Validation of a numerical software for the simulation of the pollutant dispersion from traffic in a real case: some preliminary results

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Abstract. An increasing attention of citizens and policy-makers is devoted to the monitoring and modelling of urban traffic-related air pollution (TRAP), as there is a demonstrated relationship among this and human health effects (e.g. circulatory and ischemic heart diseases, lung cancer, asthma onset in children and adults, and acute lower respiratory infections in children). In this work, we investigate the capability of the ENVI-met[®] software to reproduce the concentrations of pollutants, emitted from vehicular traffic, and the meteorological parameters, both measured by a specific monitoring station, to evaluate its potential use for the TRAP prediction. Starting from the meteorological and traffic flow data of a specific day, a number of simulations, with different configurations, have been run and the results (temporal and spatial distribution of meteorological parameters and pollutants concentrations) have been compared with the monitored data, provided by the ARPAS (Agenzia Regionale per la Protezione dell'Ambiente della Sardegna – Regional Agency for the Protection of the Sardinian Environment) and measured by the weather station and the air quality monitoring station CENCA1 in Cagliari (Italy). The results of these comparisons are encouraging and can help, among the others, in better understanding the urban traffic pollutant dispersion and in optimizing the location of the air quality monitoring stations.

1 Introduction

The latest World Health Organization (WHO) reports highlight the significance of air pollution as a major environmental risk factor for the health of the world's population. The reports describe, through the use of upto-date databases on annual particulate matter (PM₁₀ and PM_{2.5}) concentrations, how outdoor and indoor air pollution affects all areas of the planet and impacts the health of populations without distinction between age groups, gender and socioeconomic status. In this regard, the WHO estimates a "burden of disease" particularly borne by developing countries, but also in the European Region, and highlights that air pollution is an important human health risk factor linked to the exposure to the respirable fraction of particulate matter, nitrogen oxides (NO_x) and ozone (O_3) [1]. The main concern, in terms of health effects, however, is with suspended particulate matter, particularly the finest fractions (PM₁₀ and PM_{2.5}), which are classified by the International Agency for Research on Cancer (IARC) as a Group 1 human carcinogen and considered a multiple component pollutant: in addition to being a risk factor by itself (regardless of its chemical composition), it is a carrier of numerous toxic and carcinogenic agents, such as metals (e.g., arsenic, lead, cadmium, nickel), polycyclic aromatic hydrocarbons (PAHs) (e.g., benzo[a]pyrene), dioxins and furans.

Urban areas represent the territorial contexts most at risk from this point of view, as most of the pollution and most of the population is concentrated in these areas. In Italy, about 70% of the population lives in urban areas, with projected growth in the coming years, which will imply further pressures on the environment with consequences for outdoor and indoor air quality.

Vehicular traffic is the main cause of this pollution, in varying proportions depending on the different geographical contexts. In northern Italy, for example, contributions due to domestic heating and industrial activities have a significant weight on urban air quality when compared to central and southern Italy, where the predominant contribution to air pollution is due to private vehicular traffic and public transport, consisting almost entirely of diesel-powered buses.

According to conservative estimates, air pollution related to motor vehicles causes 1% (184,000 deaths) of all deaths related to air pollution in the world [2]. Exposure to air pollution has been linked to premature mortality and cardiovascular disease [3], stroke [4], respiratory disease [3] and lung cancer [5]; complications of pregnancy [6], early childhood pneumonia [7], childhood asthma [8], as well as congenital heart abnormalities [9], deep vein thrombosis [10] and type 2 diabetes mellitus [11]. As research progresses, this list of health-related effects continues to grow, and the list now includes effects that some

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decades ago were not associated with traffic-related air pollution, including: autism and the behavioral problems of children [12], cognitive decline [13], dementia [14-15], and also obesity in children [16]. Many pathological mechanisms lend biological plausibility to the epidemiological results outlined above [1].

