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REVIEW ARTICLE

A review of AirQ Models and their applications for forecasting the air pollution health outcomes

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Abstract Even though clean air is considered as a basic requirement for the maintenance of human health, air pollution continues to pose a significant health threat in developed and developing countries alike. Monitoring and modeling of classic and emerging pollutants is vital to our knowledge of health outcomes in exposed subjects and to our ability to predict them. The ability to anticipate and manage changes in atmospheric pollutant concentrations relies on an accurate representation of the chemical state of the atmosphere. The task of providing the best possible analysis of air pollution thus requires efficient computational tools enabling efficient integration of observational data into models. A number of air quality models have been developed and play an important role in air quality management. Even though a large number of air quality models have been discussed or applied, their heterogeneity makes it difficult to select one approach above the others. This paper provides a brief review on air quality models with respect to several aspects such as prediction of health effects.

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Introduction

Clean air is considered as a basic requirement to maintain human health (Chiu and Yang 2015; Gibson 2015; Welker-Hood et al. 2011). However, air pollution continues to pose a significant threat to health in developed and developing countries alike.

The WHO estimates that some 80% of premature deaths are due to ischemic heart disease and stroke caused by outdoor air pollution, 14% are due to chronic obstructive pulmonary disease or acute lower respiratory tract infections, and 6% are due to lung cancer. Children are particularly susceptible due to their fast metabolism (Ferrante et al. 2012; Danysh et al. 2015; Rodriguez-Villamizar et al. 2015). The "WHO Air quality guidelines" provide global guidance on thresholds and limits for key air pollutants harmful for human health. According to the WHO, a reduction in particulate matter (PM_{10}) pollution from 70 to 20 μg/m^3 can reduce air pollution-related deaths by 15% (WHO 2006).

Accurate evaluation of the concentrations and effects of air pollutants is therefore increasingly important. Over the past few years, modeling approaches based on mathematical and numerical techniques have been used more and more often to explore the relationships between air pollution and diseases or deaths, raising important questions on the significance of the data collected and on the need for appropriate training of professionals in these fields. This paper provides a brief review of the different guidelines and approaches—including air modeling systems like the Air Quality model (AirQ model) and AirQ Software 2.2—adopted by different countries over the past 6 years to assess air quality and the health impacts due to exposure to classic and emerging air pollutants.

Search strategy and selection criteria

The PubMed, Web of Science, Scopus, and Cochrane databases and reports of European and non-European environment agencies were searched for case reports, editorials, and expert opinions published in English, Italian, and French from January 2010 to June 2016. Search terms were "Air quality guidelines," "Air pollutants," "Air Quality Models," "Air Q software," "air pollution," and "health."

Air quality guidelines and comparison between emerging and developed countries

The guidelines apply in all WHO regions and regard particulate matter (PM), ozone (O_3), nitrogen dioxide (NO_2), and sulfur dioxide (SO_2) (see Table 1).

The European Commission's Thematic Strategy on Air Pollution set the goals of improving human health and the environment through the improvement of air quality by the year 2020. The EU air quality legislation stresses the need for improving air quality monitoring and assessment, to provide better "information to the public" (Directive 2008/50/EC).

PM, O_3, and NO_2 are currently Europe's most problematic pollutants in terms of damage to health (Mills et al. 2015; Choi et al. 2015; EEA 2010). Generally, the effect of air pollution on health and relevant policymaking can be explained through the Driving force-Pressure-State-Exposure-Effect-Action (DPSEEA) model (Corvalán et al. 2014). Ideal policymaking to protect human health involves a reduction of exposure to environmental risks at all stages of the process. However, policy-based interventions are not simple, since the time lag between the reduction of exposure to the environmental risk factors and its effects on disease prevalence, as well as other variables, makes interventions hard to implement (Ha 2014). The DPSEEA model (Fig. 1) is closely related to the establishment of air quality standards, because setting up those standards can lead to management and reduction of pollution sources, reducing pollutant concentrations and associated health risk factors to ensure a healthy environment for citizens (Corvalán et al. 2014). Air quality standard setting may be considered as a reliable method for reducing human exposure to air pollutants.

The US Environmental Protection Agency (EPA) has set National Ambient Air Quality Standards (NAAQSs) for six principal pollutants, called "criteria" pollutants (US EPA 2014). The Ambient Air Quality and Cleaner Air for Europe (CAFE) Directive (2008/50/EC) was published in May 2008, replacing the Framework Directive and the first, second, and third Daughter Directives.

