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PMSS AND GRAL INTER-COMPARISON: STRENGTHS AND WEAKNESSES OF THE TWO MODELS IN REPRODUCING URBAN NOX LEVELS IN A REAL CASE APPLICATION

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Abstract: Air dispersion models are useful tools for quantifying pollutant concentrations in urban environment however many issues related to the dispersion estimation within urban canopy still persist. Most of them concern the emissions estimation, the flow field reconstruction between obstacles (buildings, bridges, tunnels, etc.) and the pollutant dispersion driven by the estimated flow field. This study presents results of a model inter-comparison conducted in a real case study, focusing on a 6 km x 6 km square domain covering the city of Modena (Italy), between two Lagrangian dispersion models set-up with the aim of estimating the NOx concentrations produced by traffic flow within the urban area of the city. Comparisons are made between the Graz Lagrangian Model (a.k.a. GRAL) and the Parallel Micro SWIFT and SPRAY (a.k.a. PMSS) modelling suite, in terms of dispersion concentrations and computing cost. The horizontal resolution for both the models is set to 4 meters and the traffic emissions estimation is based on a bottom-up approach: the PTV VISUM traffic model is used to estimate traffic flows on the Modena urban road network and the EMEP/EEA cold and hot emission factors are employed to estimate related emissions. All the other urban emission sources were considered to contribute to the regional background concentrations and estimated with the WRF-Chem model, which estimates also initial and boundary meteorological conditions (multi-scale approach). The general objective of the inter-comparison is to use equivalent input data for both the models keeping the emissions and the meteorological initial and boundary /condition consistent so that any discrepancies in output would be the results of differences in the micro-scale dispersion models. Since different turbulence parametrisation and dispersion scheme are implemented in the two models, the goal of this study is to identify the strengths and the weaknesses of both the models in reproducing urban NOx concentrations, in a real case application, at urban traffic and urban background sites.

Key words: *microscale simulation, lagrangian particle dispersion model, urban air quality*

INTRODUCTION

Urban areas generally experience degraded air quality due to the large emissions occurring within their area. Environmental policies, emission regulation and atmospheric research rely heavily on modelling tools in order to take decisions regarding actions, to grant permissions or to improve the scientific understanding. Lagrangian particle dispersion models are simulation tools which are commonly used to investigate dispersion of primary emissions within urban areas. Few of this type of models are available for the community: some are fully proprietary, some are free to use but with a proprietary code, some are free to use and open source.

Among two models under active development there are the Parallel Micro SWIFT SPRAY (PMSS, Arianet Milan, Italy and Aria Technologies, Paris, France) and the Graz Lagrangian Model (GRAL): the former is a proprietary code, the latter is a free and open code (Oettl, 2015). Both the codes are largely used in the scientific community (e.g. Veratti et al., 2020; 2021) and for regulation purposes (e.g. Oettl and Ferrero, 2017), and both are able to account for buildings and obstacles in their wind fields and dispersion. Within the project "TRAFAIR – Understanding traffic flow to improve air quality" the GRAL model is applied to provide a daily NOx forecast service for 6 European cities at a "microscale". In order to have a preliminary assessment of the scientific and computing resources of the project, a very preliminary comparison of PMSS and GRAL was performed.

MATERIALS AND METHODS

Both PMSS and GRAL simulate the advection and diffusion of inert species in the atmosphere, producing 3D concentration fields. The models have a distinct difference in the parallelization level: PMSS applies a MPI protocol for parallelization, while GRAL implements a simple parallelization strategy that can enable the usage of multiple cores within the same computing node. Other differences mainly regard the computation of the flow field within the complex urban environment: PMSS interpolates heterogeneous meteorological input data imposing impermeability conditions on the ground and at building surfaces. A RANS flow solver can be optionally used to simulate accurate velocity and pressure fields in the built-up environments. On the other hand, GRAL in the prognostic approach simulates the flow around obstacles by solving the RANS equations, neglecting molecular viscosity, Coriolis and buoyancy forces, and utilizing an eddy viscosity turbulence mode. PMSS uses the Thomson's approach (Thomson, 1987) to solve Langevin equations and Hanna's (1982) for the parametrisation of boundary-layer turbulence i.e. the scale variables need to be provided to PMSS. In GRAL the solution of the Langevin equations for the computation of the turbulent horizontal velocity component follows Anfossi et al. (2006): although it is possible to use vertical profiles, the recommended operation is to provide wind speed, wind direction and stability classes, which are used to compute the friction velocity and the Obukhov length according to Venkatram et al. (1997) and VDI 3783-8 respectively.

