaluate the performance of DAUMOD-GRS in relation to a widely used complex model, and
2) To explore the potential role of processes and sources not considered in previous studies.

Methodology

Simulation periods (2012):

- Winter month: 16 July to 11 August

- Spring month: 5 November to 1 December

Input data:

- Boundary conditions: clean air

- Emission inventory of NOx and VOCs from area sources in the MABA (1 km, 1h) (Venegas et al., 2011)

Analyses:

1. Hourly concentrations of NO_2, NOx and O_3 at: CEN (UB), and LB and ACU (RI)

2. Sensitivity to changes in background O_3 and f-NO_2

3. Comparison with CMAQ using 4 nested domains + power plant emissions

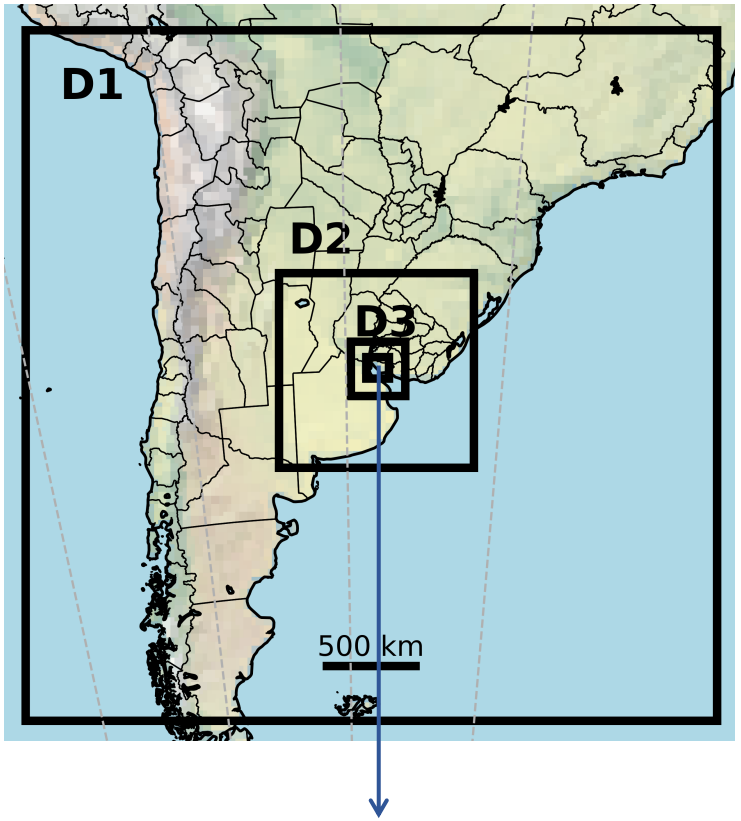
Venegas et al., 2011: https://www.intechopen.com/chapters/16157

Methodology

WRF-CMAQ in the MABA

WRFv4.2.1:

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



CMAQv5.4:

