T5: Inverse modelling, source identification and apportionment

Source apportionment analysis for NO$_2$ concentrations in Buenos Aires from high resolution CMAQ-ISAM simulations

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1. INTRODUCTION

Source Apportionment

- Key for designing effective mitigation strategies

- Several techniques

  - Emission Reduction Impact methods (*e.g. brute force*)

  - Incremental methods

  - **Mass-transfer methods → Integrated Source Apportionment Method (ISAM, CMAQ)**

1. INTRODUCTION

Source Apportionment

· Since CMAQ v5.4, several tagging options   · Tagging method affects considerably results and interpretation

ISAM option	Reactants Assigment	cb6r3 species
Option 1 (legacy)	All	All
Option 2	Nitrogen	NO, NO_2, NO_3, $HONO$, HNO_3, N_2O_5, ANO_3
Option 3	VOCS + radicals + nitrogen	NO, NO_2, NO_3, $HONO$, HNO_3, N_2O_5, ANO_3, $FORM$, $ACET$, KET, XO_2, XO_2H, ISO_2, C_2O_3, CXO_3
Option 4	VOCs + radicals	$FORM$, $ACET$, KET, XO_2, XO_2H, ISO_2, C_2O_3, CXO_3
Option 5 (default)	If NOx limited, option 2 If VOC limited, option 4	Depending on O_3 formation regimen

$H_2O_2/HNO_3 > 0.35$
$H_2O_2/HNO_3 < 0.35$

1. INTRODUCTION

NO$_2$ and Buenos Aires

- CMAQ has been recently implemented for the first time in the Metropolitan Area of Buenos Aires (MABA) showing good performance for modeling NO$_2$ concentrations

- The MABA:

- Is a densely populated urban area covering approximately 3,830 km² and hosting a population of
- around 16 million

- Is surrounded by non urban areas and the Rio de la Plata to its east

- Has three monitoring stations

CEN – Centenario (Urban Background)
LB – La Boca (Resdential/Industrial)
ACU – Acumar (Resdential/Industrial)

1. INTRODUCTION

Objective

- Use the MABA as a case study to evaluate and understand differences between two relevant ISAM tagging options (option 2 that tracks nitrogen species and option 5 that depends on the O_3 formation regimen) for NO_2 concentrations

2. METHODOLOGY

Model configuration

- WRFv4.2.1-CMAQv5.4

- 9 vertical levels in the first 1 km above the surface
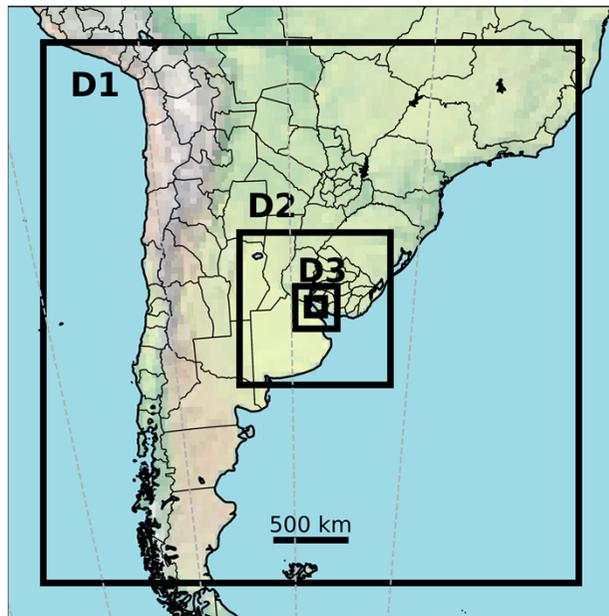
Horizontal resolution: **1 km²**

WRF Scheme	Option
Planetary Boundary Layer	BouLac
Surface Layer	Revised MM5
Land Surface	Noah
Microphysics	Thompson
Radiation	RRTMG
Urban	SLUCM
CMAQ	
Chemistry	cb6r3
Deposition	m3dry
$[O_3]_b$	20 ppb
Domain configuration	
# domains	4
Horizontal Resolutions	**1 km**, 3 km, 15 km, 45 km

