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THE DEVELOPMENT OF A BUILDING-RESOLVED AIR QUALITY FORECAST SYSTEM BY A MULTI-SCALE MODEL APPROACH AND ITS APPLICATION TO MODENA URBAN AREA, ITALY

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Abstract: One of the main critical air pollutants in terms of health effects is nitrogen dioxide (NO_2), whose levels in the last years exceeded national and WHO (World Health Organization) standards in many urban areas across the Po Valley (Northern Italy), exposing urban population to the risk of pollution-related diseases and health conditions.
The main goal of this study was to develop a multi-scale modelling system able to forecast hourly NO_2 and NO_x concentration fields at a building-resolving scale in the urban area of Modena, a city in the middle of the Po Valley, in order to support environmental policies and to take timely protective actions given a forecast of impeding poor air quality.
The modelling system relied on two different tools: the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem), which is able to compute concentration fields over regional domain by considering specific emission scenarios and the Parallel Micro SWIFT and SPRAY (PMSS) modelling suite accounting for dispersion phenomena within the urban area. PMSS was used to simulate at building-scale resolution the dispersion of NO and primary NO_2 produced by urban sources. Conversely, the WRF-Chem model was selected to reproduce the meteorological input for PMSS and to estimate the formation of secondary NO_2.
Modelled NO_2 and NO_x concentrations were compared with measurements at two urban stations, one at traffic site and at background location. Notwithstanding a slight underestimation, mainly evident at urban traffic stations for NO_x, simulated concentrations present a large agreement with related observations. The NO_2 Model Quality Objective, as defined by Fairmode guidelines, was met for both the urban stations and the other statistical indexes considered in the evaluation fulfilled the acceptance criteria for dispersion modelling in urban environment, for both NO_2 and NO_x concentrations.
In the second section of the study, the population exposure to forecasted NO_2 concentrations has been evaluated adopting a generic model of dynamic population activity. Indoor house micro-environments contributed up to 67 % of the total exposure, whilts other outdoor spaces contributed with 24% , divided between traffic environments (8 %) and other outdoor spaces (16 %). Work related buildings contributed for the ramaining share (9 %).

Key words: *WRF-Chem, PMSS, Fairmode assessment, forecast system.*

INTRODUCTION

Several forecast tools based on Chemical Transport Models (CTMs) are currently operating at European, national and also at local level. Despite nowadays high performance computing resources are becoming easily accessible and the computing efficiency constantly improving, the capability of CTMs to deliver information regarding pollutant concentrations always faces a trade-off between spatial coverage and resolution. For this reason, combined with models limitations, operational forecasting systems are rarely configured to provide concentrations at a resolution higher than 1 km. The direct consequence is that city urban environments, known to be the most sensible areas to pollution exposure, are generally represented by few model cells, making standard forecasting tools unable to capture high spatial gradients.
In contrast to CTMs, computational fluid dynamics (CFD) techniques are well suited to reproduce meteorological variables and pollutant concentrations at very high resolution (in the order of few meters), but their computing cost still rather prohibitive for all the applications that exceed the sub-city-scale.

In order to combine the advantages provided by both CTMs and CFD techniques a number of hybrid tools have been recently developed and tested in practical applications. Following similar methodology, Veratti *et al.* (2020; 2021) combined the WRF-Chem model with the Lagrangian model PMSS with the aim of providing NO_x concentrations at 4 m resolution over the urban area of Modena (a city located in the centre of the Po Valley). Analogous studies involving the use only of Lagrangian models were successfully carried out in the urban area of Zurich (Berchet *et al.*, 2017), in complex topography (Ghermandi, Fabbi, Arvani et al., 2017) and in combination with traffic field measurements in the city of Modena and Reggio Emilia (Bigi *et al.*, 2019; Ghermandi, Fabbi, Baranzoni *et al.*, 2017; Ghermandi *et al.*, 2019, 2020).
The present research has as its goal the improvment of available modelling techniques to develop a forecasting system capable of simulating hourly NO_2 and NO_x concentrations at very high resolution (4 meters resolution) for the urban area of Modena, with a time horizon of one day. The modelling system used in study is based on the WRF-Chem model (Grell *et al.*, 2005) and the Lagrangian particle model PMSS (Oldrini *et al.*, 2017). Short term hourly population exposure to forecasted NO_2 concentrations were also assessed through a dedicated module using a dynamic for population activity.

