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Numerical modelling for air quality assessment and management

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Abstract. Air quality is nowadays one of the main environmental concerns both for its impact on human health and for its effect on global climate. An effective approach to tackling this problem is represented by the paradigm *think global, act local*, since a significant amount of direct and indirect emissions are tightly related to very local activities, such as local transport and household management. This cascade of scales poses severe constraints on governance instruments, which have to be capable to follow the general guidelines issued at continental level and, at the same time, need to devise effective measures capable to produce the desired effects on a local level.
A valid aid for this complex task is represented by numerical modelling. By using numerical simulations it is possible to test *in silico* the effects of possible measures and to evaluate their cost-benefits ratio and their potential trade-offs. Apart from assessment, numerical models provide a fundamental tool to forecast potentially hazardous episodes, helping to identify the set of short-term actions that can mitigate the risky situation.

Key-words. Air quality, atmospheric pollution, numerical modelling.

1. Introduction. Air quality is not an exclusively modern concern. The Roman philosopher Seneca, in his "Letter to Lucilius", mentioned the "gravior aer" of Rome which was producing negative effects on his health and mood. However, even if atmospheric pollution is probably as old as mankind, it is clear at the same time that pollution episodes became more and more frequent after the first and second industrial revolutions. Awareness of the adverse effects of air pollution first arose in the 19th century,

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when local and national laws began to be issued to regulate the installation of industrial plants and heating devices (Stel et al. 2012). These laws became mandatory at the end of 20th century, at least in the Western World, so as to conciliate economical and social improvement with environmental issues in the so-called "sustainable development". This need, quite new for mankind (that was accustomed to consume all the available resources in an area and then move to another place or bring new resources from abroad to the pillaged area), requires new conceptual and operational tools, one of which is proven to be the recourse to numerical modelling. By way of numerical modelling, in fact, it is possible to evaluate in advance the impact of new industrial or power plants on an area, as well as to split the observed levels of pollution in the related apportioned sources. In this way, it is possible to evaluate in advance the potential effects of measures adopted to reduce the levels of pollution without wasting of funds and avoiding useless social stresses always connected with measures when applied to a real context. But numerical models can be used even in a more extreme way, that is to foresee in advance potentially critical situations for the amount or persistence of pollution. In this way, with the aid of numerical models it is in principle possible to activate measures devoted to mitigate the effects of a situation before they begin.

2. Thermo-dynamic and chemical numerical solvers. Even if pollution is a consequence of anthropogenic emissions, the yearly and monthly trends of air quality are modulated by the so-called "meteorological determinants", represented by mixing height, horizontal advection and thermo-radiative trigger, whose interplay produces the observed pollutants behaviour. For this reason, every attempt to reproduce the current or future level of air quality through numerical simulations has to be based on a trustworthy numerical weather model. This is not a trivial request, because currently available meteorological models are often calibrated to minimize uncertainty for the classical atmospheric variables like precipitation and temperature. Relatively low attention is usually devoted to other variables like mixing height, direct solar radiation or even horizontal wind speed, which on the contrary are pivotal when dealing with pollutants dispersion and transformation. The first step toward an effective simulation of air quality is then the calibration of a dynamic and thermodynamic numerical solver capable to reproduce the micrometeorological parameters which characterize the area we are interested in, with the needed spatial and temporal resolution.

But meteorology alone is not enough to describe pollution behaviour, because it is necessary to have a complete photo-chemical solver, capable to reproduce the main chemical reactions occurring in the atmosphere. In the most advanced numerical suites, dynamical and chemical solvers can be fully coupled, so that chemical reactions can modify the system dynamics and thermodynamics (e.g. aerosols favour cloud formation, then Earth's albedo, then Earth's cooling, then ground pressure gradients). The two-way coupling of chemical and dynamical solvers is surely nearer to real atmospheric behaviour than a one-way coupling, in which only dynamics can interact with chemistry, but the resulting computational overload is often too large for the benefits that it can bring. For this reason, in the large majority of situations, it is considered convenient to adopt "off-line" numerical models, which are in principle less realistic, but can perform high-resolution simulations in smaller amounts of time.

Once the chain of numerical dynamical and chemical solvers is tuned, it has to be fed by initial and boundary conditions both for the meteorological and chemical atmospheric state. Boundary conditions, in particular, are necessary when dealing with air quality at regional scale. Boundary conditions, in fact, supply the needed information on what is happening or is going to happen outside the region we are interested in and that, by way of advection, is going to perturb what is inside the region of interest. It is clear that boundary conditions increase their importance with the decreasing of the scale of the area we are interested in; in fact what is happening outside a small area can wash what is happening inside it. Differently from the dynamical counterpart, the chemical initial and boundary state of the atmosphere is difficult to depict for several reasons, primarily the weakness of the exchange of the information system. As an example, only recently the European Commission decided to foster near-real-time exchange of data (European Commission 2011) and the realization of global numerical simulations still pertains to forerunner pilot programmes like GMES (European Union 2011).

