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A MULTISCALE MODELLING APPROACH FOR EVALUATION OF URBAN AIR QUALITY IN MODENA (ITALY)

Giorgio Veratti[1], Sara Fabbi[1], Alessandro Bigi[1], Aurelia Lupascu[2], Gianni Tinarelli[3], Sergio Teggi[1], Giuseppe Brusasca[3], Tim M. Butler[2] and Grazia Ghermandi[1]

[1]Department of Engineering "Enzo Ferrari", University of Modena and Reggio Emilia, Modena, Italy
[2]Institute for Advanced Sustainability Studies, Potsdam, Germany
[3]ARIANET Srl, Milano, Italy

Abstract: A multi-scale modelling system was developed to provide hourly NO_x concentrations field at building resolving scale in the urban area of Modena. The WRF-Chem model was employed with aim of reproducing local background concentrations taking into account meteorological and chemical transformation at regional scale, conversely the PMSS modelling system was applied to simulate 3D air pollutant dispersion with a very high-resolution (4 m) on a 6 km x 6 km domain. Modelled NO_x concentrations reproduced by this modelling system show a good agreement with observation at both traffic and background urban stations.

***Key words:** WRF-Chem, PMSS, Multi-model approach, Traffic emissions.*

INTRODUCTION

One of the most critical air pollutants in terms of health effects is nitrogen dioxide (NO_2), whose levels in the last years exceed national and WHO standards in many urban areas across Europe. In Italy, and more particularly in the Po Valley, despite an overall improvement on air quality in the last 10 years (Bigi and Ghermandi, 2016), the urban population is still exposed to harmful levels of NO_2.
The current research has as its goal the estimation of the air quality in the urban area of Modena in terms of NO_x atmospheric concentrations. More in detail, the aim of the project is the tentative source-apportionment among the main pollutants sources, such as road traffic, domestic heating and regional background to support environmental policies, epidemiological studies and urban planning and management.
Current approaches to produce spatial maps of urban air pollution include the use of interpolation methods and land-use regression (LUR) models. However, all these techniques need a large number of in-situ observations at strategic locations to represent the full spatial and temporal pollutant variability and cannot be used to take into account turbulent atmospheric dispersion. For these reasons the approach used

in this study was a modelling activity based on the NO_x dispersion by coupling two different models: the Weather Research and Forecasting (WRF) model coupled with Chemistry (Grell et al., 2005), able to computes concentrations fields over regional domain, and the Parallel Micro SWIFT and SPRAY (PMSS, Oldrini et al., 2017, Trini Castelli et al., 2018) modelling system accounting for dispersion phenomena within urban area.

The choice of this modelling chain was based on the WRF-Chem ability to simulate the emissions, transport and chemical transformations simultaneously with meteorology at large scale, and on the PMSS capability to provide high resolution air quality maps over an entire urban domain, with a reasonable computation time (Ghermandi et al., 2015).

In this study the PMSS modelling system was used to simulate at building scale resolution the NO_x dispersion produced by urban traffic flows in the city of the Modena. Conversely, the WRF-Chem model was performed to estimate the NO_x background concentrations on a multiple domains with a nesting technique, in order to take into account emissions both at regional and local scale.

WRF-CHEM SETUP

For this application the Weather Research and Forecasting model with chemistry (WRF-Chem), version 3.9.1, was applied over three one-way nested domains, centred in urban area of Modena, at 15, 3 and 1 km horizontal resolution respectively (Figure 1). The model top was set at 50 hPa, using 35 vertical levels with the first model layer approximately at 30 m. The MOZART gas-phase chemical mechanism and the MOSAIC aerosol model were used to simulate airborne pollutants over the nested domains. MOSAIC employs 4 sectional aerosol bins and includes both inorganic and organic aerosols. Processes involving secondary organic aerosols were represented by a volatility basis-set (VBS) approach.