Ambient air quality has been regulated in China since 1982, with initial limits for total suspended particulate (TSP), SO_2, NO_2, Pb, and benzo(a)pyrene (BaP). In 1996, the standard was both strengthened and expanded under National Standard GB 3095-1996, but in Ministry of Environmental Protection Announcement No. 1, the standard was updated with less stringent limits for some pollutants (Category Emissions Standards China 2014).

Brazil's National Environmental Council (CONAMA) and the core agency National Environment System (SISNAMA) have set the country's air quality guidelines, but the national standards are to be applied only in the absence of local ambient air quality standards (http://transportpolicy.net/index.php?title=Brazil:_Air_Quality_Standards). The most recent worldwide environmental laws are based on the Kyoto protocol.

Classic and emerging pollutants and their health effects

PM_{10}, $PM_{2.5}$, CO, O_3, NO_2, and SO_2 are defined "classic or traditional" air pollutants

CO is a ubiquitous toxic gaseous pollutant in the atmosphere generated by natural and anthropogenic combustion, by photochemical oxidation of methane and other volatile organic compounds (VOCs), and by vegetables (ATSDR 2009). Outdoor air pollution by CO is dangerous for individuals with heart disease (Lee et al. 2015) and is associated with an increased risk for thromboembolism (De Matteis et al. 2015), osteoporosis, and migraine (Chiu and Yang 2015; Chang et al. 2015). A potential connection with neurodevelopmental outcomes has also been suggested (Levy 2015).

Fossil fuel combustion is a major source of PM_{10}, $PM_{2.5}$, CO, O_3, NO_2, and SO_2 (Ferrante et al. 2012). The lower use of high-sulfur coal for domestic and/or industrial purposes is contributing to the reduction of urban and rural concentrations of SO_2, and this trend is widely recorded in several European countries (Masiol et al. 2014). The significant reduction in SO_2 emissions achieved since the 1970s is one of the success stories of Europe's earlier air pollution strategy (Ferrante et al. 2012). Indeed, every 10 $\mu g/m^3$ increase in PM_{10} and SO_2 was associated with an increase of about 1.012 (95% CI 1.002, 1.022) and 1.021 (95% CI 1.002, 1.040) in mortality from ischemic heart disease, respectively (Lin et al. 2014; Liu et al. 2015a; Suissa et al. 2013).

Some reports have raised concerns over the health effects of outdoor air pollution mixtures.

Classic air pollutants (Chen and Kan 2008; Gloag 1981) are associated with low-term birth weight (Qian et al. 2013) and increased limb defects (Lin et al. 2014), pre-eclampsia in pregnancy (Yorifuji et al. 2015), acute bronchitis (Nahidi et al.

Table 1 Air quality guidelines in some emerging and developed countries

Pollutant	WHO	NAAQS	CAFE	China	Brazil
PM 2.5	10 μg/m^3 annual mean	12 μg/m^3 annual mean	20 μg/m^3 annual mean	15 μg/m^3 annual mean	–
	25 μg/m^3 24 h mean	35 μg/m^3 24 h mean		35 μg/m^3 24 h mean	
PM 10	20 μg/m^3 annual mean	150 μg/m^3	40 μg/m^3 annual mean	40 μg/m^3 annual mean	–
	50 μg/m^3 24 h mean		50 μg/m^3 24 h mean	50 μg/m^3 24 h mean	
O3	100 μg/m^3 8 h mean	0.075 ppm	120 μg/m^3 8 h mean	100 μg/m^3 8 h mean 160 μg/m^3 1 h mean	160 μg/m^3 1 h mean
NO2	40 μg/m^3 annual mean	53 ppb	40 μg/m^3 annual mean	40 μg/m^3 annual mean	100 μg/m^3 annual mean
	200 μg/m^3 1 h mean	100 ppb	200 μg/m^3 1 h mean	200 μg/m^3 1 h mean	320 μg/m^3 1 h mean
SO2	20 μg/m^3 24 h mean	75 ppb 1 h mean	350 μg/m^3 1 h mean	50 μg/m^3 24 h mean	80 μg/m^3 annual mean
	500 μg/m^3 10 min mean	0.5 ppm 3 h mean	125 μg/m^3 24 h mean	150 μg/m^3 1 h mean	365 μg/m^3 24 h mean
CO	100 μg/m^3 15 min mean	–	10,000 μg/m^3 (Not to be exceeded)	4000 μg/m^3 24 h mean	40,000 μg/m^3 1 h mean
	30 μg/m^3 1 h mean			10,000 μg/m^3 1 h mean	10,000 μg/m^3 8 h mean
COV	–	–	–	–	–
Nafthalene	10 μg/m^3 annual mean	–	–	–	–
B(a)P	8.7×10^{-5} (UR/lifetime)	No safe level can be recommended.	0.001 μg/m^3 annual mean	0.001 μg/m3 annual mean 0.0025 μg/m3 24 h mean	–
Tetrachloroethylene	250 μg/m^3 annual mean	–	–	–	–
Formaldehyde	100 μg/m^3 30 min	–	–		–
Benzene	No safe level of exposure can be recommended.	No safe level can be recommended.	5 μg/m^3 annual mean	No safe level can be recommended.	No safe level can be recommended.
Toluene	260 μg/m^3 7 days 1000 μg/m^3 30 min	–	–	–	–