In order to perform a model intercomparison, both GRAL and PMSS were initialized with the same meteorological and emissions inputs. The focus was the urban area of Modena a 180 000 inhabitants in the Po valley, Italy, among the European regions with the worst air quality, and also one of the cities involved in the TRAFAIR project; the atmospheric pollutant considered was NOx. The domain is about 6 km x 6 km at 4 m resolution, accounting for the presence of buildings (Figure 1, on the right).

The Weather Research and Forecasting model coupled with chemistry (WRF-Chem) was applied over two one-way nested domains, at 15 and 3 km horizontal resolution respectively (Figure 1, on the left) to generate the initial and boundary meteorological conditions of the two models. The WRF-Chem 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 NOx concentration fields were observed within the layer ranging at 0 – 3 meters and 1.5 – 4.5 meters above ground for PMSS and GRAL respectively. GRAL is optmised to simulate atmospheric conditions which are classified according to wind speed, wind direction and stability class. Wind conditions were taken from the WRF-Chem output at 35 meters above the ground in the cell over the central area of Modena; these, along with global solar radiation, were used to estimate the stability class according to a modification of the SRDT scheme by Berchet et al. (2017). It is worth noting that WRF-Chem wind field was provided directly to GRAL, notwithstanding the use of the meteorological pre-processor GRAMM (Graz Mesoscale Model, Oettl and Veratti, 2021) is recommended.

For PMSS, wind and temperature input fields were extracted from nine WRF-Chem vertical profile spanning across 1 km from the ground, located within and in the nearby area of Modena. Atmospheric turbulence parameterisation was assessed by the means of the SUR-face-atmosphere interFace PROcessor (SURFPRO) through the estimation of the Planetary Boundary Layer height, Obukhov length, friction velocity and convective scale velocity.