3. Emission inventories. Differently from what happens in meteorology, where the only atmospheric constituent which has sources and sinks is water vapour, when dealing with air quality we need to take into account a huge variety of minor constituents (parts per million or even billion) that are continually emitted by human or natural activities and, at the same time, are depleted from the atmosphere. For this reason, a fundamental and basic step for the simulation of air quality is that to realize an emission inventory that might supply and estimate the amount of pollutants emitted as well as their diurnal, weekly and seasonal cycle. This activity is by far the most complicated to accomplish, because it requires a wide variety of expertise, spanning from that of industrial processes up to the knowledge of animals and plants physiology. Once these emissions are estimated at a regional level, they have to be distributed on the territory with a spatial resolution that is comparable to that of the numerical simulations we are interested in. This task is usually carried out using informations based on land-use and land-cover characteristics.

Another important aspect that has to be determined in order to carry out numerical simulations of air quality is the periodical aspect of emissions. For example, road transport is not homogeneously distributed during the day, the week or the year. The same happens for industrial emissions and for energy production and consumption. All these aspects have to be tuned on the area to be analyzed, because local behaviour and culture differs from place to place and they impact differently on pollutants dispersion and transformation.

Particular attention has to be paid to industrial emissions. Since a significant amount of these emissions is forced into chimneys, it is characterized by an emission eight (the height of the stack), a flux and an emission temperature. These aspects are extremely important because they influence the so-called "plume raise", e.g. the overshooting of the pollutants with respect to ground level, which is the level we are interested in. In other words, difference is made on the same amount of pollutant released at ground level and at air temperature (e.g. road transport emissions) or released from a tall stack and with a high temperature. In the latter case, in fact, the pollutant has a higher degree of dilution, but the capability to affect wider areas.

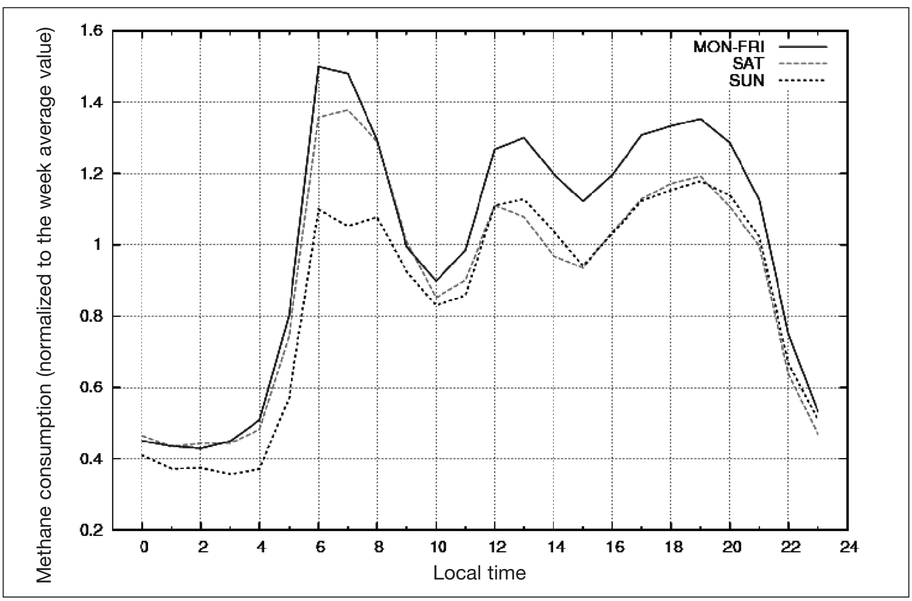

Figure 1. Diurnal methane consumption in domestic usage and for services over the Friuli Venezia Giulia region and for different days of the week. Values are normalized with the weekly daily consumption. It is assumed that this behaviour might be the same for the other energetic vectors. Courtesy SNAM Rete Gas.

Table 1. Pollutants emissions pertaining to Friuli Venezia Giulia, ascribed to several social sectors, expressed in ton/year and referring to the year 2007.

Pollutants	*Energy Production*	*Industry*	*Domestic*	*Road Transport*
CH4	91	367	2,294	321
CO	910	5,896	38,505	26,381
COV	91	683	9,482	3,293
N2O	16	133	251	93
NH3	0	47	68	423
NOx	6,144	7,267	7,627	10,764
PM10	19	134	1,991	1,064
SO2	9,853	5,828	316	94

4. Air quality state and source apportionment. Once the driver represented by meteorology is defined, jointly with orographic boundaries and together with the emission pattern and timing, numerical simulations can be carried out. These numerical simulations can be devoted to define the current status of air quality (e.g. to determine the portions of an area where limit values fixed by human or environmental health constraints can be exceeded) or to evaluate the relative weight of different sources or source classes (called "source apportionment"). The former activity is important in order to single out potentially critical areas, e.g. where to adopt a set of mitigation actions, while the latter is fundamental to single out the best suited set of mitigation actions, minimizing costs and maximising effects, keeping at an acceptable level the social stress that every policy brings with itself.

