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EXTENDED ABSTRACT

A hybrid modelling system for high-resolution urban air quality assessment with integrated source apportionment

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Introduction

Accurate assessment of air quality is essential for managing pollution exposure and protecting public health, particularly in cities with complex emission sources and concentration patterns. This work proposes a modelling approach designed to estimate urban air quality at building-scale resolution, enabling the identification of localized hotspots of elevated pollutant concentrations. To assess the contributions of all emission sources affecting the urban air quality with both high temporal (hourly) and spatial (a few meters) resolutions on a target domain, a Hybrid Modelling System (HMS) is proposed.

The HMS couples a Eulerian Chemical Transport Model (CTM) with a high-resolution Lagrangian Particle Dispersion Model (LPDM), which can explicitly resolve the effect of buildings on pollutant dispersion. Its design conceptually relies on the hypothesis that, due to its typical spatial resolution of the order of a kilometer, the CTM can represent the city's background concentration accounting for regional and local sources, while the LPDM can accurately capture traffic-induced street-level increments that cause concentration hotspots. Accordingly, the HMS performs two independent simulations with an hourly timestep, each using one of the two models. Each model operates at its typical resolution: the CTM covers a broader area, typically at least 30×30 km^2 with kilometer-scale resolution, while the LPDM focuses on the target domain with meter-scale resolution. To maintain consistency, both models use the same meteorological and topographic inputs, and the CTM incorporates the same traffic emission data as the LPDM, along with other regional sources. The results are then combined over the high-resolution domain to sum background and street-level contributions, using a coupling procedure that prevents double counting of emissions.

A first version of the HMS was developed and validated in Barbero (2021), coupling the CTM FARM (Flexible Air quality Regional Model, Silibello et al., 2008) with the high-resolution modelling suite PMSS (Parallel Micro Swift Spray, Oldrini et al., 2017). In this version, the background concentration was estimated by FARM through a simulation including all sources within the urban domain except local traffic, handled by PMSS. Hourly total concentrations were obtained on the target grid by summing the background concentrations with the street increment modelled by PMSS in a simulation specifically focused on traffic emissions. This approach inherently avoids double counting of emissions and produced promising results, providing essential information about traffic hotspots. However, the chemical equilibrium among all sources is altered in the FARM simulation due to the exclusion of local traffic sources, and the contribution of secondary pollution from traffic-related chemical reactions is neglected.

This work introduces a new HMS configuration, hereafter the "advanced HMS", built on the same hypotheses and models but designed to overcome these two limitations. Its key innovation is the integration of an On-line Reactive Source Apportionment (ORSA) algorithm in FARM (Calori et al., 2024), which allows direct identification of both primary and secondary pollution contributions from traffic sources during the simulation. The following paragraph details the use of the ORSA algorithm within the HMS and its associated coupling procedure. This new configuration is then compared with the first HMS setup and validated through a dedicated test case, which is subsequently presented along with a discussion of the main results.

Hybrid Modelling System with On-line Reactive Source Apportionment

The ORSA algorithm in FARM was developed to simultaneously track the contributions to pollutant concentrations from different groups of emission sources, as well as from initial and boundary conditions, throughout the simulation. In ORSA, each tagged group of sources is defined by a dedicated emission input representing a subset of the total emissions and pollutants from each group are tracked using a set of reactive tracers.

In the HMS, FARM ORSA is applied in a simulation that includes all sources affecting urban air quality, in order to track the traffic sources also represented in the PMSS simulation and to quantify their primary and secondary contributions. Therefore, the background concentration is directly computed from all sources not tagged as PMSS traffic sources., i.e., remaining emissions, boundary and initial conditions. Subsequently, the total concentration on the target grid is obtained, as in the first HMS configuration, by summing on an hourly basis the background concentration and the street increment modelled by PMSS. Moreover, for species that undergo secondary formation, such as PM10, the background concentration includes an additional term quantifying the secondary pollution attributable to PMSS traffic sources. An additional note concerns the computation of NO_2 in the HMS. Since PMSS simulates only non-reactive primary pollutants, NO_2 values are derived from NO_x concentrations directly calculated by the model using a nonlinear polynomial relationship. The coefficients are calibrated for each application with FARM NO_x/NO_2 data and validated against measurements, to ensure chemical consistency with FARM. This advanced configuration of the HMS still inherently avoids double-counting of emissions; moreover, by using this algorithm, it prevents any alteration that could result from removing a group of sources in a simulation, and it also allows the secondary pollution contribution to be estimated when needed.

