

**23rd International Conference on
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EXTENDED ABSTRACT

Source apportionment analysis for NO₂ concentrations in Buenos Aires from high resolution CMAQ-ISAM simulations

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Abstract: This study compares two Integrated Source Apportionment Method (ISAM) options within CMAQ applied to the Metropolitan Area of Buenos Aires (MABA) for NO₂ source apportionment. Option 2 attributes contributions solely to nitrogen species, while Option 5 also considers VOCs under VOC-limited O₃ production conditions. Simulations are run for four representative periods, tracking boundary (BCO), biogenic (BIO), area (GR), and point (PT) emission sectors. Results show major differences in BCO and BIO contributions: Option 2 assigns up to 12% and 1% of total average NO₂ concentrations to these sources, respectively, while Option 5 assigns up to 54% and 17%. These differences arise from how each option handles the NO + O₃ → NO₂ reaction. Option 5 attributes part of NO₂ to background O₃, emphasizing its role in ambient concentrations. The choice between options should reflect the study's objective, whether to understand total chemical influences (Option 5) or to assess local contributions (Option 2).

Keywords: *source apportionment, ISAM, urban scale, NO₂*

INTRODUCTION

Identifying and understanding air pollutant sources is a key step in designing effective mitigation strategies. Aided by air quality models, several source apportionment approaches exist, ranging in complexity from simple brute-force, where simulations with and without specific emissions are compared, to more sophisticated techniques such as mass-transfer and tagging methods. In particular, the Integrated Source Apportionment Method (ISAM), implemented in the Community Multiscale Air Quality (CMAQ) model (Byun et al., 1999; Byun et al., 2006), enables the tagging and tracking of emissions from a specific source types or region, and has been widely applied at the urban scale (e.g., Kitawa et al., 2021; Xian et al., 2024; de la Paz et al., 2024). However, differences between ISAM tagging configurations, which can significantly influence apportionment results and their interpretation, are scarcely studied.

The main objective of this work is to evaluate and understand the differences between two relevant ISAM tagging options for nitrogen dioxide (NO₂) concentrations, using the Metropolitan Area of Buenos Aires (MABA), a densely populated urban area, as a case study.

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METHODOLOGY

The WRFv4.2.1-CMAQv5.4 configuration, based on sensitivity studies performed by Luque et al., (2024a) and (2024b), is described in Table I with the innermost domain covering the whole MABA.

WRF scheme	Option
<i>Planetary boundary layer</i>	BouLac
<i>Surface layer</i>	Revised MM5
<i>Land surface</i>	Noah
<i>Microphysics</i>	Thompson
<i>Radiation</i>	RRTMG
<i>Urban</i>	SLUCM
CMAQ	
<i>Chemistry</i>	cb6r3
<i>Deposition</i>	m3dry
Domain configuration	
<i># domains</i>	4
<i>Horizontal resolutions</i>	1 km, 3 km, 15 km, 45 km

Table I: Model configuration

The EDGAR HTAPv2 inventory (Janssens-Maenhout et al., 2015) is used for the coarser domains (D1–D3), while a high-resolution local inventory (1 km, 1 h) developed by Venegas et al. (2011), which includes emissions from aircraft, residential, commercial, small industrial sources, and traffic, is applied for the MABA. In addition, a point source emissions dataset representing power plants along the coast, based on the JICA (2012) report, is incorporated. Biogenic emissions are calculated inline by CMAQ using MEGANv3.2 (Guenther et al., 2012).

Since CMAQ version 5.4, ISAM provides five tagging options, which differ in how reactant species are weighted in each chemical reaction. The default option is option 5, which attributes ambient concentrations to nitrogen-containing reactants (NO, NO₂, NO₃, HONO, HNO₃, N₂O₅ and ANO₃ for the cb6r3 chemistry mechanism used in this work) or VOCs and radicals (ALD₂, ALDX, FORM, ACET, KET, XO₂, XO₂H, ISO₂, C₂O₃, CXO₃), depending on the ozone (O₃) formation regime (NO_x-limited or VOC-limited, respectively). Option 2 which only considers nitrogen species in the weighting, can also be used for tracking NO₂ source contributions. In both cases, when neither nitrogen species or VOCs and radicals are involved, all available reactants are weighted according to stoichiometry.

In this study, source apportionment for NO₂ concentrations according to these two tagging options is compared at the available monitoring sites in the MABA: Parque Centenario (CEN, urban background), La Boca (LB, residential/industrial), and Acumar (ACU, residential/industrial). This is done during four representative days selected based on two criteria: (1) good model performance at depicting total NO₂ concentration and (2) variability in wind directions and pollutant concentrations both above and below the observed mean, in order to capture different meteorological and pollution conditions. Each simulation includes a two-day spin-up period. Two of the selected