2014), chronic obstructive pulmonary disease (COPD) (especially asthma) (Guo et al. 2014; Ghozicali et al. 2015; Miri et al. 2016), hypertension and increased blood pressure (Dong et al. 2014), cardiac arrhythmia and cardiovascular diseases (Zhao et al. 2014; Jevtić et al. 2014; Miri et al. 2016), and autism spectrum disorders (Jung et al. 2013).

It is difficult to draw conclusions about the effects of emerging air contaminants on health for a number of reasons, including data heterogeneity, small numbers of studies, and investigations limited to a small number of regions (Singh et al. 2014). Heavy metals, persistent organic pollutants (POPs), and VOCs, the major emerging air pollutants, exert a variety of harmful effects on human health (Ferrante et al. 2012).

Heavy metals can cause harm at low concentrations and are toxic and carcinogenic; their relative toxic/carcinogenic potencies are compound-specific. Exposure has been related to developmental retardation, various cancers, kidney damage, and even death in some instances of exposure to very high concentrations.

POPs are a group of chemicals that persist in the environment for a very long time, exerting a potentially significant impact on human health. Their stability and ability to be transported make them ubiquitous; POPs are also found in arctic regions (Singh et al. 2014; Wang et al. 2015; Fernández-González et al. 2014). The United Nations Environment Programme (UNEP) has listed 12 POPs as the "dirty dozen." Nine are old organochlorine pesticides (aldrin, DDT, chlordane, dieldrin, endrin, heptachlor, hexachlorobenzene, mirex, and toxaphene). Atmospheric polycyclic aromatic hydrocarbons (PAHs) can also cause adverse effects on human health, but the relative contribution of this route of exposure is still unclear (Ferrante et al. 2012). The production and use of some POPs have been banned in most countries, resulting in reduced air concentrations (Morales et al. 2014; Augusto et al. 2015). Three other POPs that raise concern are industrial chemicals, including polychlorinated biphenyls (PCBs), polychlorinated dibenzodioxins (PCDDs or dioxins), and polychlorinated dibenzofurans (PCDFs or furans) (Crinnion 2011).

Several epidemiological studies have highlighted an association between POPs and chronic diseases like diabetes (Kim and Lee 2014; Ngwa et al. 2015; Jaacks and Staimez 2015), birth defects (Ren et al. 2011), genotoxic effects, serum abnormalities (Li et al. 2014), autism spectrum disorder (Mitchell et al. 2012), endocrine disruption effects (Crinnion 2011), reproductive and immune dysfunction, and cancer (Crinnion 2011; Vested et al. 2014).

VOCs are ubiquitous domestic pollutants. Industry, transports, and residential sources are the major anthropogenic sources (Ferrante et al. 2012). Many VOCs are classified as known or possible carcinogens (Manno 2013), irritants, and toxicants and have a role in the development of asthma and allergy and their exacerbations (Nurmatov et al. 2015; Oliveri Conti et al. 2011; Chin et al. 2014).

AirQ models

The concentrations of substances measured in the atmosphere derive by some variables as transport, diffusion, chemical reactivity, and ground deposition. The phenomena of transport are due to mean fluid's velocity, and it has been measured and studied for centuries instead; the study of diffusion or turbulent flow is more recent.

Air pollution's monitoring gives important quantitative information about air pollutant's concentrations and their deposition, but it can only describe air quality without giving clear identification of causes of pollution. Air pollution's modeling, instead, can give a most complete and deterministic description of air pollution, including an analysis of emission sources, meteorological processes, and physical and chemical changes, but also is useful for monitoring the effects of implementation of mitigation measures and for forecast for the human outcomes (Daly and Zanetti 2007).

