22nd International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
10-14 June 2024, Pärnu, Estonia

APPLICATION OF AIR QUALITY MODELS IN THE PO VALLEY. RESULTS FROM THE PREPAIR PROJECT

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Abstract: EU legislation on air quality (AQ) requires a comprehensive and consistent assessment, including pressure factors and status indicators, through complementary and synergistic use of measurements, emission inventories and chemical transport models (CTMs). Furthermore, CTMs must rely on emission inventories with adequate spatial and temporal resolution to provide a comprehensive estimate of pollutant concentrations in the atmosphere. The Integrated LIFE PREPAIR project "Po Regions Engaged to Policies of Air" (https://www.lifeprepair.eu), started in 2017 and now nearing completion, has developed various tools to enhance AQ estimation and management in the Po Valley. In this work the results of the application of different CTMs in the project domain (Po Valley and Slovenia) will be presented. Over the years, three updates to the emissions dataset have been carried out, combining the top-down estimation methods described in the EEA/EMEP Guidebook with the local-scale bottom-up inventories. These emissions datasets were the basis for the modelling simulations. Five different CTMs were used to evaluate the annual state of air quality in the years 2020, 2021 and 2022. For each year, the statistical indicators specified by the European AQ Directive were calculated and combined following an ensemble approach. Various data fusion techniques were applied to the raw results of the models to improve indicator estimation. The performance of each CTM and data fusion method was evaluated using cross-validation techniques. Some of these models are used to provide daily forecasts and analysis. These outputs are shared through a dedicated platform for the analysis of scenarios of interest to the administrative bodies involved in PREPAIR.

Key words: *Air quality assessment, CTM, Emission inventories, Po Valley, Italy*

INTRODUCTION

Air pollution represents one of the main environmental factors that affect the health of European citizens, as most of the population is exposed to concentration levels of pollutants exceeding the limits that community legislation considers for the protection of human health. The Po basin, despite the significant improvements recorded in recent years, represents one of the most critical European areas, particularly in relation to pollution from particulate matter, nitrogen dioxide and ozone. The LIFE Prepair project fits into this context, involving all the regions of the Po basin and neighboring Slovenia with the aim of facilitating the adoption of shared reduction measures through the implementation of the respective regional air quality plans. Previous experiences demonstrate that in this area coordinated and large-scale actions on different sources of pollutants are necessary to further reduce pollution levels and achieve compliance with the limit values established by current legislation. In support of the institutional activity of the Regions and ARPAs

(Environmental Protection Agencies) within the Prepair project, the aim was to provide an important contribution to the knowledge of the state of air quality in the Po basin and in Slovenia with the publication of annual reports. Starting from the year 2020, three reports (Bande et al., 2021, Bande et al., 2022, Bande et al., 2023) provide a synthetic vision of air quality on a basin scale. In fact, European legislation requires that every year an assessment be carried out of the concentration in the air of regulated pollutants and of the population exposed to levels that do not comply with the legislation itself. The significant contribution of the project is represented by the use of the observed data provided by all the partners with a high level of validation and by the application of five modeling chains with different characteristics, to provide an overall vision of a territory that shares problems, and therefore common solutions.

MATERIALS AND METHODS

An evaluation of the annual air quality for the years 2020, 2021 and 2022 was conducted using five distinct air quality (AQ) modeling systems. These systems, namely NINFA-ER, PieAMS (Giorcelli et al.,2013), SMAL-LO, SPIAIR and CAMX-SLO, are employed by regional agencies involved in the PREPAIR project. They utilize three unique chemical transport models (CTMs): CHIMERE, FARM (Gariazzo et al,.2007), and CAMx to analyze the dynamics of gases and particulates in the atmosphere. Despite sharing the same Prepair emissions inventory, these AQ modeling systems exhibit differences in gas-phase and aerosol chemical mechanisms, domain size and location, meteorological input, parameterization, as well as spatialization and emission speciation/disaggregation.