2. METHODOLOGY

Period selection

- Four days selected, each with two spin up days, selected based on:

1. Good model performance at depicting total NO_2 concentrations

2. Variability in wind direction at the monitoring sites to capture emissions from different surrounding cells

3. Variability in modeled NO_2 concentrations (both above and under the observed mean) to capture different pollution conditions

- 7/19/12: Winter day with "high" concentrations and Ws ≈ 2 m/s from the NW

- 7/26/12: Winter day with "low" concentrations and Ws ∈[4, 8] m/s rotating from NW, SW to SE

- 11/20/12: Spring day "high" concentrations and Ws ∈ [0, 8] m/s rotating from SE to NE

- 11/22/12: Spring day with "low" concentrations and Ws ∈[4, 10] m/s rotating from SE to NE

2. METHODOLOGY

Emissions, tracked sectors

- Regional emissions from EDGAR HTAPv2 (Processed by Hermes) ⟶**BCO**

- Local NOx and VOCs emissions (1 km, 1 h)

    - Area sources (Aircraft, residential, commercial, small industries, **traffic**) ⟶**GR**

    - Point sources (Power plants) ⟶**PT**

- Biogenic emissions from MEGANv3.2 ⟶**BIO**

ISAM options tested

- Option 2 (Nitrogen species)

- Option 5 (Nitrogen or vocs and radicals depending on O_3 formation regimen)