Air pollution models represent an important tool in environmental and epidemiological science. Only these methods allow the deterministic relationship's quantification between emissions and concentrations/depositions, including the consequences of past and upcoming scenarios and the determination of the effectiveness of air pollution management strategies. This makes air pollution models indispensable in several research applications.

The problem of assessing air quality over large regions is complex under several aspects (Finazzi et al. 2013). AirQ models use mathematical and numerical approaches to simulate the physical and chemical processes undergone by air pollutants and to simulate their dispersion and reaction in the atmosphere. The aim of these models is to relate mathematically the effects of source's emissions with the level concentrations and to establish if permissible levels are, or are not, being exceeded.

Several AirQ models are available in literature for air quality forecasting, but like most of statistic models, they are applicable in specific conditions (Gottschalk et al. 2013). For these motifs, it is very important to describe their possible applications and the vantages and advantages of each group of models; in fact, a better knowledge of these will be of help for workers on health and environment for a better management of the air quality and its health effects. However, the specialists in health cannot do without a collaboration with the AirQ experts (physicists and chemists) for the complexity of the AirQ model's approach that need a specific and deepened knowledge.

Firstly, the researcher can choose to study primary or secondary air pollutants. The secondary pollutants are the primary pollutants (e.g., NO, SO_2, O_2, etc.) modified in their molecular and toxicological characteristics due to involvement in chemical reactions in the atmosphere.

AirQ models, in fact, can be distinguished in two big groups based on the chemical reactions involved.

The so-called non-reactive models are applied to pollutants such as CO and SO_2 for the simple manner in which their chemical reactions can be described (Luong 2014). In contrast, "*reactive models*" address complex mechanisms common to atmospheric photochemistry and regard pollutants such as NO, NO_2, and O_3. AirQ models, which also involve GIS matching (Batterman et al. 2010), fall into three major categories: dispersion, photochemical models, and receptor models (Luong 2014). Generally, an AirQ model does not contain all characteristics of the real system but contains the features of interest for the scientific problem we wish to solve through its use.

Dispersion model

An atmospheric "*dispersion model*" is a mathematical simulation of the physics and chemistry governing the transport, dispersion, and transformation of pollutants in the atmosphere. When we want to estimate the concentration of air pollutants at ground-level receptors near emission sources or we want to determine the compliance of concentrations measured with respect to the national or international Air Quality standards (see Table 1), the dispersion model can be used. So, the dispersion models are widely used in the risk assessment of hazardous effects of air pollution on humans and the environment (Van Leuken et al. 2016). However, large is the range of its possible applications: assessment of emission compliance with guidelines, criteria, and standards for a clean air; evaluation of environmental impact of new plants; determination of appropriate chimneys' heights; management of emissions already existing; planning of air monitoring networks; identification of the main sources to air pollution; evaluation of the efficacy of mitigation strategies around air emissions; forecast of pollution episodes, etc.

Modern dispersion models are computer programs that calculate the pollutant concentration downwind of a source using information on the following:

- Contaminant emission rate
- Characteristics of the emission source
- Local topography
- Meteorology of the area
- Ambient or background concentrations of pollutants

The dispersion models are most useful for pollutants that are dispersed over large distances and that may react in the atmosphere with O_3, NO_2, etc. The dispersion models can be applied for the simulation of air pollutant concentrations from different emission sources (line, point, and area sources) at both local and regional scales (Luong 2014; Irwin 2014; Pan et al. 2014; Batterman et al. 2010).

This model is carried out through four stages: data input, dispersion calculations, derivation of concentrations, and finally, analysis. The accuracy and uncertainty of each stage must be known and evaluated to ensure a reliable assessment of the significance of any potential adverse effects.

There are two levels of the dispersion model: the simple *screening dispersion models* and the more sophisticated models also called *refined dispersion models*.

In fact, when the screening model (use preset, worst-case meteorological conditions with the aim of eliminating the need of more detailed modeling for those sources) proves clearly that there are no expected concentrations in excess with respect to the legal air standards, we do not need a second-level model. When the concentrations exceed the legal air standards, the more sophisticated model should be applied by scientists. All analytical techniques that allow a more complete treatment of physical and chemical atmospheric processes represent the second level of the model. More detailed and accurate input data are needed for this approach. Through these models, scientists are capable of making an accurate estimate of the source impact and the effectiveness of control strategies. The combined approach of the two models would be desirable; however, very often, the only screening is the only viable option for estimating the source impact.

The sources of pollutants can be classified as point, line, and area/volume sources.