In Italy, the various legislative and technological interventions put in place over the past 15 years have certainly produced a benefit, introducing new air quality standards, regulating the use of fuels, the use of the best available techniques for the control of industrial emissions and, at the same time, implementing the number of control units and pollutants measured in air quality monitoring networks. The period of high pollution that affected the whole country during the winter of 2015-2016, determined by the peculiar meteorological conditions adverse to the dilution of pollutants in the atmosphere (long period of absence of precipitation, high pressure, thermal inversion in the lower layers of the atmosphere), has lead to buffer solutions, such as vehicular traffic interruption, that can only mitigate, often with little success, contingent situations but not systematically address the problem of long-term exposure to air pollution. On the opposite, during recent lockdown periods due to the Covid pandemic, a significant improvement in the air quality was recorded: this has made the correlation between air quality and vehicular traffic more evident.

In this perspective, the identification of interventions aimed at planning a better "organization" of activities and mobility in urban areas can bring a number of benefits comparable to those achievable through structural interventions, which aim at reducing the number of primary sources of emissions (such as the reduction of circulating motor vehicles, the adoption of district heating in urban areas to reduce the sources due to domestic heating systems) and their improvement in terms of quality (efficient urban transport and with electrified vehicles or running on natural gas instead of diesel). For these reasons, identifying and implementing efficient long-term mitigation strategies, supported by reliable data, is a strongly needed.

The choice of numerically simulating the dispersion of pollution caused by vehicular traffic in the urban environment is an increasingly used approach, but the validation of the simulation results depends on the compliance of the model and weather conditions to the reality that wants to be represented and, finally, to its calibration to make the values optimal and reliable. On turn, the databases of the mentioned data also depend on the environmental monitoring network in the territory: for instance, in Sardinia (Italy) there is the Sardinian Regional Network, that was designed and built in a relatively distant period of time. The location and type of monitoring stations, for example, thought more to determine the highest concentrations in industrial and urban areas, did not always meet the requirements of representativeness indicated by the new laws on air quality, mainly related to human health and natural ecosystem protection (for example, some pollutants now being considered by the regulation, such as benzene, PM₁₀ and PM_{2.5}, were not at the time of construction of the network). In the metropolitan area of Cagliari, the regional network consists of (see Fig. 1) the traffic station of Cagliari, located in via Cadello (CENCA1), and of the stations of Monserrato (CENMO1) and Quartu Sant'Elena (CENQU1).



Fig. 1. Position of the monitoring stations of the Metropolitan City of Cagliari.

In this paper, we present the preliminary results of the capability of a numerical software, namely ENVImet[®] (version 5.0.2), to reproduce the concentrations of pollutants, emitted from vehicular traffic, and the meteorological parameters, both measured by a specific monitoring station (the above mentioned CENCA1), to evaluate its potential use for the Traffic Related Air Pollution (TRAP) prediction. More in details, the targets are:

1. investigating the capability of the ENVI-met[®] software to reproduce the meteorological data and the concentration of pollutants, released from vehicular traffic, measured by a specific monitoring station;

2. studying the trend of dispersion of pollutants produced by vehicular traffic and their temporal and spatial distribution in an actual urban area, belonging to the municipality of Cagliari (Sardinia, Italy).

2 Materials and methods

ENVI-met[®] is an environmental and microclimate simulation software that operates at an urban microscale level and, through thermo-fluid dynamic equations, allows the behaviour of a three-dimensional climate model to be reproduced [17]. Developed by the Environmental Modelling Group of the University of Mainz (Germany) led by Michael Bruse, ENVI-met[®] can simulate the interactions between buildings, surfaces, vegetation, and air and energy flows within the urban built environment. Considering that the main use of ENVI-met[®] is for external comfort, its validation for the traffic pollutant dispersion simulation through the comparison with in-field measured data is needed.

For this target, we have chosen to simulate the pollutant dispersion from vehicular traffic emissions in the area around the quoted monitoring station CENCA1 in Cagliari (Italy), showed on Fig. 2. This study area is of about 306,000 square meters, $(426m \times 720m)$, with

the highly congested road via Cadello (an essential road for the access and exit from the city of Cagliari) in the middle and the Monte Claro park in the south. Between the street and the park there is a wall about 3 m high, which flanks the road on both sides of the road and for most of its extension. The maximum height has been chosen in order to be three times the maximum building height in the area. The model is built on a threedimensional grid composed by $213 \times 360 \times 45$ cells, with a resolution of $2m \times 2m \times 2m$ (equivalent to 426m \times 720m \times 90m). The closets cells to the ground have a higher resolution, being divided into 5 sub-cells to guarantee a more precise and accurate result at pedestrian level, where the wind velocity profile has the highest curvature.