3. RESULTS

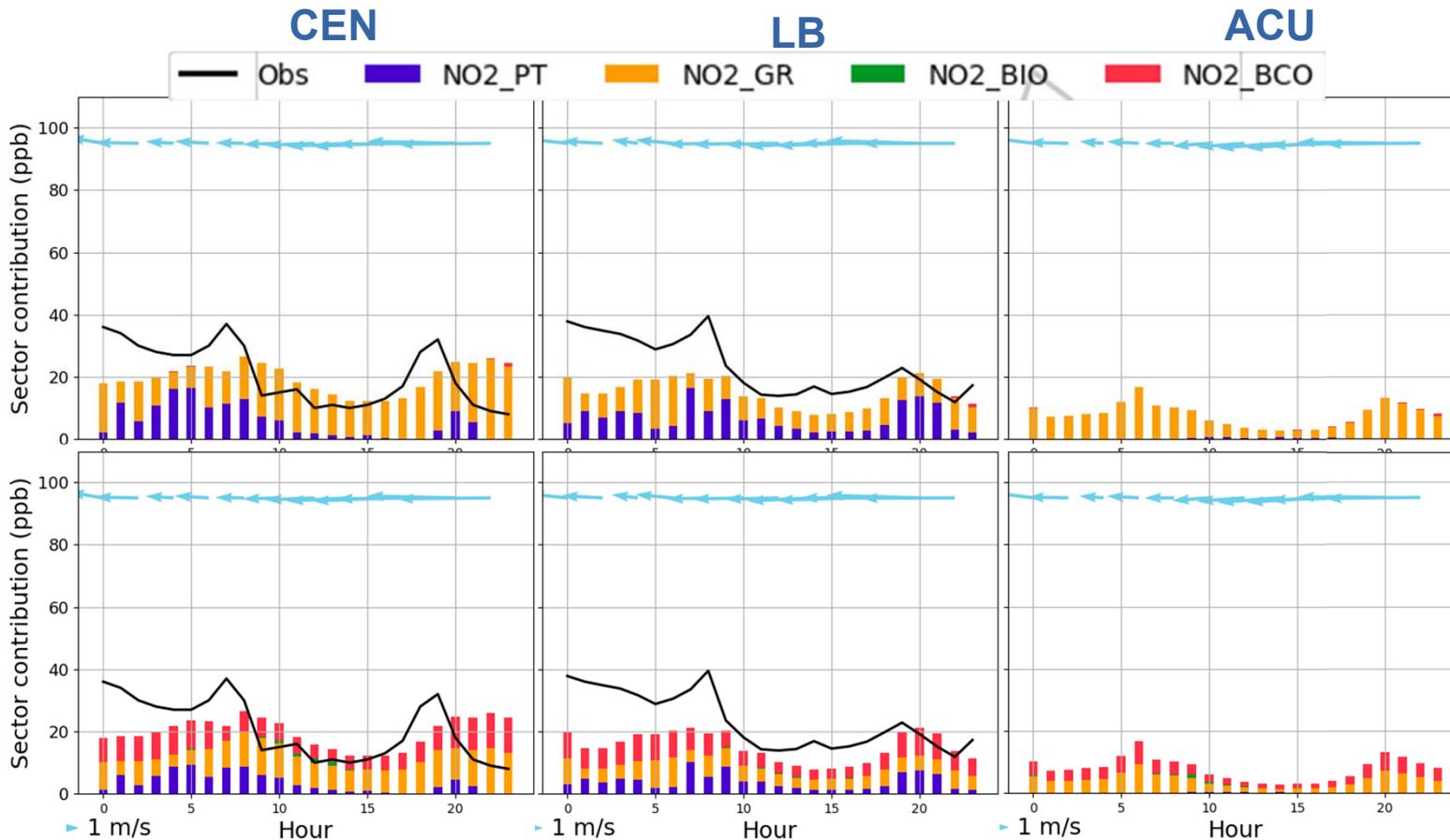## Hourly variations at monitoring sites (7/19)