EMISSION INVENTORY

The LIFE PREPAIR project enabled the creation of a unified database of air pollutant emissions in the Po basin and Slovenia (Marongiu et al., 2022). The emissions were calculated following the EEA-EMEP Guidebook methodology mainly with the INEMAR system (INEMAR ARPA Lombardia, 2023) and were compared among the various regions and autonomous provinces. Considering the reference year 2017, the analysis of the database showed that the main sources of primary emissions of PM_{10}, CO and NO_x are non-industrial plants (e.g. heating) and road traffic, while the agricultural sector (especially livestock and mineral fertilizers) is the major source of NH_3. The emissions of SO_2 are due to the sulfur content in the fuels used in the industries.

The emissions were divided into point and diffuse sources. For diffuse sources, the vertical allocation was different depending on the system used: SPIAR assigned the emissions to the first layer of the model (between the ground and 20 m), while NINFA-ER, SMAL-LO and PieAMS used specific vertical profiles for the SNAP emission sectors or activities. Also, the temporal and spatial models for distributing the annual emissions in hours were different for each AQ modelling system.

The emissions from natural (biogenic) sources and fires were included in the PREPAIR database but not in this study. The emissions of biogenic VOCs were estimated with the MEGAN model in all systems, while fires were excluded because the data were not extendable to different years.

CHEMICAL TRANSPORT MODELS

The specific differences for each CTM are detailed in table 1. The chemical transport models employ different gas-phase chemical mechanisms:

- MELCHIOR2 (CHIMERE): used for regional tropospheric chemistry modeling. It accurately simulates concentrations of ozone, carbon monoxide, nitrogen oxides, and other organic and inorganic compounds under various atmospheric conditions. It encompasses 120 chemical reactions involving over 40 gaseous species.
- SAPRC-99 (FARM) (Carter, 2000): used for reactions of volatile organic compounds (VOCs) and nitrogen oxides (NO_x). These reactions result in the formation of ozone and secondary organic aerosols in the lower troposphere. It includes 215 chemical reactions involving more than 140 species.
- CB05 Mechanism (CAMx): used for atmospheric chemistry modeling and pollutant formation. It describes 156 chemical reactions involving 51 species and explicitly incorporates the treatment of methyl peroxy radicals for simulating hydrogen peroxide under low NO_x conditions.

Different modeling systems use different aerosol models to describe how aerosols are distributed by size. NINFA-ER splits the aerosol into 10 size bins, from 10 nm to 40 µm in diameter. PieAMS and SMAL-LO use the AERO3 (Binkowsky, 1999) module, which has three size modes for aerosols: Aitken, accumulation and coarse. $PM_{2.5}$ is the sum of the Aitken and accumulation modes, while PM_{10} is the sum of all three modes. The aerosol module, used by SPIAIR, has two size modes for aerosols: fine ($PM_{2.5}$) and coarse. Fine aerosols include all secondary aerosols and some primary aerosols, while coarse aerosols, the difference between PM_{10} and $PM_{2.5}$, include only primary aerosols.

Table 1. Chemical transport modelling systems

Name	CTM	meteorological driver	chemical boundary conditions	data fusion method	domain	available period
NINFA-ER (Arpa Emilia Romagna)	Chimere 2017 r4v1	COSMO-5M	kAIROS	kriging with external drift	Po Valley and Slovenia	2020-2023
SPIAIR (Arpa Veneto)	CAMx v6.5	COSMO-5M	kAIROS	multiple linear regression & interpolation of residuals	Po Valley	2022-2023
PieAMS (Arpa Piemonte)	FARM v4.13	COSMO-5M	Prev'Air / FORAIR	kriging with external drift	Po Valley	2020-2023
SMAL-LO (Arpa Lombardia)	FARM v4.13	WRF-ARW	QualeAria	SCM/optimal interpolation	Po Valley and Slovenia	2020-2023
CAMx-SLO (ARSO Slovenia)	CAMx v6.2	Aladin	MACC renalysis	kriging with external drift	Po Valley and Slovenia	2021-2023