Test case

The test case used to evaluate the HMS focuses on an 8×8 km^2 target domain with a horizontal resolution of 5 m, centered on the city of Milan. The study specifically addresses NO_2 and PM10, two of the most critical pollutants in urban environments. The selected study period spans from June 27 to July 5, 2017, chosen based on the availability of data related to emissions, meteorology, and air quality measurements. FARM was applied over a broader 35x35 km^2 domain with a horizontal resolution of 500 m including the whole Milan metropolitan area, while PMSS operated on the target domain.

Meteorological data and initial and boundary conditions for FARM were provided by the air quality forecasting system QualeAria (Kukkonen et al., 2012). Both models in HMS utilize topographic data from the EU-DEM (Digital Elevation Model over Europe) and land use data from the Corine Land Cover 2012 (CLC-2012) dataset.

Traffic emissions within the municipality of Milan were derived from traffic data provided by the AMAT agency (Agency for Mobility, Environment, and Territory). PM emissions include both exhaust and non-exhaust sources, accounting for mechanical abrasion and resuspension. The estimation of regional emissions was based on the INEMAR (INventario EMissioni ARia) emissions inventory, referring to 2014 data.

To validate the results given by the HMS, data from the monitoring network managed by the ARPA Lombardia Regional Environmental Protection Agency were used. **Table 1** shows both the stations' positions and the classifications, according to the prevalent local emissions (Traffic – Background).

Table 1 *- Monitoring system stations inside Milan PMSS domain*

Station	*Position [UTM32]*	*Classification*	*Location*
Liguria	513134 5032273	Urban traffic	Near four-lane road, traffic light
Marche	514918 5038105	Urban traffic	Near four-lane road
Pascal	518405 5036190	Urban background	Near single-lane road
Senato	515435 5035238	Urban traffic	Near junction of three single-lane roads
Verziere	515270 5034443	Urban traffic	Near double-line road

Results

To assess the differences between the first and advanced HMS configurations, total concentrations from both were compared. Because the PMSS street increment is identical in both setups, any observed differences highlight the variations in the background concentration calculated by each configuration. **Figure 1** displays the differences in NO_2 and PM10 concentrations, averaged over the simulation period, between the advanced HMS and the first HMS configuration within the FARM domain. The figures indicate that both NO_2 and PM10 were underestimated with the first HMS configuration. The absolute differences are greater for NO_2, reaching a maximum of 4 $\mu g/m^3$, while those for PM10 remain minimal, with a maximum of only 0.20 $\mu g/m^3$. This pattern extends to relative differences as well: daily percentage changes for NO_2 reach up to 40% at specific points within the domain, whereas PM10 varies between -3% and +2%. The analysis of the figures shows that NO_2 concentration patterns differ noticeably from PM10. The largest differences for NO_2 appear within the PMSS domain, near traffic sources, which were absent from the FARM simulation in the first HMS. Smaller differences are also observed along the city plume generated by traffic emissions. Being highly reactive, NO_2 forms rapidly near its sources, which explains its sharper spatial gradients within the city and why its chemical equilibrium is more strongly influenced by PMSS traffic sources.

In contrast, differences in PM10 concentrations are smaller within the target domain, though more noticeable along the city plume, reflecting its lower reactivity, with chemical transformations occurring more gradually over time and space.