Fig. 2. The case study area (source: Google Earth); the red line delimits the domain, the orange dot represents the CENCA1 monitoring station position, while the blue lines delimit the peculiar sub-areas.

The study area is divided into sub-zones (see Fig. 2), with peculiar features. The area marked with the letter A includes buildings consisting of several housing units arranged on several levels, of the total height of 16 m. The road network is represented by via del Seminario (one lane per direction), via Agostino Pipia (one lane) and via Monsignor Parraguez (one lane); depending on the number of lanes, the width of the carriageways varies from 3 m to 6 m. Between the buildings there are small areas covered by variegated vegetation. With the letter B is marked the area owned by the Archbishop's Seminary of Cagliari with the seminar facilities and a multipurpose sports complex. With the exception of the paved paths dedicated to internal roads, the soil surrounding the structures and playgrounds is natural and mostly uncultivated; a few vegetation is found along the perimeter wall shared with via Agostino Pipia and is composed of broad-leaved trees of considerable height. The area marked with the letter D is a classic neighborhood, with character almost exclusively residential, of independent dwellings built on a maximum of three levels, reaching an average height of the order of 8 m. Here the access is regulated by via Monsignor Giuseppe Cogoni and via Monsignor Paolo Botto, for the practically exclusive use of residents. This area borders to the north-west with another area (marked with the letter C), occupied by buildings consisting of several units of housing arranged on several levels and sharing the same architectural style, with a height of about 23 m and a flat roof; the spaces between them are

dedicated to parking and are paved. Here the vegetation, which is mainly in the form of bushes, hedges and grass, is sporadic and does not reach high heights. Next to the Monte Claro park, only partially contained within the perimeter highlighted in F, is the territory of relevance of the Metropolitan City of Cagliari (letter E). The building that houses some offices has a flat cover, reaches the height of about 30 m and, in continuity with the park, is surrounded by low shrubs typical of the Mediterranean scrub, meadows, bushes and hedges; the vegetation is completed with conifers of considerable height thickened in the northern area and bordering the via Cadello. The monitoring air quality station CENCA1 and the coupled weather station are located in the same area and marked with an orange rectangle. Eventually, the areas indicated by the letters E and F enclose most of the vegetated surfaces of the domain. The most relevant road crossing the domain is so via Cadello, whose geometry consists of a single track, about 14 m wide, and two lanes per direction. This relevance is also due to the north-east intersection with another major road, the Asse Mediano di Scorrimento (an expressway), which crosses much of the city and consists of two separate carriageways, each with two lanes in each direction. The three-dimensional domain is represented in Fig. 3.



Fig. 3. The three-dimensional domain.

The CENCA1 monitoring system is installed above a cabin, which, being located on a raised base of 0.8 m, reaches a height of 3.3 m. The above mentioned wall separating via Cadello from the sub-area E is 2.5 m far. The system is able to sample, at a fixed frequency, carbon monoxide (CO), nitrogen oxides (NO_x), nitrogen monoxide (NO), nitrogen dioxide (NO₂), ozone (O₃), particulates (PM) with a diameter of less than 2.5 μ m (PM_{2.5}), PM with a diameter of less than 10 μ m (PM₁₀), sulphur dioxide (SO₂), benzene (C₆H₆), toluene (C₇H₈), xylene (C₈H₁₀) and black carbon (BC). As above stated, the monitoring station is coupled with a weather station, able to measure wind direction, wind speed, air temperature, relative humidity and atmospheric pressure.