COSMO-5M is a limited area atmospheric model for the Mediterranean region that provides weather forecasts and thus the inputs for NINFA-ER, PieAMS and SPIAIR. COSMO-5M is managed by ARPA-SIMC Emilia-Romagna in collaboration with CNMCA of the Italian Air Force and the National Civil Protection. COSMO-5M has a horizontal resolution of 5 km and a vertical structure of 45 levels, covering the national territory and part of Europe and Africa. COSMO-5M runs twice a day, at 00.00 and 12.00, providing forecasts up to 72 hours, based on the analysis of observational data and the boundary conditions of the global model IFS of ECMWF. COSMO-5M also performs a continuous assimilation phase with deviation technique, to have a continuous analysis dataset. SMAL-LO model uses the Weather Research and Forecasting (WRF) model as meteorological input, which has a horizontal resolution of 4 km. WRF is an atmospheric model that simulates the behavior of the atmosphere based on the initial conditions and the observed data. WRF is re-initialized every day with 12 hours of spin-up and the boundary conditions are taken from the global model GFS.

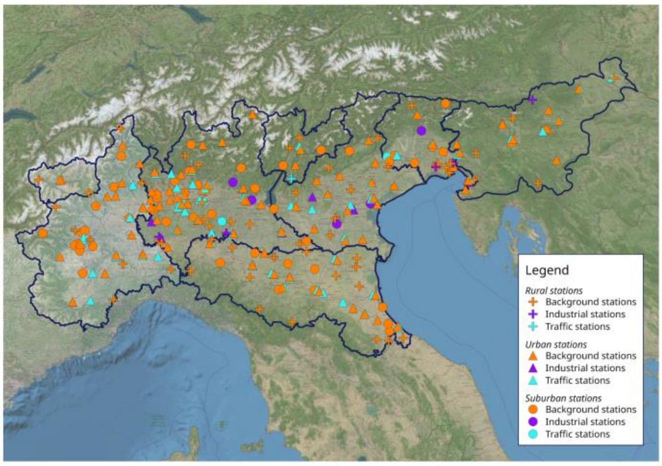

Figure 1. Spatial distribution of monitoring stations available in observation dataset.

AIR QUALITY OBSERVED DATA

The observational database (Figure 1) used in data fusion procedures was built with the support of PREPAIR partners providing revised validated data. This dataset is composed of pollutant concentrations measured by monitoring stations, divided following both zone type classification (e.g. urban, sub-urban and rural categories) and station type classification (e.g. background, industrial, and traffic). The dataset contains hourly measurements of nitrogen dioxide (NO_2) and ozone (O_3), hourly and daily measurements of particulate matter PM_{10} and $PM_{2.5}$. The database used in data fusion procedures has been chosen based on the following main criteria:

- only background stations (urban, suburban or rural) have been chosen;
- only stations with data capture percentage of 75% or higher have been selected.

DATA FUSION

Data fusion is considered one of the techniques of data assimilation (Lahoz et al. 2014) where we combine the results of numerical models and the point measurements (Schneider et al, 2015). There are various known statistical and geo-statistical approaches to the data fusion (Berrocal et al, 2012). NINFA-ER, PieAMS and CAMx-SLO use Kriging with External Drift (Wackernagel 2003, Cressie 1993) as a data fusion technique, with slight differences in the algorithm implementation. All three systems use CTM concentration fields and terrain height as external drift. SMAL-LO adopted the Optimal Interpolation (Kalnay, 2003) approach for the data fusion process in the 2022 assessment and the Successive Correction Method (Bratseth, 1986) in 2020 and 2021. Finally, SPIAIR uses a two-step procedure (Horalek et al, 2007) involving first a linear regression with observations as dependent variable and CTM output and terrain elevation as independent variables and then an IDW (inverse distance weight) algorithm interpolation of the regression residuals.
For all models the data fusion simulation is validated by means of a cross validation. The leave-one-out methodology has been applied to obtain a set of independent observations to verify the spatial prediction performance. The results show satisfying performances for data fusion methodologies for almost all air quality indexes. More details on the data fusion techniques used can be found in Bande et al. 2023, Bande et al., 2022, Bande et al., 2021.