MODELS SET-UP

With respect to a previous study focusing on the same area (Veratti *et al.*, 2020), the novelty and the enhancement introduced in this work regards mainly the WRF-Chem run strategy and the interplay with PMSS. In particular, with the aim of avoiding the double counting of the emissions on the overlapping area between the two models domains and to simulate at the same time the formation of secondary pollutants, WRF-Chem is run twice. The first run is a standard CTM simulation accounting for all set of reactions occurring among pollutants (full-run), while in the second run only the dispersion and diffusion were considered (tracer-rum).
The WRF-Chem model, version 3.9.1, was applied over two one-way nested domains, centred in urban area of Modena, at 15 and 3 km horizontal resolution respectively. 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. The meteorological and chemical parameters necessary for initial and boundary conditions were respectively provided by the Global Forecast System (GFS) model and by the Whole Atmosphere Community Climate Model (WACCM).
Anthropogenic emissions were taken from the TNO-MACC III inventory which was further downscaled to the resolution of the model grid (3 km) to better reproduce surface observations of key trace gases in the province of Modena. The emission categories involved in the downscaling procedure were residential and other non-industrial combustion, industry combustion and waste management, conversely traffic emissions were computed using a bottom-up approach relying on local traffic fluxes, vehicle fleet composition and COPERT5 emission factors.
PMSS, which is composed by the diagnostic wind field model Micro-SWIFT and the Lagrangian particle model Micro-SPRAY, was run on a 6 km x 6 km square domain covering the city of Modena with a horizontal grid resolution of 4 m. To represent the flow entering the micro-scale computational domain, 9 vertical profiles of temperature, wind speed and direction from the inner most domain of the WRF-Chem simulation were extracted on an hourly basis. 3D fields of wind, temperature and turbulence were obtained for 20 vertical levels from 3 m up to 200 m above the ground using the Micro-SWIFT model using the RANS flow solver option. Regarding the Micro-SPRAY set-up, the horizontal grid was chosen to be identical to that of the Micro-SWIFT and the vertical grid structure consisted of 10 levels with a linear progression up to 200 m above the ground level with 3 m height for the first layer close to the soil. This arrangement leads to a configuration of 1504 x 1504 x 10 nodes and a total number of $2.26{\cdot}10^7$ cells. In order to ensure consistency between WRF-Chem and PMSS simulated concentrations, the emissions used to feed both the models were the same.
Simulations were performed for all the days of February 2019, which were characterized by weather condition typical for winter in the central Po Valley with a very little atmospheric circulation due to recurrent thermal inversions at low altitude, low mixing layer heights and persistent foggy and hazy events which lasted also during day time. Recurrent wind calm episodes and high-pressure conditions enhance persistence and homogenization of air masses on a regional scale: the characteristic climate

conditions, along with the strong anthropic pressure in the area, lead to long-lasting high concentrations of pollutants also at remote rural sites.

DYNAMIC POPULATION EXPOSURE

Personal exposure is mostly determined by the air pollutant concentrations in different city environments where people spend their time as well as the amount of time they spend within each environment. Therefore, the exposure cannot simply be assessed by the pollutant concentrations. Other key factors are the number of people exposed to those air pollutant concentrations and the time spent in contact with those concentrations. Consequently, total exposure represents the exposure in all micro-environments (ME) both indoors and outdoors.

To estimate the population mobility within the urban area of Modena different micro-environments were defined and identified as follow: road traffic ME, work ME, house ME and other outdor environments. The data used to distinguish different micro-environments was taken from the Geoportale Regione Emilia-Romagna (https://geoportale.regione.emilia-romagna.it/) and relied on geographical information such as street carriageways, city buildings, industrial areas and public parks.

The population was further distributed during the hours of the day to all micro-environments according to generic diurnal profiles derived from population activity in different European countries (Borrego *et al.*, 2009). These diurnal displacement patterns were further modified to account for typical traffic behaviour for the city of Modena and a distinction between weekdays and weekends was also made.

RESULTS

Modelled concentrations were compared with observations at two urban stations: the first one at a traffic site, located in the proximity of a busy street close to the urban ring road (UT) and the second one at background site, within a public park to the West of the historical city centre (UB).

Predicted NO_2 and NO_x concentrations by the hybrid modelling system present a high level of agreement with related observations at both the stations, showing particularly good capability in reproducing NO_2 trend with Normalized Mean Bias (NMB) equal to -9 % at urban background and -24 % at traffic site and linear correlation respectively equal to 0.60 and 0.70. The NMB presented by the hybrid system at the same two stations for NO_x concentrations are equal to -14 % and -30 % and the linear correlations with observation are respectively 0.41 and 0.58.

A quantitative estimation of the agreement between simulated and observed concentrations was also assessed following the statistical metrics proposed by Hanna and Chang (2012) for urban dispersion model evaluation. Fractiona Bias (FB), Normalized Mean Sqaure Error (NMSE), Factor of two (FAC2) and Normalized Average Difference (NAD) were computed for both the urban stations located in Modena. Table 1 summarizes all the computed statistics.

Table 1. Statistics of hourly NO_2 and NO_x concentrations computed for the period between February 1and February 28, 2019

Station	Pollutant	FB	NMSE	FAC2	NAD
UT	NO_2	0.20	0.26	0.71	0.20
	NO_x	0.30	0.80	0.59	0.30
UB	NO_2	0.09	0.23	0.69	0.22
	NO_x	0.15	0.89	0.53	0.33

The statistical analysis shows that PMSS combined with WRF-Chem at both the urban stations fulfill the acceptance criteria defined by Hanna and Chang (2012). Regarding the FB, the results are always less than the threshold of 0.67, in particular at urban background site the outcomes of this metric are particularly good. At urban traffic station the results are larger than the previous one indicating that the models tend to underestimate more the mean concentrations but nevertheless in well agreement with the reference benchmark. As far as the NMSE is concerned, the hybrid modelling system shows its best performances with scores largely lower than the acceptance benchmark (6), with a maximum value of 0.89 at urban background station for NO_x, meaning that predicted values very rarely differ strongly from observations.