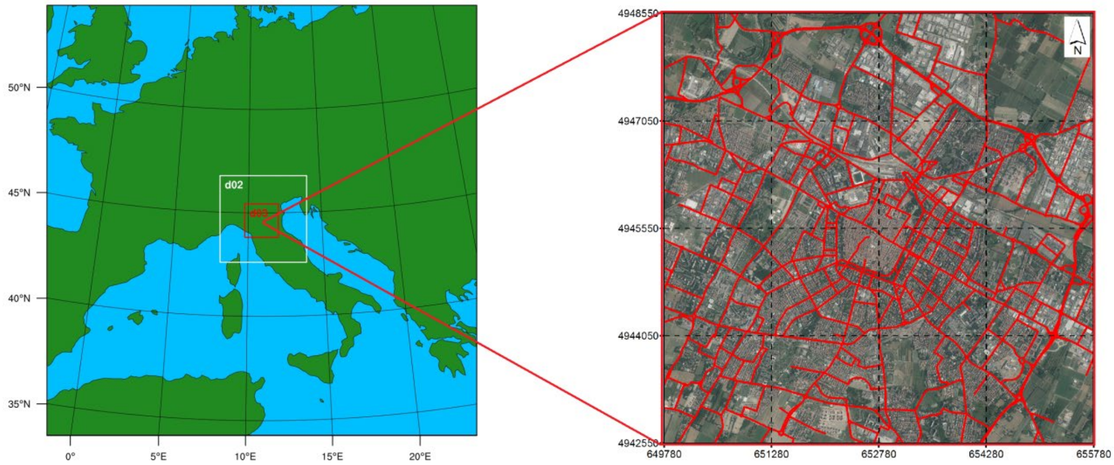

Figure 1. WRF-chem model domains (on the left) and PMSS domain with the considered street network represented as red lines (on the right).

Meteorological initial and boundary conditions were provided by the 6-hourly ECMWF analysis field (ERA5 dataset) with horizontal resolution of 0.25° x 0.25°, interpolated to 37 pressure levels from 1000 to 1 hPa. Data included 3D field of temperature, specific humidity and wind speed components. 2D surface parameters such as mean sea level pressure, sea surface temperature, soil temperature and volumetric soil water content were also considered. As to land use, the Corine Land Cover (CLC) dataset was adopted after reclassifying it into the 33USGS classes to match the WRF land use tables.

The anthropogenic emissions used in this study for the parent and the nested domains were taken from TNO-MACC III inventory, available on a regular grid with a horizontal resolution of 0.125° x 0.0625°, which contains emissions for air pollutants such as NO_x, SO_2, NMVOC, NH_3, CO and primary particulate matter ($PM_{2.5}$ and PM_{10}).

In order to avoid the double counting of the traffic emissions placed inside the urban area of Modena and to better represent the spatial distribution of this type of sources in the nearby territory, a downscale procedure was conducted for the 71-75 SNAP sectors. The original dataset (resolution ca. 14 km x 7 km) covering the inner most WRF-Chem domain was subdivided to a finer grid with a horizontal resolution of

1 km x 1 km. In collaboration with the municipality of Modena, the PTV VISUM model was employed to estimate traffic fluxes of light and duty vehicles at rush hour (from 7:30 a.m. to 8:30 a.m.) on the main roads of the province of Modena. These data were used as a proxy variable to distribute TNO-MAC III traffic emissions covering the province of Modena, to the portion of the land interested by PTV VISUM road network: the more traffic fluxes were estimated for a specific road segment, the more emissions were assigned to its related territory cell (1 km x 1 km).

Once the downscaled grid dataset was created, a spatial surrogate function was implemented to identify the TNO-MACC III traffic emissions within the PMSS domain. This function returns zero if the territory cell is completely inside the PMSS domain, one if the territory cell is completely outside and a value between zero and one (proportional to the area outside the PMSS domain) if the territory cell crosses the domain boundaries. Finally, to exclude TNO-MACC III emissions from the PMSS domain, the spatial mask created with the surrogate function was multiplied by the downscaled traffic emission inventory.

TNO-MACC III emissions are provided as annual totals, therefore for each SNAP category was applied a multiplication factor to take into account monthly and daily (weekend or weekday) variation, as suggested by Kuik et al. (2018).

Dust, sea salt and biogenic emissions were calculated on–line, the latter using the Model of Emissions of Gases and Aerosol from Nature (MEGAN v2).