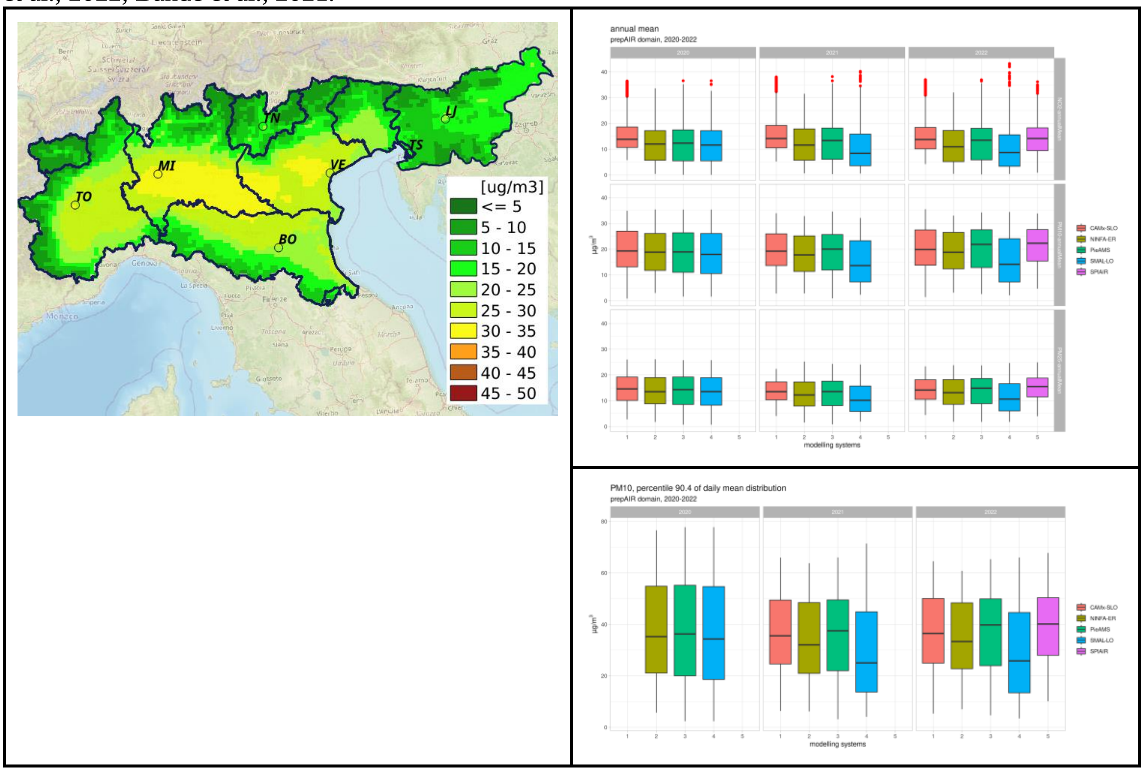

Figure 2. Left) Maps of PM_{10} annual mean produced by the ensemble of the five data fusion systems and right) Boxplots of grid point concentration distributions grouped by modelling system and year. Top: NO_2, PM_{10} and $PM_{2.5}$ annual mean, bottom: percentile 90.4 of PM_{10} daily values.

RESULTS

The Air Quality Assessment reports offer a comprehensive overview of air quality conditions in the Po Valley and Slovenia. These reports focus on PM_{10}, $PM_{2.5}$, nitrogen dioxide and ozone, pollutants that in some cases exceed legal thresholds. The assessments have been carried out with a state-of-art approach that uses data fusion techniques to integrate information coming from air quality monitoring networks and CTM modelling systems.

The results show that the most critical indicators are the 93.1 percentile of ozone and the 90.4 percentile of PM_{10}. For the former there are not substantial differences over the three examined years and the exceedances are widespread the entire study area; for the latter (Figure 2 bottom right) higher levels are observed during 2022 and 2020, with the most critical areas concentrated in the main urban centers and in the plain central areas of the Po valley, between Piedmont, Lombardy, Veneto and Emilia. Annual average concentrations are everywhere below the legal limits for PM_{10} and NO_2, and around this value or slightly below for $PM_{2.5}$ in many areas (Figure 2, left and top right).

Finally, it must be underlined that although the five CTM systems have different setup (resolution, boundary condition, meteorological data and data fusion technique), the model outputs are similar to each other showing the reliability of this multi-model assessment.

ACKNWOLEDGMENTS

This research was funded by LIFE-IP PREPAIR (LIFE15 IPE/IT/000013).

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