The meteorological data used as input to a dispersion model should be selected on the basis of spatial and temporal representativeness. The representativeness of data is dependent on the following:

1. The proximity of the meteorological monitoring site with respect to the analyzed geographical area
2. The geomorphology of land (plains, hill's presence, etc.)
3. The exposure of the meteorological monitoring site
4. The period of time during which input data are collected

In particular, more attention should be dedicated to topographic data because they can to lead evaluation errors (Luong 2014; Irwin 2014).

The most commonly used dispersion models are Box, Gaussian plume, and Lagrangian models.

Box model

The Box model is the simplest of the dispersion model types, assuming that the airshed or a given volume of atmospheric air has a box shape. It also assumes that the air pollutants inside the box are homogeneously distributed and uses that assumption to estimate the average pollutant concentrations anywhere within the box. However, although useful, this model is very limited in its ability to accurately predict the dispersion of air pollutants over an airshed because the assumption of homogeneous pollutant distribution is much too simple and not real.

Gaussian plume model

The Gaussian plume model is the oldest (ca. 1936) and most commonly used model type. It assumes that the air pollutant dispersion has a Gaussian distribution, so that the pollutant distribution has a normal probability distribution. Gaussian models are most often used for predicting the dispersion of continuous air pollution plumes originating from ground-level or elevated sources. Gaussian models may also be used for predicting the dispersion of non-continuous air pollution plumes also called "puff models." Several primary algorithms are used in Gaussian modeling.

Lagrangian model

The Lagrangian model is a dispersion model that mathematically follows pollution plume particles. In fact, using this approach is possible to show how the particles move in the atmosphere, and they model the motion of the parcels as a random walk process. The Lagrangian model then calculates the air pollution dispersion by computing the statistics of the trajectories of a large number of pollution plume parcels. A Lagrangian model uses a moving frame of reference as the parcels move from their initial location; in fact, it is said that with a Lagrangian model, we follow along with the plume.

Eulerian model

An Eulerian dispersion model is similar to a Lagrangian model but differs in that the Eulerian model uses a fixed three-dimensional Cartesian grid as a frame of reference rather than a moving frame of reference as in the Lagrangian model.

Computational fluid dynamics

CFD is a model for an area's wind and turbulence and both the contaminant's transport and dispersion. It is becoming the more accepted AirQ model by the community as a useful means to understand the complex flow and the resulting dispersion behavior. Zhong has been using the alternative of the computational fluid dynamics or CFD (a numerical simulation). The CFD model gives an insight into flow patterns that are difficult, expensive, or impossible to study using traditional (experimental) techniques. CFD provides a qualitative and/or quantitative prediction of fluid flows (Tong et al. 2016; Sun et al. 2015) through the following:

- The mathematical modeling (partial differential equations)
- The numerical methods (discretization and solution techniques)
- Software tools (solvers, preprocessing and post-processing utilities)

CFD allows scientists and engineers to perform certain numerical experiments using some computer simulations for the virtual flow laboratory tests. Normally, CFD does not replace the field measurements completely, but the amount of experimentations and the overall costs can be significantly reduced. Indeed, both the equipment and personnel are very difficult to transport with respect to CFD software that is easily portable and easy to use and modify. However, the results of a CFD simulation are not 100% reliable for many reasons as the following: the input data may involve imprecision; the mathematical model chosen may be inadequate; and finally, the accuracy of results is limited by the available computing power. The reliability of CFD simulations however is more affordable for laminar/slow flows, for single-phase flows, and for chemically inert systems. In addition, CFD is a highly interdisciplinary research area which needs concepts of physics, applied mathematics, and computer science. The most comprehensive applications of CFD have been based on Reynolds-averaged Navier–Stokes (RANS) equations and large eddy simulation (LES). RANS can only predict mean information about the flow and pollutant fields, while LES also provides turbulence information about unsteadiness and intermittency (Zhong et al. 2015). Zhong's study (dispersion and transport of reactive pollutants in a deep urban street canyon using LES) demonstrates the validity of this approach to quantify parameters for a simplified two-box model, which could support traffic management and urban planning strategies and personal exposure assessment (Luong 2014; El-Fadel and Abi-Esber 2012; Di Menno di Bucchianico et al. 2014).