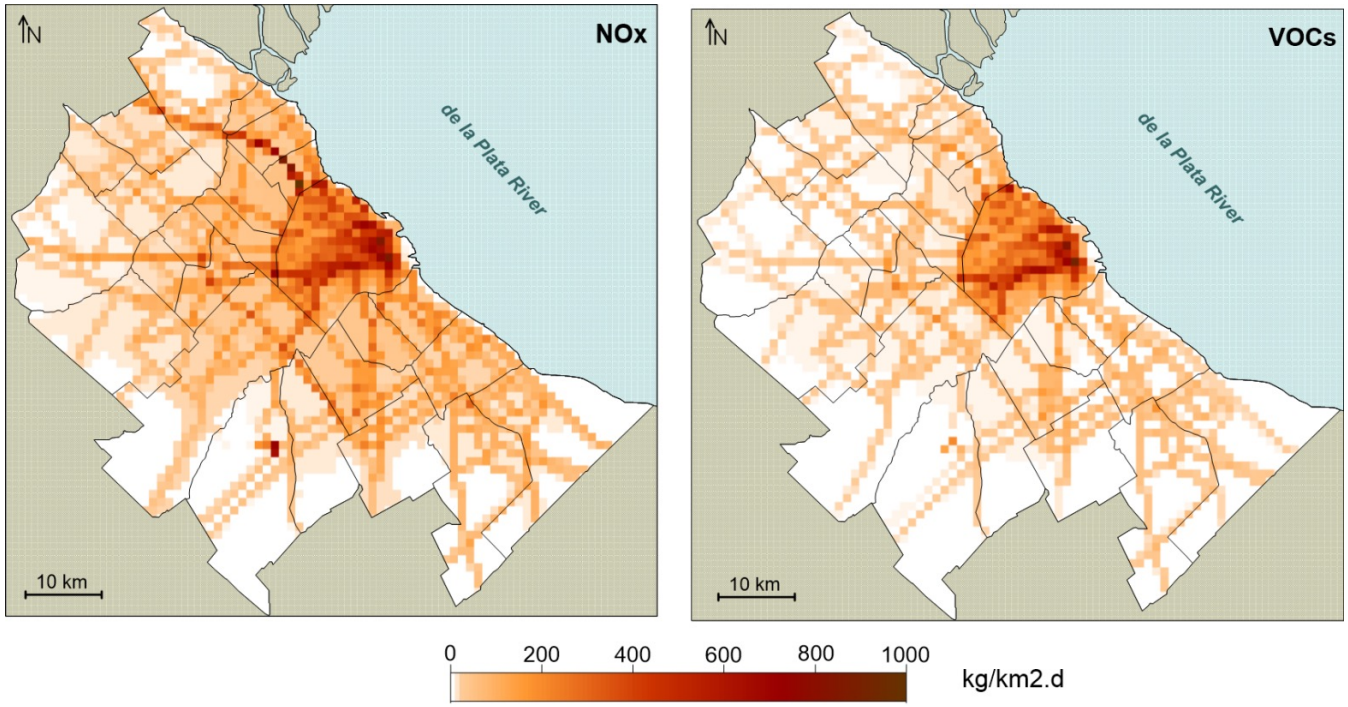
- CB6r3_ae7_aq
- bVOCs emissions from MEGAN
- Deposition using default values
- 8 vertical layers within the first km
- Horizontal resolutions: Resolución: 45 km, 15 km, 3 km, **1 km (D4)**

Luque et al., Air Qual Atmos Health, 2025: https://doi.org/10.1007/s11869-025-01810-8

Methodology

Emissions