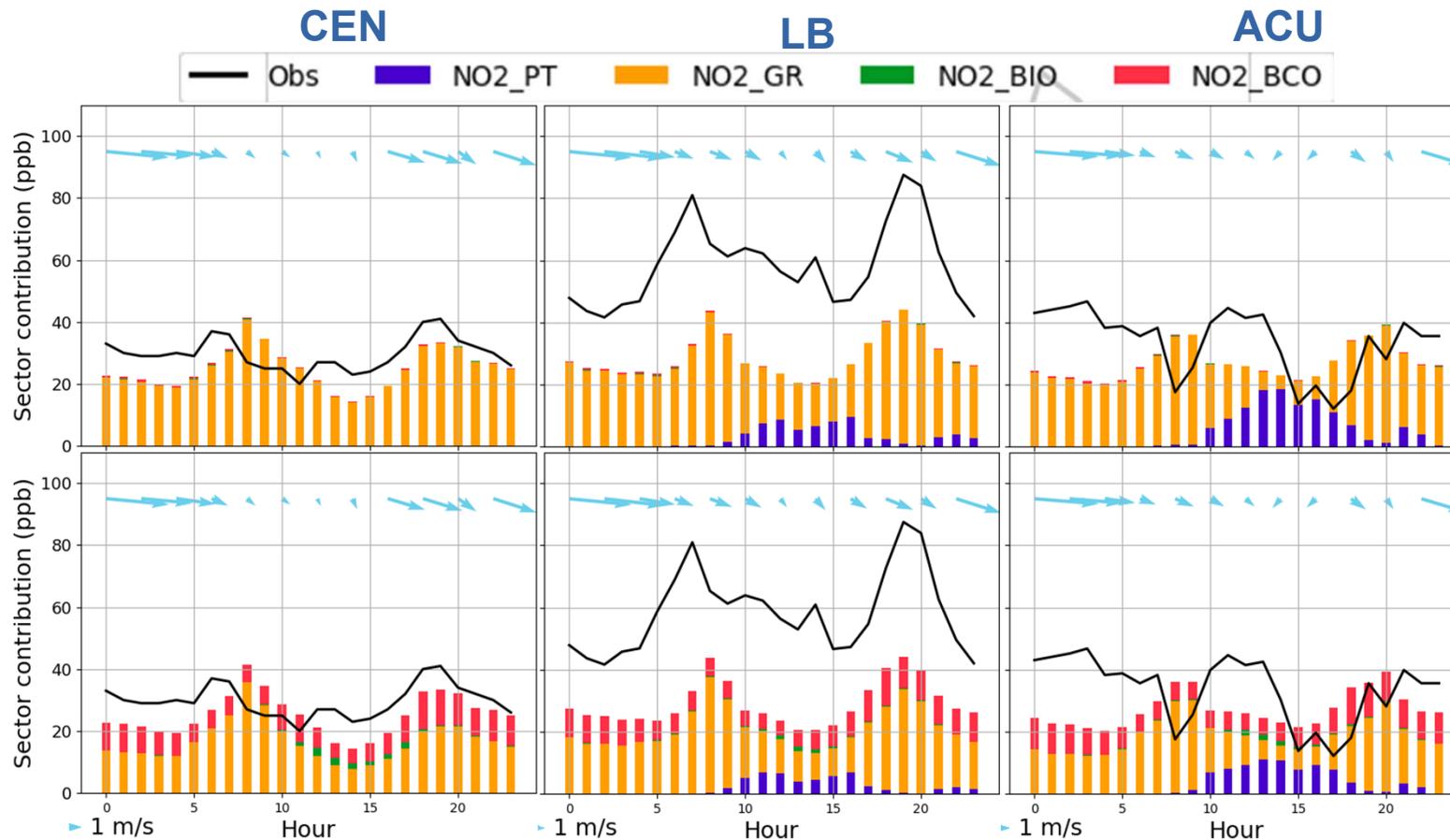
- **PT** contribution is heavily dependant of site location (Wind direction)