Regarding the traffic related pollutant emissions, ENVI-met[®] employs a static model for generating the emission profile of pollutants, based on the characteristics of the road section, on the modal partition and on the emission factors of each included vehicular category. Among the different typologies of traffic roads included in the software, the typology of traffic assigned to each road included in the domain has been chosen to be as close as possible to the actual specific type of each road traffic, according to the traffic data provided by the Transport Section of the Department of Civil-Engineering Environmental and Architecture (DICAAR) of the University of Cagliari (Fig. 4). The modal partition was as follows: Light Duty Vehicles/Transporter (LDV): 5%; Heavy Duty Vehicles (HDV): 2.50%; Motorcycles (MC): 0.50%; Public Transport (Urban Bus): 3%; Coaches: 1%; Passenger Cars (PC): 88%. The emission sources of pollutants generated by vehicular traffic are linear sources, arranged in succession so as to outline the travel lanes and at a height of 30 cm from the ground (Fig. 5). It has to be highlighted that the references for the emission factors considered by ENVI-met® for each vehicle category comes from the emission factors for road transport in Germany, Austria, Switzerland, Norway and France. These values were employed in the preliminary simulations, but was then substituted with the average emission factors for road transport in Italy by the ISPRA (Istituto Superiore per la Protezione e la Ricerca Ambientale - Italian Institute for Environmental Protection and Research), because the local vehicle fleet (especially in the southern area) is incomparable, in terms of composition and age (and therefore also of emissions), to that taken into account in the software.



Fig. 4. Daily traffic distribution on via Cadello.



Fig. 5. Plan view of the domain with the linear pollutant source emissions highlighted.

The day chosen for the simulation was selected as the one in 2020 (the last year with available data from the CENCA1) with the lowest daily-averaged wind speed: this because the chosen validation procedure implies to perform the simulations and compare the obtained data with the in-field measured ones on the three most frequent wind situation in Cagliari, i.e. calm, Mistral and Sirocco. This day comes out to be the 16 December 2020, with a daily-averaged measured wind speed of 1.24 m/s, from the south direction. These data (and the other meteorological ones), measured from the mareographic station placed in the Cagliari harbor, has been subsequently used as boundary conditions for all the simulations.

Various simulations were carried out, starting from the standard parameters of the software and updating them to refine the simulations, as the first simulations highlighted the difficulties of the software to match the measured data in the present case. In the next section we will focus on the results from the last simulation. Among the various refinements, the most relevant are listed in the following:

- the value of the input wind speed has been reduced from 1.24 m/s to 0.51 m/s to better fit the ones measured by the weather station coupled to the CENCA1;
- the type of source (among the ones included in the software) has been varied from pointwise to linear;
- the location of the linear sources has been moved from the road center to the boundary lines of the road lanes;
- background air concentrations of the pollutants were added, while in the firsts simulations they were neglected;
- the pollutant emission factors for the vehicular traffic included in ENVI-met[®] have been replaced with the ISPRA ones.

3 Results

In this section, some preliminary results obtained from simulations performed with ENVI-met[®] will be presented. Multiple simulations were led with different configurations. The results (temporal and spatial distribution of meteorological parameters and pollutants concentration) were compared with the monitored data, provided by the ARPAS (Agenzia Regionale per la Protezione dell'Ambiente della Sardegna – Regional Agency for the Protection of the Sardinian Environment) and measured by the weather station and the air quality monitoring station CENCA1 (Cagliari, Italy), respectively.

The use of multiple simulations was necessary to refine the modelling and the configuration process; in particular, we refined the boundary conditions, the choice and arrangement of source type that would model the pollutant emissions generated by vehicular traffic, and the inclusion of emission factors (for each vehicle category) representative of the study context. In the absence of this fine-tuning, first simulation results highlighted a significant underestimation of pollutant concentration values, which were several orders of magnitude (up to 10^5 times) lower than those actually measured by the CENCA1 monitoring station.

In the following, this section is divided into three subsections: in the first one, the temporal distribution of meteorological parameters measured by the weather station (wind direction and speed, air temperature, relative humidity) will be compared with analogous simulated distribution; in the second one, the same type of comparison will concern pollutants concentration (NO, NO₂, PM_{2.5}, PM₁₀) measured by the CENCA1 monitoring station. These comparisons were made to investigate the capability of the ENVI-met[®] software to reproduce pollutants concentration, emitted by vehicular traffic, and meteorological parameters, in order to evaluate, as previously stated, its potential use for the Traffic Related Air Pollution (TRAP) prediction. In the third subsection, the spatial distribution of meteorological parameters and pollutants concentration throughout the case study model will be shown, in order to highlight the most exposed areas to pollutant accumulation under the particular atmospheric conditions examined.