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

Results

Performance metrics - hourly NO_2

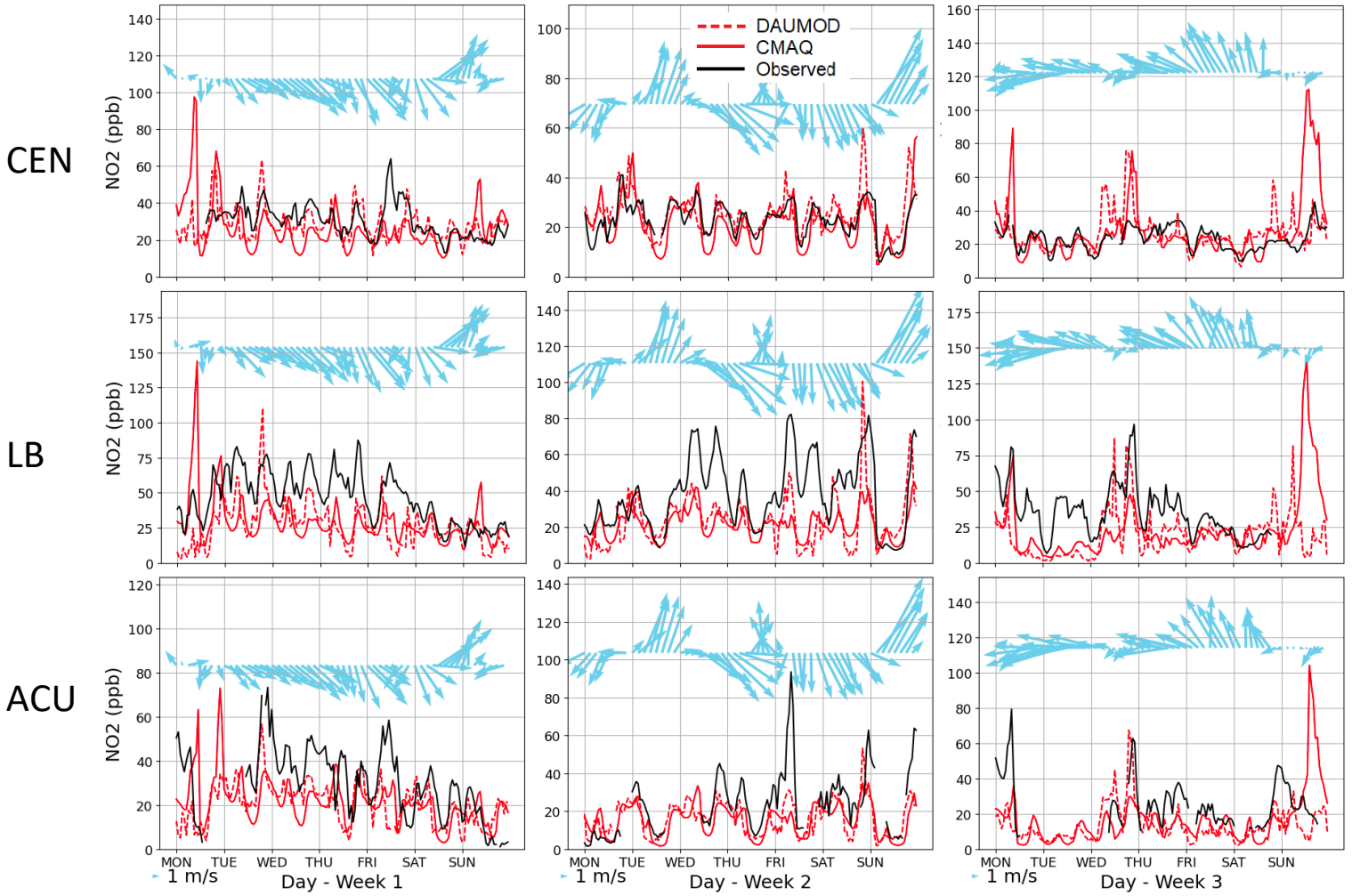
WINTER	WRF-CMAQ					DAUMOD-GRS				
	N	FB	NMSE	FA2	R	N	FB	NMSE	FA2	R
CEN (UB)	578	-0.02	0.25	0.92	0.40	576	-0.06	0.14	0.94	0.45
LB (RI)	575	0.48	0.57	0.62	0.47	573	0.55	0.63	0.58	0.51
ACU (RI)	458	0.36	0.66	0.60	0.33	456	0.40	0.57	0.65	0.47