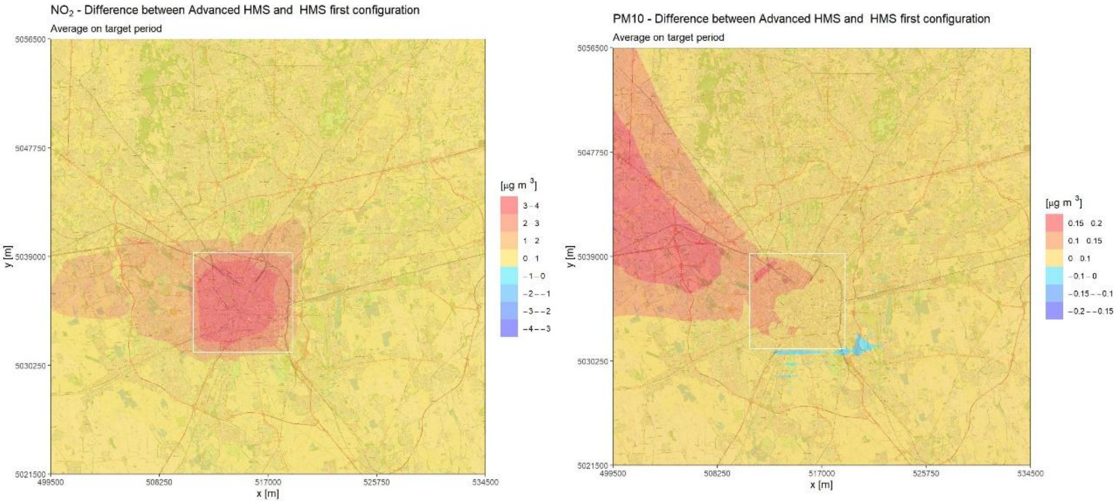

***Figure 1** - NO₂ and PM10 maps of the difference between concentration maps averaged on the simulation period resulting from advanced HMS and first HMS configuration. The maps are focused on the 35x35 km² domain, the PMSS target domain is shown in white.*

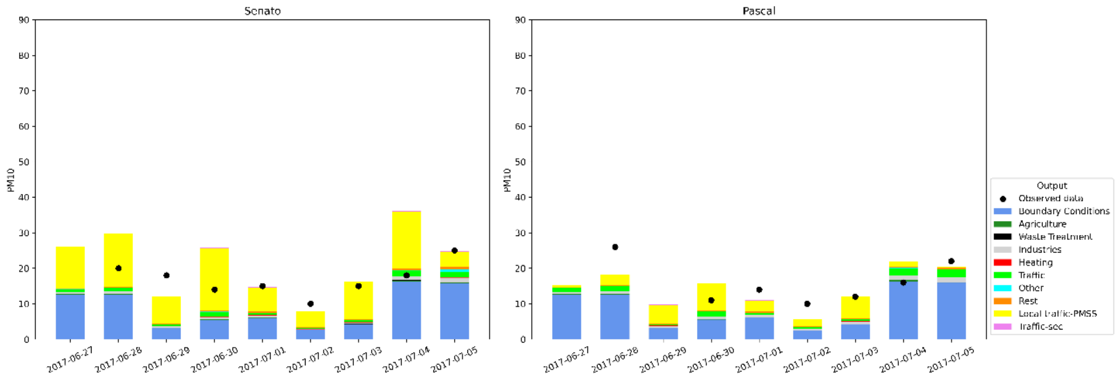

***Figure 2** – Comparison between observed (black dots) and modelled HMS daily PM10 concentrations at monitoring stations. The figure also reports the contribution of different groups of sources tagged by FARM ORSA in HMS.*

Subsequently, the advanced HMS was validated against observational data. **Figure 2** presents, as an example, the time series of daily averaged PM10 concentrations, computed with the advanced HMS at representative stations, alongside corresponding measurements. The comparison is shown for Senato (urban traffic) and Pascal (urban background). These figures illustrate not only the contribution of traffic sources simulated with PMSS (Traffic – PMSS) but also those from different tagged source groups provided by the FARM simulation, as well as the secondary pollution from these traffic sources (Traffic – sec). The purpose is to exemplify the type of additional insights that the advanced HMS can offer, enabling the estimation of the impact of various source categories on urban air quality. It can be noted that the contribution to PM10 from secondary pollution due to traffic sources is small, indicating that the underestimation present in the first HMS was not significantly high. Overall, the advanced HMS confirms its ability to reproduce the spatial concentration gradients typical of cities, mainly due to the varying contributions from PMSS-simulated traffic sources across stations. While a longer simulation period would be required for a more robust assessment of HMS performance, **Table 2** presents the statistical evaluation of the advanced HMS. The results indicate that the model meets the urban air quality model performance criteria (Hanna and Chang, 2012), although both pollutants were slightly overestimated in this one-week simulation.

Table 2 *– Statistical evaluation of advanced HMS performance for hourly NO_2 and daily PM10 concentration values.*

	n. data	Mean obs	Mean HMS	SD obs	SD HMS	IA	FAC2	FB
NO_2	960	37.21	43.40	21.01	28.15	0.40	0.56	0.15
PM10	23	16.52	18.72	4.41	8.53	0.65	0.96	0.12

Conclusion

In conclusion, the advanced HMS demonstrates good accuracy in urban environments, effectively capturing spatial variability. Compared to the previous configuration, the integration of the source apportionment algorithm enhances background concentration estimates by maintaining chemical balance among pollutants and enables the quantification of contributions from different source groups and secondary pollution from traffic, offering more detailed insights to users.

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