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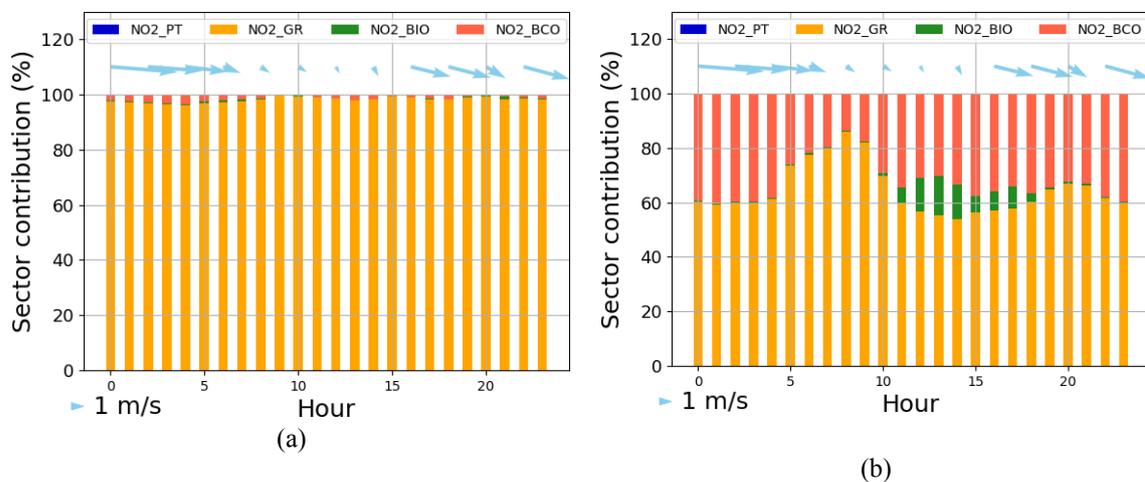
days correspond to winter (July 19 and 26), and two to spring (November 20 and 22) of the year 2012. The sectors tracked are boundary (BCO), biogenic (BIO), area (GR), and point (PT) emissions. It should be noted that area emissions are not disaggregated, but correspond mostly to traffic-related sources, while point emissions correspond exclusively to power plants.

RESULTS

Figure 1 shows the hourly relative contributions of BCO, BIO, GR and PT sectors to total NO₂ concentrations at CEN during 7/19 and 11/20 along with wind vectors displayed at the top of each figure. A marked difference in behaviour is observed at this site between the two days: the contribution of point sources on 19/7 is negligible, whereas on 11/20 they account for up to 74% (under ISAM option 2) and 40% (under ISAM option 5) of the total NO₂ average hourly concentration. This contrast is most likely driven by differences in wind patterns: on the 7/19 winds are from the NW, while on 11/20 wind consistently blows from the E where power plants are located (Pineda Rojas et al., 2020).

The largest differences between ISAM options are observed in the BCO contributions. Across all sites and days, BCO contributions range from 0% to 12% with option 2 and from 14% to 54% with option 5. In order to understand this, it is important to consider the most important reaction for NO₂ formation: $\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2$. When assigning BCO contributions, option 2 weights only the NO that is either advected from the border or formed by species originating from the boundary. In contrast, option 5 weights both NO and O₃, resulting in a greater BCO contribution. This highlights the significant role of background O₃ in NO₂ formation.

Likely for similar reasons, another difference between ISAM options is observed in BIO contributions. With option 2, which considers only soil NO emissions, BIO contributions reach at most 1% of total NO₂ concentrations. In contrast, option 5 can attribute up to 17% of total concentrations to the BIO sector, as it also accounts for the O₃ formed through reactions involving biogenic VOCs emissions. Its largest relative contribution is during hours of low traffic activity and higher temperatures.



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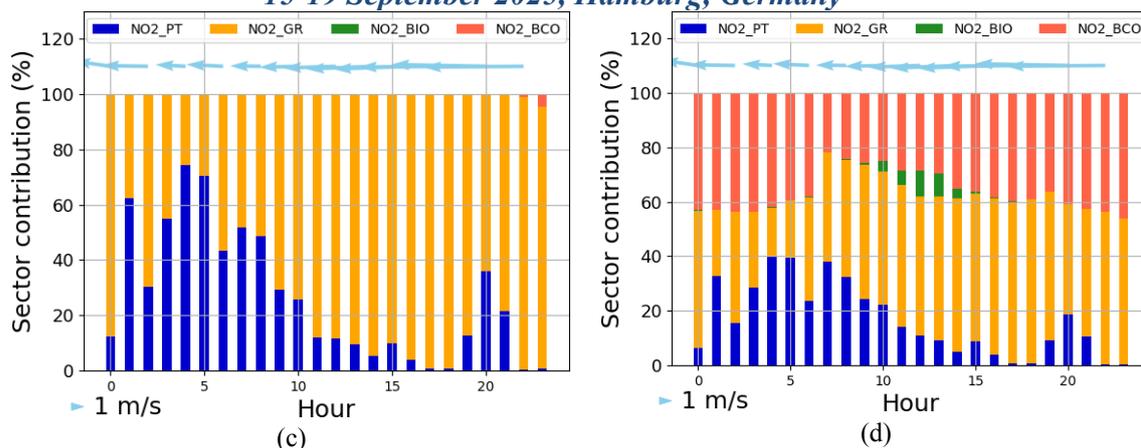


Figure 1: Sectors relative contributions to NO_2 concentrations at CEN under option 2 (left column) and option 5 (right column) for (a, b) the 7/19 and (c, d) 11/20

CONCLUSIONS

Results highlight the substantial impact that the choice of ISAM configuration can have on source apportionment analyses. While option 5, CMAQ default, captures a wider range of chemical pathways, including those involving O_3 and VOCs, it tends to allocate a larger proportion of NO_2 to less actionable sources like boundary and biogenic emissions. In contrast, option 2, which emphasizes nitrogen contributions, may lead to a stronger attribution to locally emitted sources. While option 5 provides a more complete view of the origin of pollutants, option 2 may be more informative of potential actions within controllable sources. Therefore, selecting the appropriate configuration depends on the intended application and requires transparency regarding the methodological assumptions involved.

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