3.1 Temporal distribution of meteorological parameters

Fig. 6 shows the daily distribution of the wind direction measured by the weather station (the solid line in red). The measurements took place 10 m above the ground level and their average (the red dashed line) is around 195° N, so a wind coming from the South. The dashed line in blue refers to the average of the simulated wind direction at the cell whose centre of gravity is placed at approximately the same height as the actual measurements were sampled. The velocity direction and intensity oscillations in the simulations are very small, because of the constant forcing conditions imposed because, as already stated, among the targets of this paper there is the evaluation of the capability of the software to predict the TRAP and, consequently, to provide affordable results even with raw input data. The resemblance of the simulated and measured mean wind direction is remarkable, in particular taking in mind that the input data for the simulations come from a different weather station.



Fig. 6. Simulated (blue line) and measured (red lines) wind direction temporal distribution.

Fig. 7 presents the comparison between measured and simulated wind speed: also in this case, the agreement between mean measured and simulated values is very good. At 1 p.m., the wind speed measured by the weather station reaches its maximum value and, at the same time, so does the air temperature, showed in Fig. 8: this can be explained with the wind direction which, as above shown, comes roughly from the south, and it is consequently a warm wind in the chosen location.

Fig. 8 shows that the simulated air temperature trend is qualitatively similar to the measured one. However, during the hours when the measured temperatures are lower, the simulated values are overestimated; the opposite occurs during the hottest hours of the day, where the measured temperatures exceed the simulated ones. Furthermore, the greatest excursion is observed in the measured data series.

It can be observed, on Fig. 9, that the simulated relative humidity also has a qualitatively similar trend to the measured one. In this case, the simulated values tend to be always lower, as well as earlier, than those measured. Moreover, the increase in wind speed, observed in Fig. 7, also affects the relative humidity, which in that hour is close to its minimum value.



Fig. 7. Simulated (blue line) and measured (red lines) wind speed temporal distribution.



Fig. 8. Simulated (blue line) and measured (red line) air temperature temporal distribution.

In summary, we can state that the results of the simulations show a good correspondence with the meteorological parameters measured by the weather station associated with CENCA1.



Fig. 9. Simulated (blue line) and measured (red line) relative humidity temporal distribution.

3.2 Temporal distribution of pollutants concentration

On Fig. 10, Fig. 11, Fig. 12 and Fig. 13, the comparison between measured and simulated traffic related pollutants (NO₂, PM_{2.5}, PM₁₀ and NO, respectively) is shown. The simulated pollutants concentration shows a good quantitative correspondence with the measured concentration (Fig. 10, Fig. 11, Fig. 12), with the exception of nitrogen monoxide (NO) (Fig. 13).

The measured concentrations appear mostly higher than those simulated, except for particulate matter (PM_{10}) (Fig. 12). In this regard, it should be pointed out that the availability of the daily average value of the PM_{10} measured concentration only, does not allow any kind of assessment on the hourly distribution of the compared time series, but forces a comparison imprinted only on the daily averages.

The time series of the simulated concentrations show the projection of a single peak, shifted a few hours forward from the first peak of the time series of measured concentrations; after the peak, the values of the simulated concentrations decrease, but much more slowly than the measured ones do.

Although the typical concentration peaks, observed in the time series of measured concentrations at times when vehicular traffic activity is commonly most intense, were not reproduce by the simulations, the results achieved in this study are encouraging for a potential use of the software as a forecasting tool.

3.3 Spatial distribution of meteorological parameters and pollutants concentration

This subsection presents the simulated spatial distribution that meteorological parameters and pollutants concentrations assumed at 4 p.m. on the day



Fig. 10. Temporal distribution of simulated (blue line) and measured (red line) nitrogen dioxide (NO₂) concentration.



Fig. 11. Temporal distribution of simulated (blue line) and measured (red circles) fine particulate matter (PM_{2.5}) concentration.



Fig. 12. Temporal distribution of simulated (blue lines) and measured (red line) coarse particulate matter (PM_{10}) concentration.

studied and at 1 m above the ground level. 4 p.m. corresponds to the moment when the sources, according

to the hourly emission profile, release the greatest amount of pollutant into the atmosphere (see Fig. 4); the distance from the ground level was chosen to match, as much as possible, the height of pedestrians' upper airways.