Many dispersion models have been validated as, e.g., the following:

- *ADMS*: the ADMS or the atmospheric dispersion modeling system is the latest atmospheric pollution dispersion model used for the calculation of concentrations of air pollutants emitted both continuously from point, line, volume, and area sources and intermittently from point sources. The ADMS 5 Service Pack 1 is the modern version (2013) and was developed by Cambridge Environmental Research Consultants in collaboration with other UK Agency and Universities in 1993. This version allows up to 300 sources, 30 line sources, 30 area sources, and 30 volume sources which may be modeled. This model includes algorithms which consider downwash effects of nearby buildings within the path of the dispersing pollution plume; the effects of complex terrain; effects of complex terrain; wet deposition, gravitational settling, and dry deposition; short-term fluctuations in pollutant concentration; chemical reactions, etc. The system also includes a meteorological data input preprocessor. The ADMS model allows to simulate passive or buoyant continuous plumes but also short-duration puff releases. It characterizes the atmospheric turbulence by two parameters, the boundary layer depth and the Monin–Obukhov length.
- *AERMOD*: it was introduced in USA by the American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee (AERMIC), and it was used instead of the old ISC3 (Gaussian plume model) (Silverman et al. 2007). AERMOD is an air dispersion model on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, as well as simple and complex terrains. The AERMOD modeling system is based on two input (regulatory components) data processors: AERMET, a meteorological data preprocessor that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, and AERMAP, a terrain data preprocessor that incorporates a complex terrain using USGS Digital Elevation Data. AERMOD includes also AERSCREEN, a screening version of AERMOD, AERSURFACE, a surface characteristics preprocessor, and BPIPPRIME, a multibuilding dimensions program incorporating the GEP technical procedures for PRIME applications; all of them are non-regulatory components. At this time, AERMOD does not calculate design values for the lead NAAQS (rolling 3-month averages), so a post-processing tool named LEADPOST is available to calculate design values from monthly AERMOD outputs (EPA 2005). Frost carried out an evaluation through the steady-state dispersion model AERMOD to determine its accuracy at

predicting hourly soil concentrations of SO_2 by comparing model-predicted concentrations to monitored data in a year. This study showed to overpredict and to underpredict bias that is outside of acceptable model performance measures (Frost 2014).

- *ATSTEP* is a Gaussian puff model used for the assessment and forecasting of the atmospheric dispersion, deposition of gamma radiation, and doses of released radioactivity in case of accidents in nuclear power plants or during transport of nuclear technologies. This forecasting AirQ method was developed by the Karlsruhe Institute of Technology (KIT) of Germany and is designed for running in the Real-time On-line DecisiOn Support (RODOS) system for nuclear emergency management. RODOS is used for radiation protection and for test operations in many European countries.
- *CMAQ* or the Community Multi-scale Air Quality Model is a very sophisticated atmospheric dispersion model developed by the US EPA to manage the regional air pollution problems (e.g., fine particulate levels exceeding the US health standards). In addition, it is used to simulate the emission, diffusion, and deposition of air pollutants that occur in the lower atmosphere. CMAQ has also the capacity to exactly predict air pollutant concentrations resulting from secondary pollution formation. CMAQ is the most used model for its capability in assessing the efficacy of emission control strategies in reducing regional air pollution levels.
- *DISPERSION21* or 2.1 is a local-scale atmospheric pollution dispersion model developed by the Swedish Meteorological and Hydrological Institute in Norrköping. DISPLAY21 has several basic features and capabilities similar to the CALPUFF model.
- *OSPM*: The Operational Street Pollution Model (OSPM) is an atmospheric dispersion model used for simulating the dispersion of air pollutants in so-called street canyons. It is a model developed by the Department of Atmospheric Environment of National Environmental Research Institute of Denmark, and the model has been maintained by the Department of Environmental Science at Aarhus University since 2011. OSPM has been used in many countries for several finalities including urban pollution assessment, evaluation of data by monitoring campaigns, assessment of effectiveness of pollution abatement strategies, etc., during about 20 years. OSPM is considered as a state of the art on the field of urban pollution modeling. The model is designed to work with both input and output (as 1-h averages). The turbulence produced by the road traffic (TPT) is acting in addition to the turbulence caused by the roof level wind. This results in a faster dispersion of the direct plume but also an improved air exchange at roof level between the street canyon and the background air (Ottosen et al. 2015).
- *RIMPUFF*: this model is a local-scale puff diffusion model developed in Denmark. It is a model aimed at helping emergency management organizations toward chemical, nuclear, biological, and radiological releases to the atmosphere. It is being used in several European national emergency centers for preparedness and in the prediction of nuclear accidental releases, chemical gas releases, and the airborne spread of foot and mouth disease virus. Its range of application covers distances up to ~1000 km from the source. RIMPUFF calculates the instantaneous atmospheric dispersion and wet and dry deposition, taking into account the local wind variability, turbulence levels, and other meteorologic factors. Puff diffusions are parameterized for travel times in the range from a few seconds up to 1 day.
- *TSCREEN*: The Toxics Screening Model (TSCREEN) is a Gaussian model that implements the procedures to correctly analyze toxic emissions and their subsequent dispersion from one of several different types of possible releases for superfund sites. It contains three models: SCREEN3, PUFF, and Relief Valve Discharge (RVD). The TSCREEN model is quite useful for screening level analyses; it is user-friendly and is accompanied by a user's guide and a document "Workbook of Screening Techniques for Assessing Impacts of Toxic Air Pollutants (Revised)," containing useful information on air toxics modeling concepts. Banerjee et al. (2011) reported a comprehensive study on the application of mathematical modeling for source contribution assessment (for both industrial and vehicular emissions) in terms of regional air quality in India.
- *SAFE AIR* or Simulation of Air pollution From Emissions Above Inhomogeneous Regions is an Italian advanced dispersion model for calculating air pollutant concentrations released both evermore or intermittently from point, line, volume, and area sources. It uses an integrated Gaussian puff modeling system and is based on three main parts: a meteorological preprocessor Wind-field Interpolation by Non Divergent Schemes (WINDS) to calculate wind fields, the Acquisition of Boundary Layer parameters (ABLE) meteorological preprocessor to calculate atmospheric pollutants, and finally, a Lagrangian multisource model named P6 (Program Plotting Paths of Pollutant Puffs and Plumes) to plot pollutant dispersion. SAFE AIR is used both by the European Environment Agency (EEA) and the Italian Agency for the Protection of the Environment (APAT).
- *CALINE3* or CAlifornia LINE Source Dispersion Model is a Californian steady-state Gaussian dispersion model planned to identify pollution concentrations at receptor locations downwind of highways located in relatively uncomplicated terrains.