- **BIO** contribution is higher during hours with low traffic activity and higher temperatures

- Largest differences:

  - **BCO** (3% vs 43%)
  - **BIO** (1% vs 14%)

3. RESULTS

Hourly variations at monitoring sites (11/20)

- **PT** contribution is heavily dependant of site location (Wind direction)

- **BIO** contribution is higher during hours with low traffic activity and higher temperatures

- Largest differences:

  - **BCO** (12% vs 52%)
  - **BIO** (0% vs 13%)

3. RESULTS

Why such differences in BCO relative contributions?

- Most important reaction in urban environments for NO_2 formation: **$NO + O_3 \rightarrow NO_2 + O_2$**

1. Option 2: Weights only NO directly advected from the border or formed by species originating from the boundary

2. Option 5: Weights both NO and O_3 directly advected from the border of formed by species originating from the boundary

Highlights significant role of background O_3 in NO_2 formation

3. RESULTS

Why such differences in BIO relative contributions?

- Most important reaction in urban environments for NO_2 formation: **$NO + O_3 \rightarrow NO_2 + O_2$**

  1. Option 2: Weights only NO directly emitted from the soil

  2. Option 5: Weights both NO and O_3 directly emitted in the first case and formed through reactions involving VOCs in the second case

3. RESULTS

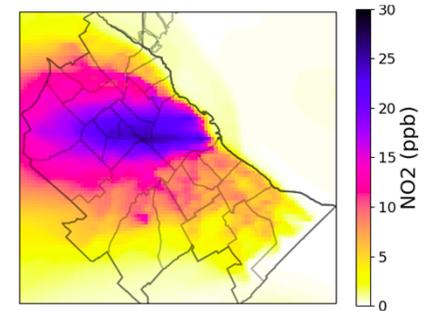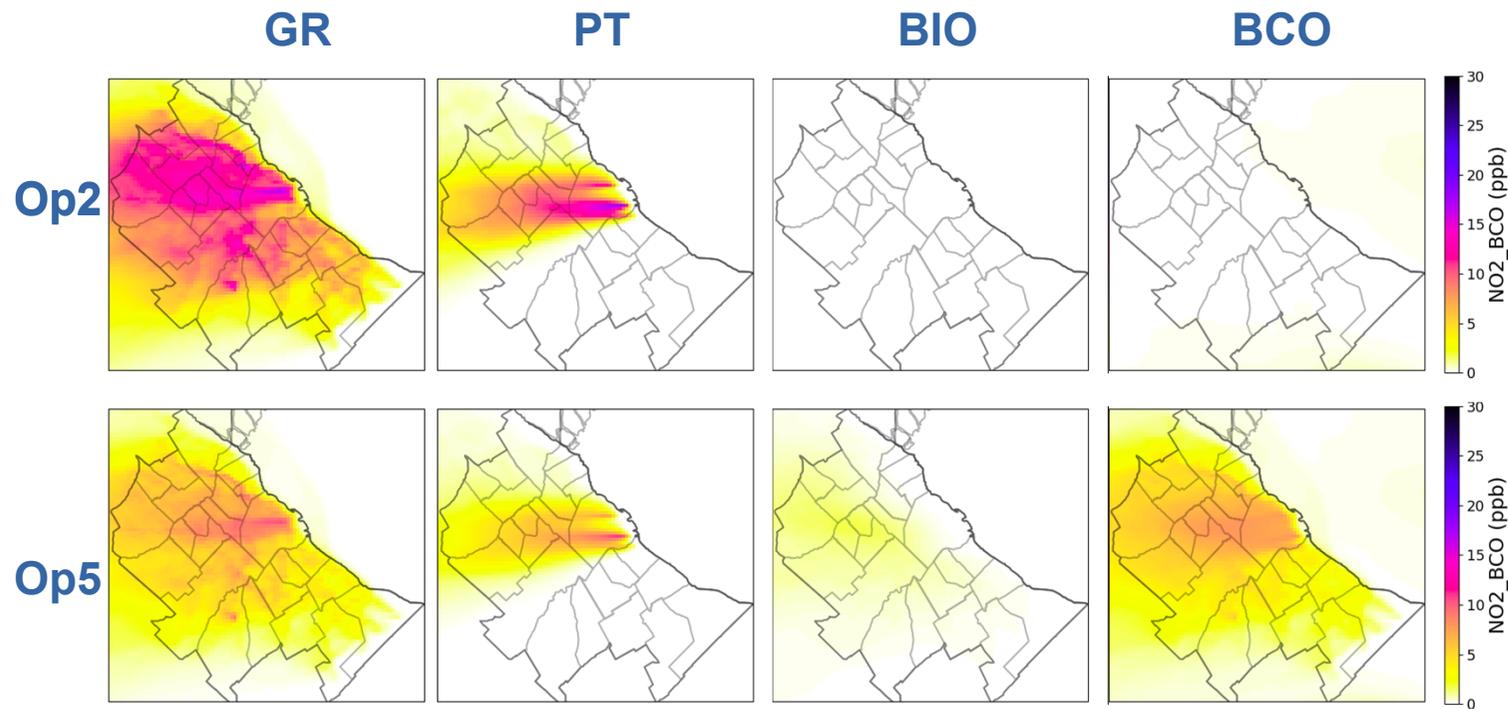## Mean daily contributions in the MABA (7/19)
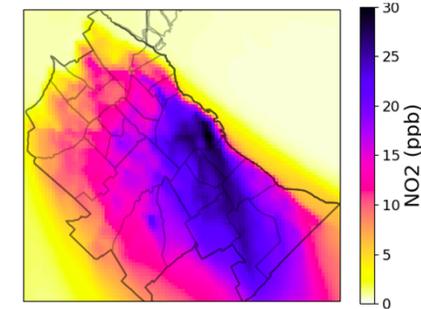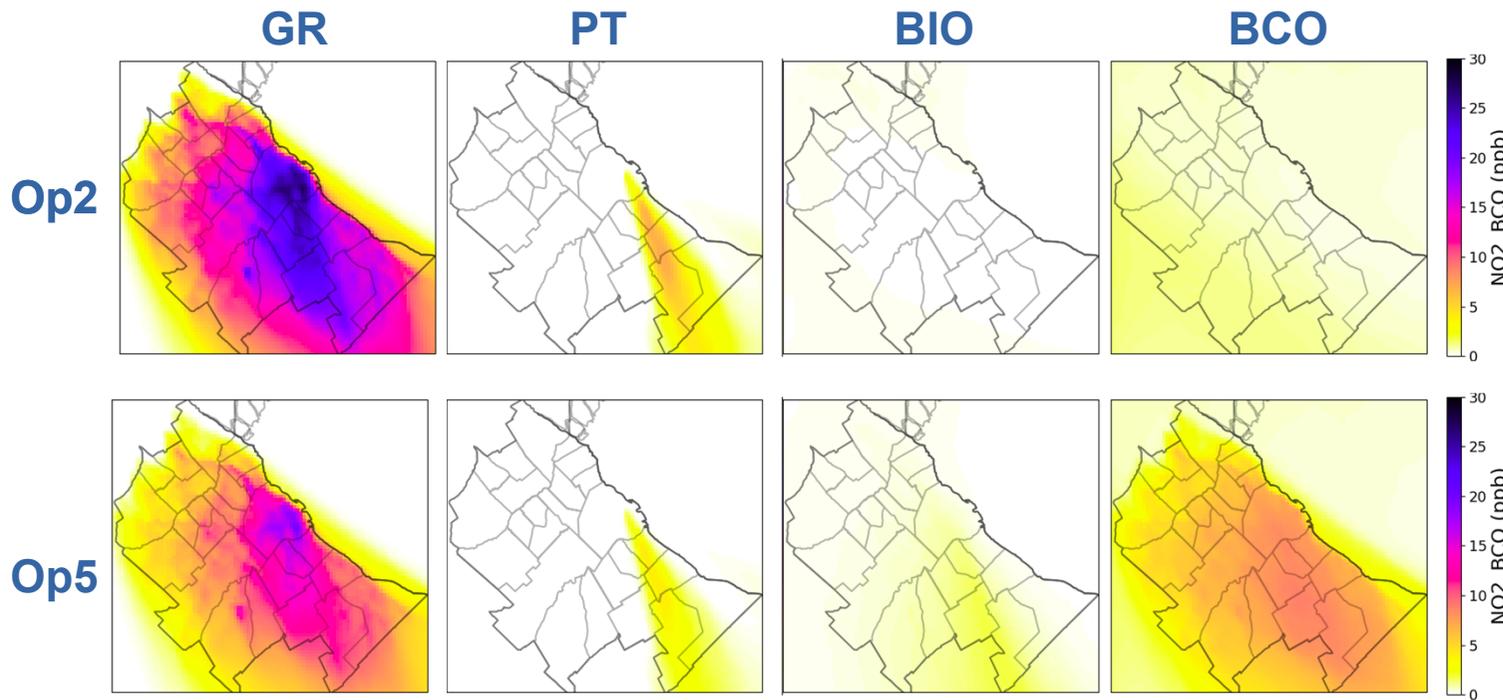
- **GR, PT** and **BIO** contributions spatial distribution follow wind predominant directions

- **GR** contributions spatial distribution highlights traffic influence

- **BCO** contribution is present in the whole MABA and is higher in the highest emissions area for option 5 where elevated NO levels promote the titration of O_3 transported from the boundaries

3. RESULTS

Mean daily contributions in the MABA (11/20)

With mosly E winds, **BIO** and **BCO** contributions in the MABA are close to 0% with option 2 as there are no NO concentrations advected from the river from these two sectors

4. CONCLUSIONS AND FURTHER WORK

- ISAM configuration has an substantial impact on source apportionment analyses

- While option 5 provides a more complete view of the origin of NO_2 concentrations, option 2 may be more informative of potential actions within controllable sources

- In the MABA, traffic emissions are the main contributors to total NO_2 concentrations

- This understanding is relevant for NO_2 concentrations, but differences between ISAM configurations behaviours are heavily dependant on the chemical reactions involved

- Selecting the appropriate configuration depends on the specie under study and the intended application and requires transparency regarding the methodological assumptions involved

- Further work includes:

  - Disaggregation of area sources

  - Analysis over longer periods of time

  - Comparison with other ISAM options