SPRING	WRF-CMAQ					DAUMOD-GRS				
	N	FB	NMSE	FA2	R	N	FB	NMSE	FA2	R
CEN (UB)	590	0.12	0.32	0.76	0.31	585	-0.17	0.20	0.83	0.61
LB (RI)	605	0.76	1.30	0.43	0.43	600	0.57	1.06	0.41	0.37
ACU (RI)	–	–	–	–	–	–	–	–	–	–

Chang & Hanna, 2005: https://doi.org/10.1007/s00703-003-0070-7 Abs(FB) < 0.30 NMSE < 1.5 FA2 > 0.50

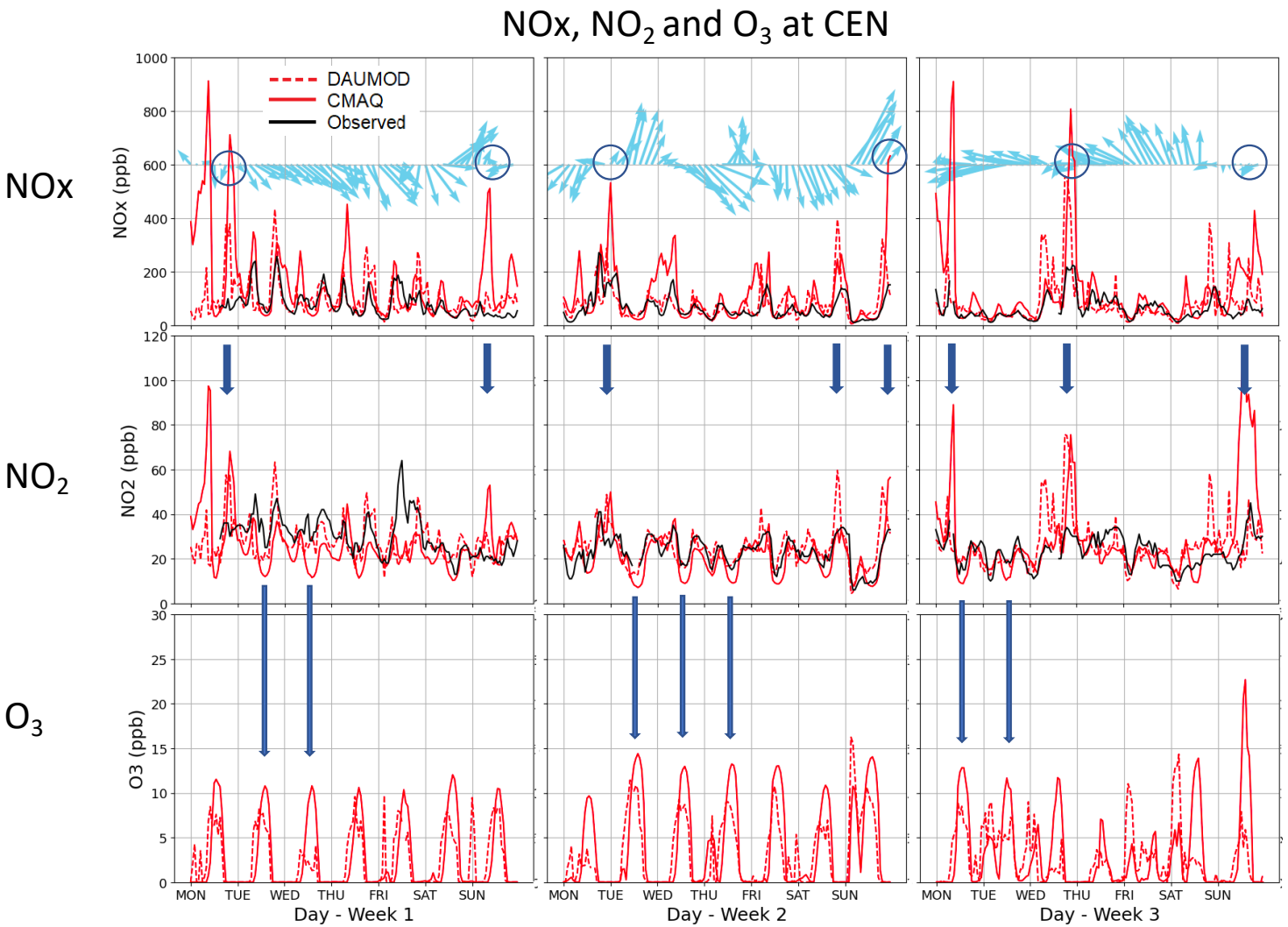
Hanna & Chang, 2011: https://doi.org/10.1007/978-94-007-1359-8_80 Abs(FB) < 0.67 NMSE < 6.0 FA2 > 0.30