- *PUFF PLUME* is a model used to forecast how air pollution disperses in the atmosphere. It is a Gaussian atmospheric dispersion model for transport chemical/radionuclide.
- *CALPUFF* is an advanced and integrated Lagrangian puff modeling system for the simulation of atmospheric pollution dispersion that has been adopted by the US EPA in its "*Guideline on Air Quality Models*". EPA uses this model for assessing long-range transport of pollutants and their impacts on US areas and on a punctual basis for certain near-field applications involving complex meteorological conditions. CALPUFF consists of three main components: CALMET (a diagnostic three-dimensional meteorological model), CALPUFF (an air quality dispersion model), and CALPOST (a data processing package). The CALPUFF model is designed to simulate the buoyant, puff, or continuous point dispersion as well as continuous line sources. The model is important because it also includes algorithms for handling the effect of downwash by nearby buildings in the path of the pollution plumes.
- *FLEXPART*: The FLEXible PARTicle dispersion model is a Lagrangian particle dispersion model used to simulate air pollutant trajectories. It can be run in either forward mode to determine the downwind concentration or mixing ratio of pollutants or in backward mode to know the origin of observed emissions. In 2013, a major update of FLEXPART-WRF was released, including a working wet deposition scheme, and new run-time options for wind fields and turbulence were added.
- *HYSPLIT*: The Hybrid Single-Particle Lagrangian Integrated Trajectory model is an Australian (Australia's Bureau of Meteorology) computer model that is used to calculate air trajectories, dispersion, or deposition of several atmospheric pollutants. HYSPLIT's back trajectories coupled to satellite images can help to understand if pollution levels are produced by local air pollution sources or moved by wind from another source area.
- NAME III is a Lagrangian air pollution dispersion model used for both short- and global-range scales. It follows the three-dimensional trajectories of parcels of the pollution plume and computes pollutant concentrations by Monte Carlo methods. NAME III has the capability to calculate several effects: the rise of buoyant plumes, wet deposition, dry deposition, plume chemistry, plume depletion for the radioactive materials, and downwash effects of buildings.

Land use regression model

For a correct epidemiologic study, exposure assessments must be carried out accurately in unmonitored areas, for a better evaluation of health effects of air pollution. In order to minimize the possible exposure misclassification, several methodologies are used. Possible methodologies include, but are not limited to, spatial interpolation, proximity models, and still dispersion modeling.

Land-use regression (LUR) modeling is also an effective and valuable method for estimating fine-scale distributions of ambient air pollutants (Oiamo et al. 2015), and generally, the LUR model has been used to identify and describe air pollution exposure and its health effects for citizens within urban areas.