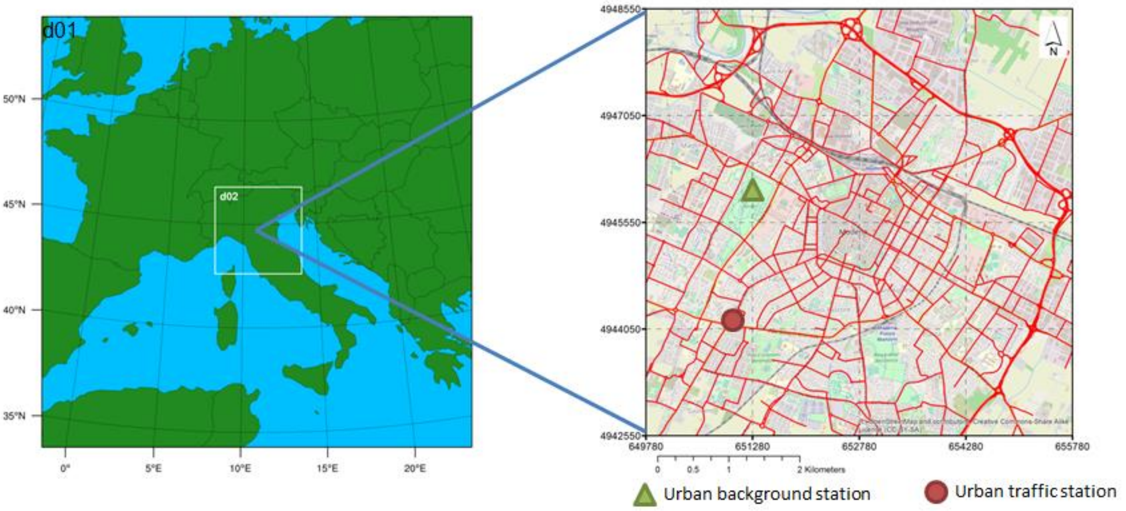

Figure 1. WRF-chem model domains (on the left) and GRAL-PMSS urban domain (on the right). Within the GRAL-PMSS domain are also depicted the location of the two urban air quality stations and the road street network considered in the simulation. Image modified from Veratti et al. (2020).

Only NOx traffic emissions were considered in the micro-scale computations, all the other emission sources were accounted in the WRF-Chem simulation along with background concentrations.. The road network accounted in the simulation (Figure 1) includes about 1100 sections with a total length of 210 km. Traffic emissions were estimated with a bottom-up approach: traffic flows were provided by the Municipality of Modena, proceeding from a simulation by PTV VISUM model of the traffic conditions at a morning rush hour between 07:00 and 08:00. A custom R package VERT (Vehicular Emission from Road Traffic (Veratti et al., 2020)) was used to estimate primary NOx emissions taking into account the traffic volume and local fleet composition. Three different modulations were applied to the emissions: two result from a Cluster Analysis of vehicle count by a set of induction loops around the city centre, one derives from a traffic measurement campaign conducted in the street facing the air quality monitoring station in urban traffic conditions (Figure 1).

RESULTS AND DISCUSSIONS

The simulation period included the week of 1st - 7th February 2019 and focus on the forecast of the NOx hourly concentration. The concentration simulated by the two models, added to WRF-Chem background concentrations, were compared with observations at two air quality monitoring sites in town, representative of urban traffic and urban background conditions (Figure 1). In Figure 2, the hourly NOx concentrations predicted by GRAL and PMSS plus the WRF-Chem contribution are compared through time series along with observations. The concentrations simulate by WRF-Chem stand-alone are also reported in the same figure.

Both models tend to underestimate the observed concentrations, particularly at the traffic and at the urban background site for GRAL and PMSS respectively. More specifically, at the urban traffic site PMSS seems to reproduce the observed pattern quite satisfactorily and during the two non-working days (Saturday Feb 2nd and Sunday February 3rd) PMSS concentrations agree with the reduction in the observations. Conversely the GRAL underestimate of NOx concentrations at the traffic site is larger than PMSS, in particular on specific days, although the concentration pattern between the two models is similar.