One of the ways in which source apportionment can be carried out is that to repeat several times the numerical simulation, neglecting each time a source or class of sources. In this way, by computing the difference between the simulation with all the sources and the simulation with all the sources but one, we can estimate the impact of this source on the level reached by all the different pollutants. It is easy to imagine that this activity requires a lot of computational resources and a lot of storage capability to save the results of numerical simulations. A positive aspect, however, is represented by the fact that this activity can be easily parallelized.

Results achieved through this source apportionment are extremely valuable for policy makers, as shown in Figure 2ab, where the contribution of several emission classes are reported for particulate matter (PM10) and nitrogen dioxide (NO2) in the four major towns of Friuli Venezia Giulia. From those figures, it is clear that domestic wood combustion represents a relevant emission source for particulate matter, while road transport represents the major source for nitrogen dioxide. Particular attention, moreover, has to be given to maritime transports as well

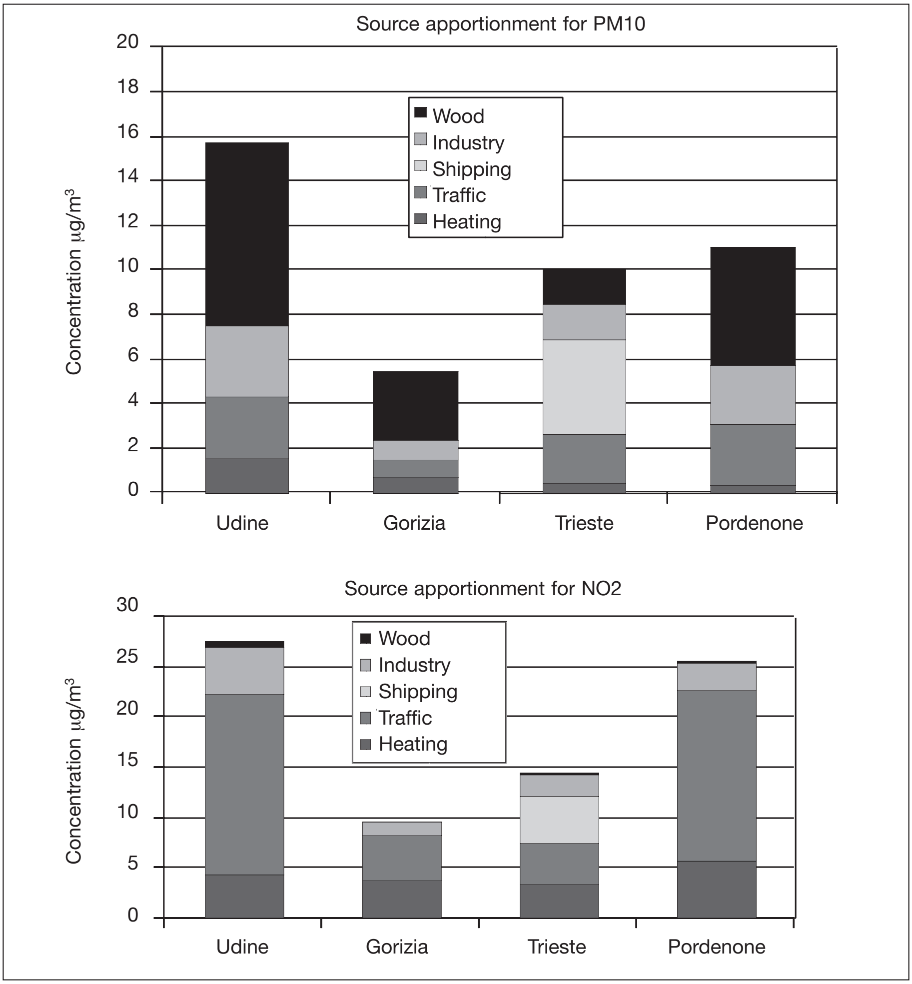

Figure 2ab. Upper panel, source apportionment for PM10 in the four major towns of Friuli Venezia Giulia. Bottom panel, source apportionment for NO2 in the four major towns of Friuli Venezia Giulia. It is clear that domestic consumption of wood is a major source for particulate matter, while road transport represents the most important source for NO2. Relevant is the source represented by shipping (Regione Autonoma Friuli Venezia Giulia 2010 and 2012).

as to trans-regional emissions. The latter aspect is particularly relevant, and worth to be underlined, because it is clear that, in particular near to the administrative borders or for small (under the emissions point of view) regions, pollution cannot be faced effectively only at regional scale.

5. Conclusions and future perspectives. Numerical simulations of air quality represent nowadays an extremely powerful tool for policy makers in order to evaluate, effectively and at a relatively low cost, the current and future level of pollution. In this way, numerical modelling permits to activate mitigation actions in advance of a full-blown pollution episode. Moreover, these mitigation actions can be chosen through a careful source apportionment, that singles out the most impacting sources or source classes. Numerical simulations, then, should become an effective governance tool to develop and test new mitigation policies. But even adaptation policies would find benefits from numerical simulations. It is in fact reasonable to imagine that, in the next future, improvements in real-time or near-real-time emission evaluations might raise the level of air quality forecasts. These improvements will bring particular benefits to the most sensitive social categories (children, elders, ill people) thanks to an increased awareness and a faster alert.

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