PMSS SETUP

A 3D wind and turbulence field and air pollution dispersion reconstruction was performed on a 6 km x 6 km square domain covering the city of Modena (Figure 1) with the PMSS modelling suite. This is a parallel system based on the coupling of the Micro-SWIFT meteorological code with a fast momentum solver and the Lagrangian particle dispersion model micro-SPRAY, working at a resolution allowing to explicitly consider the effects of the buildings. The entire domain is splitted into communicating subdomains running in parallel. Given the low altitude difference between different areas of the city, a flat domain was considered and a 3D buildings reconstruction was made by using the SHAFT pre-processor: 25,600 polygons contained in the ESRI shapefile (provided by Geoportale Regione Emilia-Romagna) were transformed into approximately 146,000 triangular prisms directly usable by Micro-SWIFT.

In order to guarantee both flow and pollutant dispersion fields at a high resolution in each part of the domain, a horizontal grid step of 4 m (square cells) was chosen. The vertical grid structure used by Micro-SPRAY consists of 10 levels with a logarithmic progression up to 200 m above the ground level with 3 m height for the first layer close to the soil to represent ground level concentrations. This arrangement leads to a configuration of 1504 x 1504 x 10 nodes and a total amount of $2.26 \cdot 10^7$ cells.

To represent the flow entering the Micro-SWIFT computational domain, vertical profiles of temperature, humidity, wind speed and direction from the inner most domain (d03) of the WRF-Chem simulation were extracted on hourly basis. In addition, mixing height values and main background turbulence parameters (i.e. friction velocity, Monin-Obukhov length and convective scale velocity) were estimated with the Mesoscale Model Interface Program (MMIF, https://www.epa.gov/scram/air-quality-dispersion-modeling-related-model-support-programs).

3D fields of wind, temperature and turbulence were obtained at a 4m horizontal resolution for 20 vertical levels from 3 m up to 200 m above the ground using the Micro-SWIFT model with the fast momentum solver option.

The PMSS modelling system was employed only to simulate traffic emissions. The methodology chosen for this source estimation was based on a bottom-up approach: traffic flows data simulated by the PTV VISUM model were employed as "activity factor" and specific emission factors were used to estimate total emissions according to the fleet composition, vehicle type, fuel, engine capacity, load displacement, slope of the road, Euro emission standard and average traveling speed.

In order to obtain detailed traffic data, the PTV VISUM simulation provided by the municipality of Modena was exploited to estimate vehicle fluxes in the urban area of the city. In addition, direct flow measurement campaigns were carried out continuously over two weeks between October 28 and November 8, 2016, with 4 Doppler radar counters (one for each road lane) in a four-lane road in the proximity of the intersection with the urban ring road. The road network considered includes about 1100 sections with a total length of 210 km.

With aim of estimating for each road segment the NO_x atmospheric emissions in terms of pollutant mass per trip unit a modified version of the R package VEIN (v0.5.2) (Ibarra-Espinosa et al., 2018) was employed. The latest Emission Factors suggested by Ntziachristos and Samaras (2016) were introduced in the package and a series of functions to automatically compute for each road of the network the total NO_x emissions were implemented. Finally, to appropriately describe NO_x emissions under typical day flow conditions, hourly modulation rates for all roads network were built by considering the real traffic flow recorded in in the mentioned measurement campaign.

MODELS SIMULATIONS

Following the setup described in the two previous sections, simulations were performed for the period between 28 October 2016 and 8 November 2016, the same period whereby the traffic measurement campaign was carried out. WRF-Chem was re-initialized every day with a 2 days spin-up to ensure consistency with meteorological and chemical fields, PMSS was re-initialized every day with 6 hours of spin-up.

RESULTS AND DISCUSSIONS

2 m temperature (T2) and 10 m wind speed (ws10) meteorological fields predicted by WRF-Chem were compared against surface observations provided by different regional networks. The statistical parameters used to evaluate the performance of the model include Mean Bias (MB), Normalised Mean Bias (NMB), Root Mean Square Error (RMSE) and Pearson correlation coefficient (r). These metrics were computed from hourly observation means and hourly modelled values. Table 1 reports these statistics for the three WRF-Chem nested domains as the average of all the considered stations.