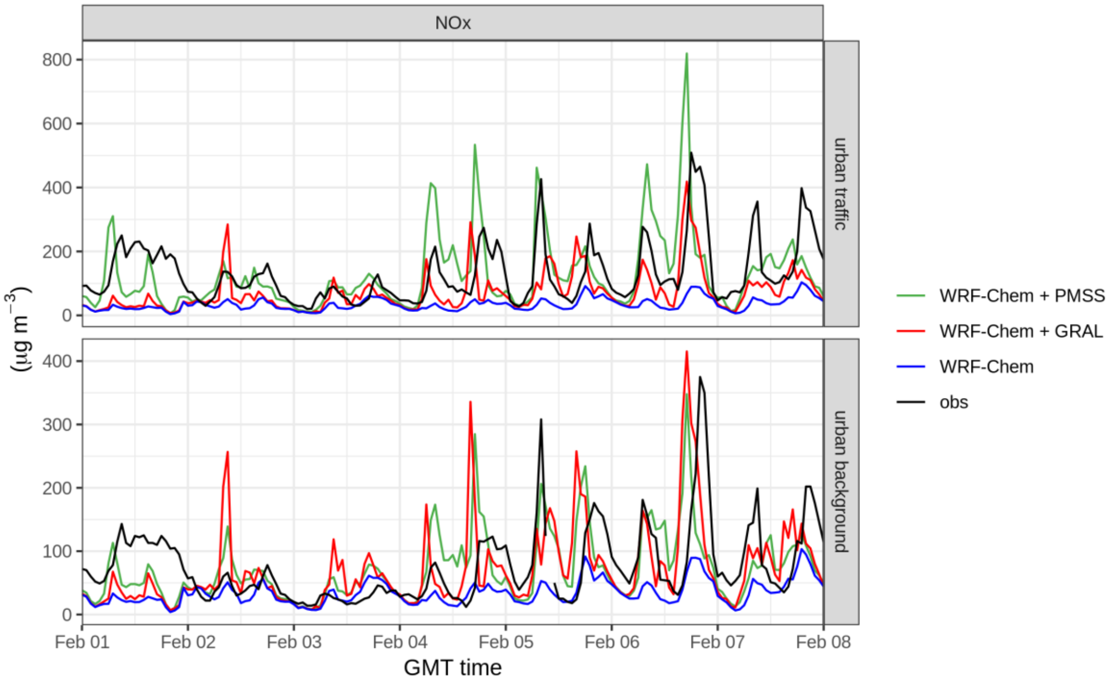

Figure 2. Hourly observed concentrations of NOx at urban traffic (top) and urban background (bottom) measurements stations along with hourly simulated concentrations by GRAL and PMSS plus the contribution of WRF-Chem and along with the concentrations reproduced by WRF-Chem stand-alone, from 1st to 7th February 2019.

Table 1. Statistics of hourly NOx concentrations computed for the period 1st – 7th February, 2019.

Station	**Model**	**NMB**	**FAC2**	***r***
urban traffic	WRF-Chem + GRAL	-0.44	0.48	0.43
	WRF-Chem + PMSS	-0.01	0.67	0.43
urban background	WRF-Chem + GRAL	-0.07	0.61	0.25
	WRF-Chem + PMSS	-0.05	0.57	0.33

At the urban background site the PMSS performance in reproducing the observed concentrations was poorer than at traffic site, while GRAL results, notwithstanding a lower correlation with the observations, showed a lower absolute bias compared to its performance at the traffic site.

The performance of GRAL and PMSS were also assessed in terms of Normalized Mean Bias (NMB), the fraction of predicted values within a factor of two of observations, also referred as Factor of two (FAC2) and Pearson correlation coefficient (*r*). Table 2 reports the statistical metrics for both the models and for both the urban air quality stations. Model intercomparison regarded also the computing resources required to perform the reconstruction of the flow field and the concentration dispersion (Table 3). Considering all the seven days of simulation between 1st and 7th February 2019, the computing resources required by PMSS to simulate only the dispersion were about 40 hours and 20 minutes, using 72 cores. By contrast to simulate only the dispersion GRAL required about 10 hours, using 24 cores. The memory consumption was quite different, around 2 GB for PMSS and around 92 GB for GRAL.

Table 2. Computing resources required for PMSS and GRAL compuation for the period 1st – 7th February, 2019.

	Index	GRAL	PMSS
Dispersion only (period 1 – 7 Feb 2019)	NCPUS	24	72
	MaxRSS	92 973 MB	2 139 MB
	Elapsed Time	09h 49m 45s	40h 19m 56s
Average 24 hour simulation (wind field + dispersion)	MaxRSS	~ 90 000 MB	~ 2 000 MB
	Elapsed Time	~ 11h 00m 00s	~ 08h 00m 00s

CONCLUSIONS

Within the framework of the project TRAFAIR, the two lagrangian particle dispersion models Parallel Micro Swift Spray (PMSS) and Graz Lagrangian Model (GRAL) were preliminarily compared in terms of NOx forecast and computing resources. Results obtained for a specific setup, in a forecast simulation, show different performance in terms of NOx prediction and computing resources. The analysis has to be considered preliminary due to the short period of analysis and the direct application of GRAL without its companion meteorological pre-processor GRAMM.

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