Regarding the FAC2 and the NAD there is a significant agreement between model results and relative acceptance criteria at both urban stations and for both the pollutants. Minimum and maximum FAC2 are equal to 0.53 and 0.71 achieved respectively at the urban background station for NO_x and at urban traffic station for NO_2 (the lower limit proposed by Hanna and Chang is 0.30). For the same locations and pollutant the maximum and the minimum NAD are 0.33 and 0.20 respectively (upper limit proposed by Hanna and Chang is 0.50).

Although statistical performance indicators provide insight on model performance, they do not tell whether model results have reached a sufficient level of quality for policy support. In this view, the Model Quality Indicator (MQI), i.e. the statistical performance indicator introduced by the FAIRMODE comunity to relate modelling results with measurement uncertanty, has been computed for simulated NO_2 concentrations. Results show that NO_2 model quality objectve (the criteria for MQI) is met at both the urban stations, with MQI lower than 1. More in detail, MQI is equal to 0.74 at UT and 0.79 at UB.

An example of modelled NO_2 concentrations (referred to Febraury 18, 2019) by the hybrid system are shown in Figure 1 with colour scaling from yellow to red. In the same figure the urban buildings are also displayed with the blue color.

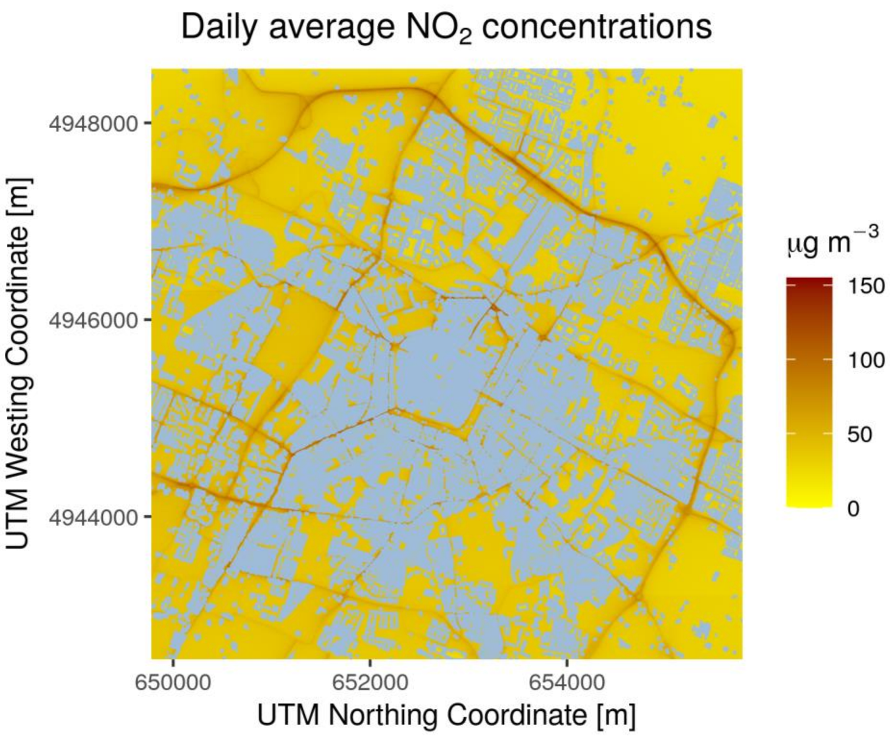

Figure 1. Daily average NO_2 concentrations simulated by the hybrid tool composed by the WRF-Chem and the Parallel Micro SWIFT SPRAY modelling suite, for Febraury 18, 2019.

According to the second objective of the study, the exposure to predicted NO_2 concentrations was assessed for each urban micro-environment using a dynamic estimate of the population. By dividing the total exposure for each micro-environment the house buildings are responsible for the 44 % of the total exposure, followed by mixed buildings composed half by house and half by work environments with 23 %, outdoor spaces with 16 %, traffic environments with 8% and finally by work related environments with 9 %.

CONCLUSIONS

Simulated and observed hourly concentrations at the two urban stations exhibit a large agreement for both NO_2 and NO_x concentrations, in particular for urban traffic site where bottom-up traffic emission estimations proved to be very successful in reproducing the observed trends. In addition, NO_2 Model Quality Objective was met for both the urban stations and additional statistical indexes considered in this

study fulfilled the acceptance criteria for dispersion modelling in urban environment, for both NO_2 and NO_x concentrations.
An additional module coupled with the modelling system suitable for population exposure assessment highlights that indoor environments are responsible for more than half of the total exposure to NO_2 concentrations.

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