Table 1. Statistics of hourly 2 m temperature (T2) and 10 m wind speed (ws10) computed for the period between October 28th and November 8th, and averaged for all the stations. MB and RMSE are in °C and m s^{-1} respectively, NMB is given in %.

Domain	Resolution (km)	Variable	MB	NMB	RMSE	r
d03	1 km x 1 km	T2	0.39	0.05	2.16	0.80
		ws10	0.02	0.06	1.35	0.36
d02	3 km x 3 km	T2	0.47	0.07	2.18	0.79
		ws10	0.01	0.06	1.37	0.35
d01	15 km x 15 km	T2	0.68	0.11	2.36	0.74
		ws10	0.09	0.12	1.39	0.36

The same statistical parameters used to analyse meteorological variables were also employed to assess the performance of WRF-Chem in modelling NO_x concentrations at rural background sites inside the inner most domain (d03). 11 stations were taken as a reference for this study: 9 of them belong to the ARPAE Emilia-Romagna network and 2 of them to the ARPA Lombardia network.

Table 2. Statistics of hourly NO_x concentrations computed for the period between October 28th and November 8th, and averaged for all the rural background stations. MB and RMSE are in μg m^{-3}, NMB is given in %.

Domain	Resolution (km)	MB	NMB	RMSE	r
d03	1 km x 1 km	-7.85	-0.04	19.00	0.23
d02	3 km x 3 km	-8.13	-0.05	17.78	0.27
d01	15 km x 15 km	-5.43	0.14	17.39	0.33

Table 2 shows the comparison between statistical indicators over the three domains as the average of all the considered stations.

As a final step of the project, PMSS was performed for the same time period (between 28 October 2016 and 8 November 2016) using the meteorology field estimated by WRF-Chem in the d03 domain and considering only traffic emissions from the urban area of Modena. PMSS output was compared with observations at two urban stations: "via Giardini" urban traffic site and "parco Ferrari" urban background site. The same comparison was carried out adding to the PMSS output the concentration estimated by WRF-Chem in the d02 and d03 domains at the stations respective points. Table 3 summarize the performance of PMSS stand-alone, PMSS combined with WRF-Chem at d02 domain (PMSS + d02) and PMSS combined with WRF-Chem at d03 domain (PMSS + d03) in term of Normalized Mean Bias (NMB), Normalized mean-square error (NMSE), Factor of 2 (FAC2), Pearson correlation coefficient (r) and Fractional Bias (FB). The results of the statistical analysis show that PMSS combined with WRF-Chem at both d02 and d03 domains fulfills the acceptance criteria defined by Hanna and Chang (2012) for urban environments. Conversely, PMSS stand-alone fulfills all the aforementioned acceptance criteria only at urban traffic site ("via Giardini" station) since FAC2 and FB at urban background site ("Parco Ferrari" station) are not within the limits defined by Hanna and Chang (2012) (respectively FAC2 > 0.30 and |FB| < 0.67).

Table 3. Statistics of hourly NO_x concentrations computed for the period between October 28th and November 8th, considering three different model configurations. NMB is given in %.

Configuration	Station	NMB	NMSE	FAC2	r	FB
PMSS	parco Ferrari	-0.69	3.30	0.25	0.37	1.06
	via Giardini	-0.36	0.89	0.49	0.46	0.45
PMSS + d02	parco Ferrari	-0.25	0.75	0.62	0.44	0.29
	via Giardini	-0.04	0.48	0.72	0.47	0.04
PMSS + d03	parco Ferrari	-0.41	1.15	0.59	0.43	0.52
	via Giardini	-0.15	0.54	0.68	0.48	0.16

CONCLUSIONS

The results obtained with this models combination show a good agreement with observations at both traffic and background urban stations, in particular for the former case where traffic emissions are expected to be the main source of NO_x. Moreover, the statistic parameters indicate that the performance of PMSS increases when it is combined with WRF-Chem, especially at 3 km resolution (d02 domain). These valuable results confirm and demonstrate how this complex modelling system can be employed to support environmental policies, epidemiological studies and urban mobility planning.

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