Hourly concentration of NO_2

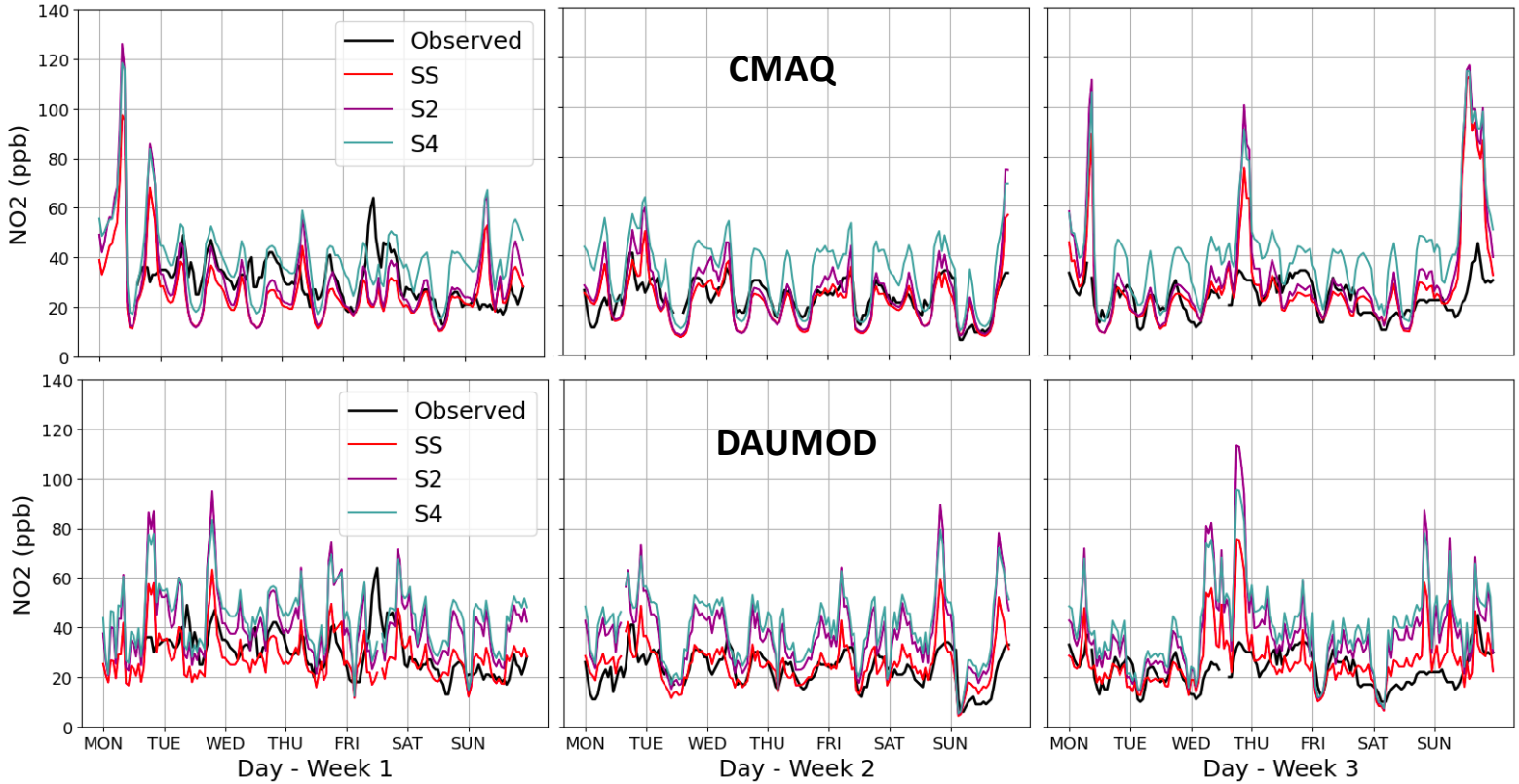


Results

WINTER



NO_2 - WINTER - **CEN**

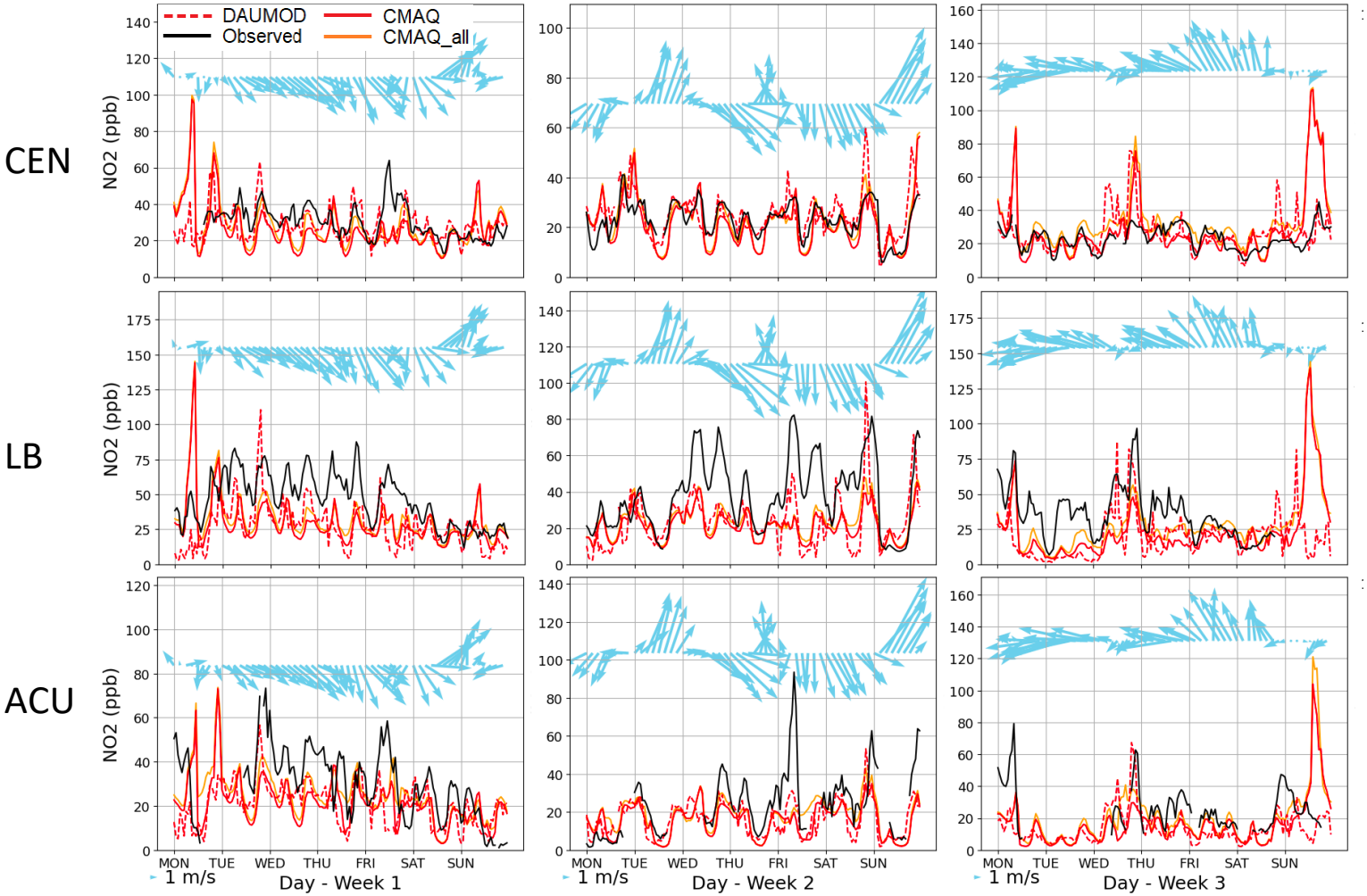


SS: Standard Simulation

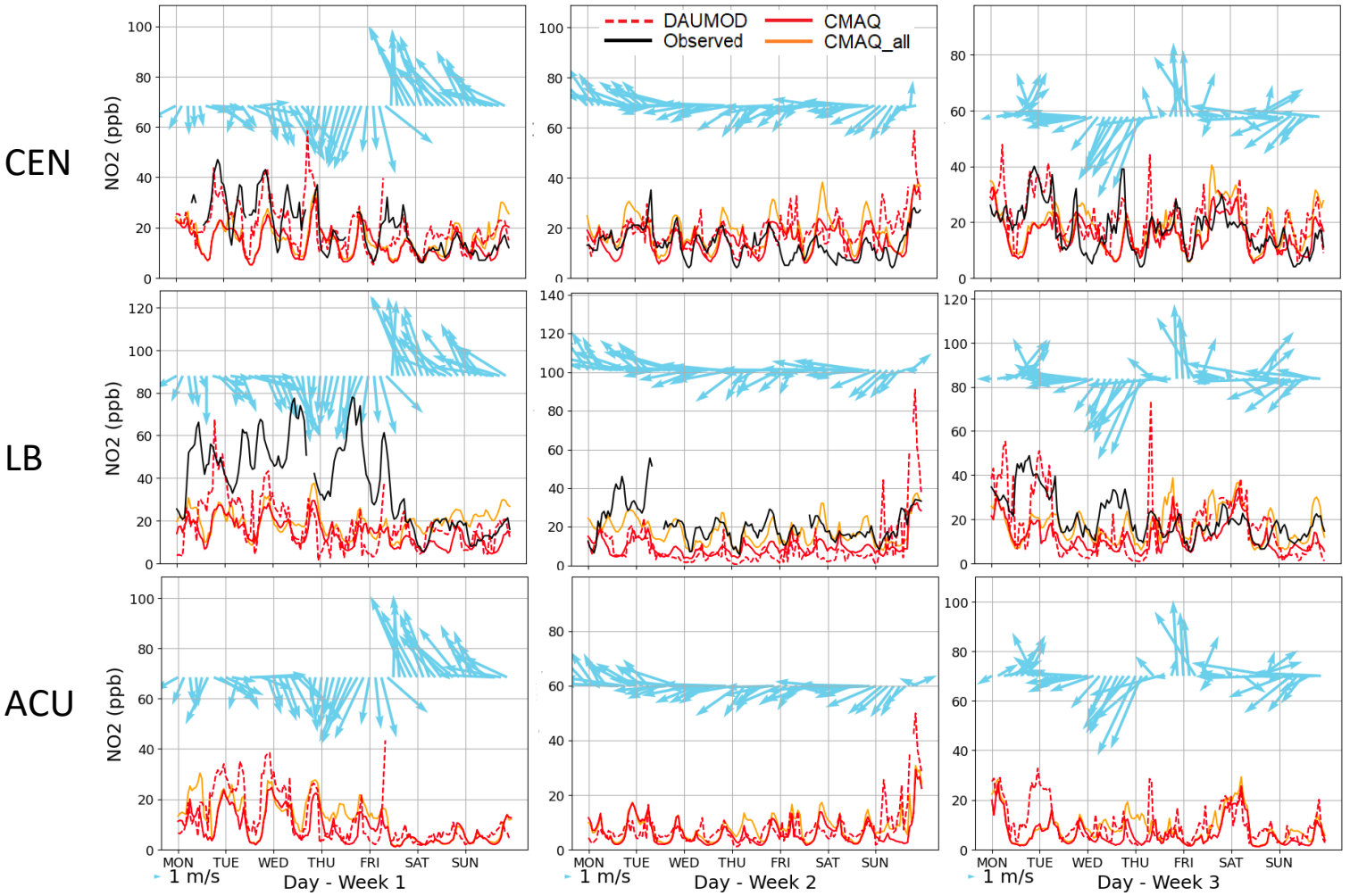
S2: f-NO_2: 0.10 → 0.15