Fig. 13. Temporal distribution of simulated (blue line) and measured (red line) nitrogen monoxide (NO) concentration.

Fig. 14 shows the spatial distribution of the wind direction and speed. Fig. 15, Fig. 16 and Fig. 17, on the other hand, concern the spatial distribution of pollutant (NO₂, PM_{2.5}, PM₁₀) concentration. However, not all pollutants were taken into account: the spatial distribution of nitrogen monoxide (NO) concentration was omitted from the plots because it was assessed to be quantitatively unreliable.



Fig. 14. Wind direction and intensity field at 4 p.m. on December 16, 2020, at 1 m above the ground level. Wind direction is displayed through oriented vectors, wind speed is displayed in false colours: fuchsia implies high speed values, dark blue implies low speed values. Air quality monitoring station (CENCA1) and its associated weather station coordinates are: X=250 m, Y=400 m.



Fig. 15. NO₂ concentration field at 4 p.m. on December 16, 2020, at 1 m above the ground level. Pollutant concentration is displayed in false colours: fuchsia implies high concentration values, dark blue implies low concentration values. Air quality monitoring station (CENCA1) and its associated weather station coordinates are: X=250 m, Y=400 m.



Fig. 16. $PM_{2.5}$ concentration field at 4 p.m. on December 16, 2020, at 1 m above the ground level. Pollutant concentration is displayed in false colours: fuchsia implies high concentration values, dark blue implies low concentration values. Air quality monitoring station (CENCA1) and its associated weather station coordinates are: X=250 m, Y=400 m.



Fig. 17. PM_{10} concentration field at 4 p.m. on December 16, 2020, at 1 m above the ground level. Pollutant concentration is displayed in false colours: fuchsia implies high concentration values, dark blue implies low concentration values. Air quality monitoring station (CENCA1) and its associated weather station coordinates are: X=250 m, Y=400 m.

The analysis of the figures from Fig. 15 to Fig. 17 suggests that the northeast section of via Cadello is highly prone to an accumulation of all the pollutants considered. The reason behind this trend could be the shelter provided by the wall (in black in the Figures) and vegetation (in green in the Figures), which prevents the wind from enhancing pollutants dispersion. The same figures also show other air pollution hotspots located along via Cadello. It is noteworthy that the highest concentration regions are not coincident with the monitoring station position, so the highest pollutant concentration measured by the monitoring station itself does not highlight the highest pollution values experienced by people in the nearby region: this kind of spatial analysis could consequently help in defining the best position for monitoring stations.

The results of this work are encouraging (and help to confirm the validity of the approach adopted so far) and could be improved introducing a temporal varying forcing and, most importantly, a vehicular emission more close to the one of the specific case (not available when the simulations were performed). Anyway, to validate the use of ENVI-met[®] as a forecasting tool in Sardinia, a more in-depth analysis of traffic information and the use of emission factors adhering to the regional context are needed.

As above stated, further future developments may concern the evaluation of the behaviour of the software when the model is subjected to different conditions of wind speed and direction (Mistral and Sirocco). Moreover, the sensitivity of the results to changes in the size of the model and the resolution of the cells could be investigated. Eventually, other areas could be modelled to verify the robustness of the results and their potential sensitivity to the peculiar location.

4 Conclusions

The aim of this study was to investigate, through numerical simulations, the ability of the ENVI-met[®] software to reproduce the concentrations of pollutants, emitted by vehicular traffic, and the meteorological parameters measured by a specific station, in order to evaluate its use in the forecasting field. The other objective was to study the pollutants dispersion and their spatial and temporal distribution in an urban area. The whole study was done in the specific case of Cagliari (Italy). Various simulations were carried out, gradually refining the simulation parameters to better match the measured data.

The results show a good correspondence with the measurements of atmospheric parameters and are promising for the concentration of pollutants. The spatial distribution of pollutants concentrations has shown that the areas of greatest concentration of pollutants are far from the air quality monitoring station (CENCA1) which could therefore measure lower concentrations than the highest one in the area and, so, not totally representative. ENVI-met[®] can therefore be a valuable tool to support the positioning of fixed air quality monitoring stations and the planning of possible measurement campaigns. In addition, it can support decision-makers in the evaluation of felling strategies and in urban and transport planning.

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