S4: [O_3]b: 20 ppb → 40 ppb

NO_2 with CMAQ_all

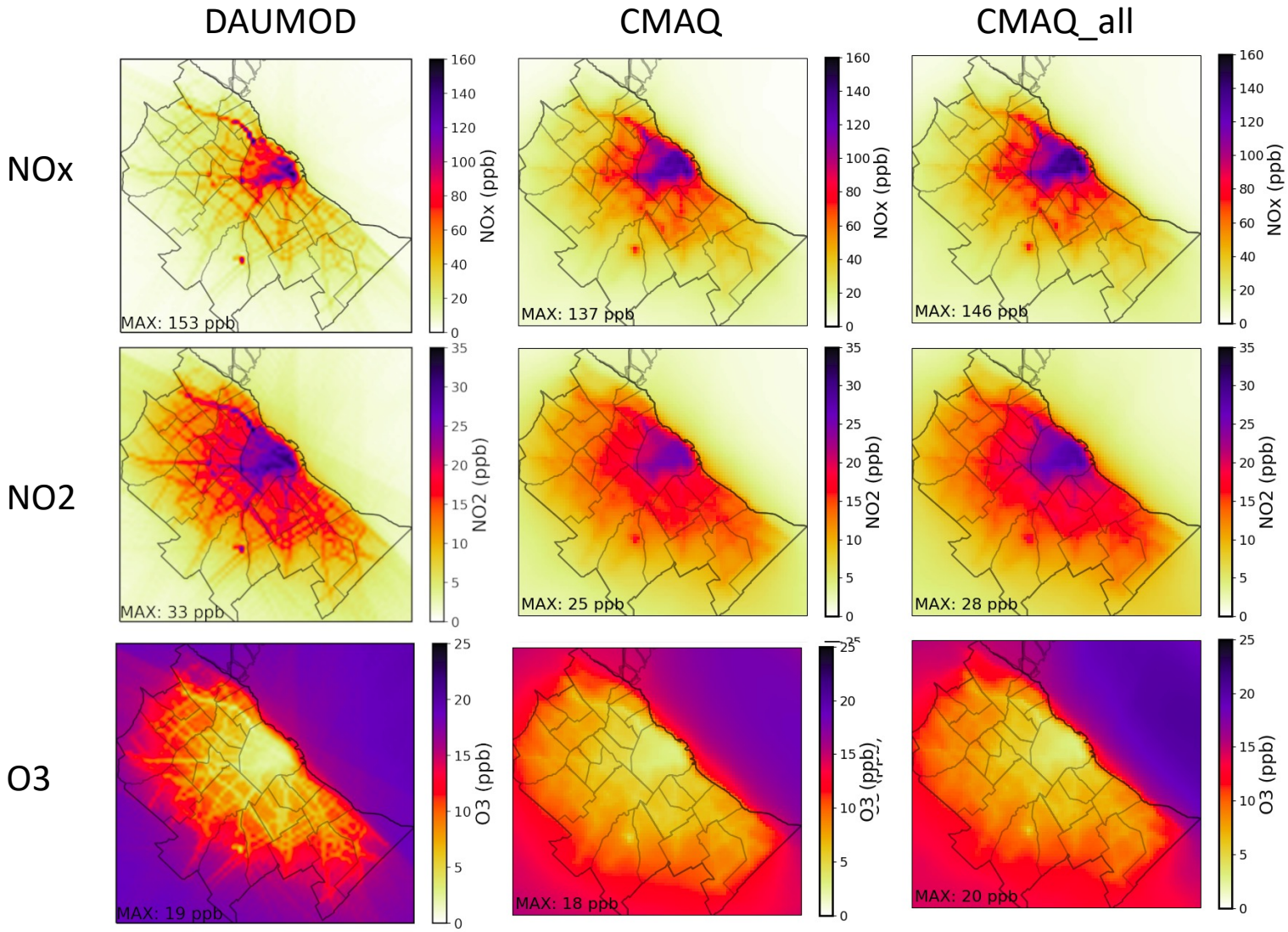


NO_2 with CMAQ_all



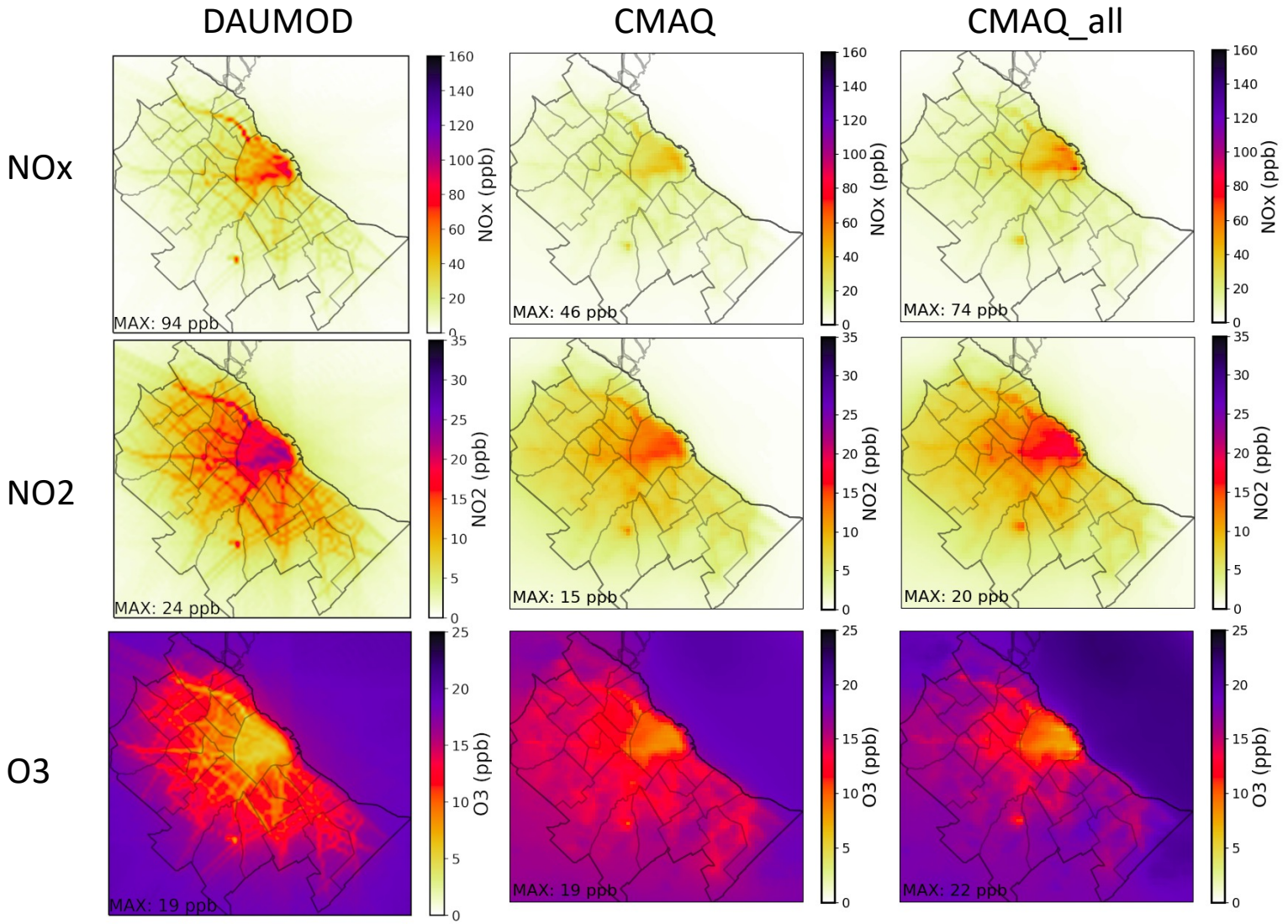
Results

WINTER



Results

SPRING



Conclusions

- Both models show acceptable and comparable performance for NO_2; best results at CEN in winter
- Large underestimations at LB and ACU under NW–N winds → likely missing industrial sources
- WRF-CMAQ: similar with 1 and 4 domains in winter; slight improvement with 4 in spring (NE winds)

Future work:

- Assess how models represent spatial variability of NO_2 using new passive tube dataset (25 sites across the city)

Thank you for your attention

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