Several studies are available with a LUR approach, but among these studies, the most used variables are road type, traffic count, elevation, and land cover (Ryan and LeMasters 2007). It is possible to use the CALINE model for this scope, but several uncertainties could cause errors of air pollution characterization; in fact, small-scale variations in pollutant concentrations are not identifiable using the interpolation techniques density monitoring and spatial distribution of traffic sources (Shmool et al. 2014). Moreover, the proximity models have a higher chance of exposure misclassifications due to the assumption of isotropic dispersion and/or the use of a categorical exposure designation as the residence (<100 m = exposed, residence >100 m = unexposed). In order to solve these limitations, LUR models have been developed and utilized to model traffic pollutants including NO_2 and $PM_{2.5}$, representing a valuable environmentally epidemiologic tool. LUR models, for the discussed motifs, have emerged as a widely used approach for characterizing long-term, local-scale spatial variability in urban air pollutants such as PM, NOx, VOCs, metals, etc. (Zhang et al. 2015). In recent times, the de Hoogh research group (de Hoogh et al. 2013) developed an LUR model for eight $PM_{2.5}$ components in over 15 European cities. LUR modeling has therefore sproven particularly useful in assessing long-term exposure to air pollution in community health studies carried out by epidemiologists (Zhang et al. 2015; Gillespie et al. 2016; Yang et al. 2016; Fehsel et al. 2016; Perron et al. 2016; Wu et al. 2016). The Health Effects Institute of Boston, Massachusetts, recommended LUR modeling as a more accurate method for estimating exposure to air pollution compared to previous methods (Health Effects Institute 2010). LUR uses the air pollutant levels of interest as the dependent variable and vehicular traffic, topography, and other geographic variables as independent variables in a multivariate regression model. By LUR, air pollutant's concentrations may be predicted for any location by the parameter estimates derived from the regression model. The addition of site-specific variables permits detection of very small area variations more effectively than other methods of interpolation (Ryan and LeMasters 2007).

Peng used a mass balance-based regression for modeling PAH accumulation in urban soils and highlighted the role of urban development in this topic (Peng et al. 2015). Peng, through this model, showed that the total PAH concentrations would increase from the baseline of 267 to 3631 ng/g during the period of 1978–2048. Peng showed also that the dynamic changes in the rates of accumulations of light and heavy PAH species were related to the shifting of sources of fuels, combustion efficiencies, and amounts of energy consumed during the course of development of Beijing (Peng et al. 2015).

Several other studies were carried out using the dispersion model; e.g., Preisler used a statistical model for determining the impact of wildland fires on particulate matter ($PM_{2.5}$) in Central California aided by satellite imagery of smoke. However, when he has matched the data with an autoregressive statistical model that uses weather and seasonal factors to identify thresholds for flagging unusual events at these sites, he found that the presence of smoke plumes could reliably identify periods of wildfire influence with 95% accuracy (Preisler et al. 2015).

Research and forecasting (WRF) model

The WRF Model is a next-generation mesoscale numerical weather prediction system designed for both atmospheric research and operational forecasting need (Karl et al. 2015). The WRF/Chem model has the advantages to integrate the meteorological and chemistry modules in the same computational grid and the same physical parameterizations and includes the feedback between the atmospheric chemistry and physical processes. The WRF system contains two dynamical solvers, referring to the Advanced Research WRF (ARW) core and the Nonhydrostatic Mesoscale Model (NMM) core. WRF is currently in use. The model serves a wide range of meteorological applications and is applied to various scales, from tens of meters to thousands of kilometers. WRF can generate atmospheric simulations using real data (observations, analyses) or idealized conditions. WRF offers operational forecasting and flexible and computationally efficient platforms, while providing recent advances in physics, numerics, and data assimilation.

In the study of Karl et al. (2015), the WRF-Chem was applied to quantify the impact of using an impact of the comprehensive photo-oxidative sequence of 2-aminoethanol (MEA) compared to using a simplified MEA scheme. The study showed that MEA emissions from a full-scale capture plant can modify regional background levels of isocyanic acid.

Gencarelli developed a modified WRF-Chem with the aim to simulate the atmospheric processes determining air Hg emissions, concentrations, and deposition online at high spatial resolution (Gencarelli et al. 2014). The model has been tested in the year 2009 using measurements of total gaseous mercury from the European Monitoring and Evaluation Programme monitoring network. The speciated measurement data of atmospheric elemental Hg, gaseous oxidized Hg, and Hg associated with particulate matter, derived from a Mediterranean oceanographic monitoring (June 2009), has permitted to show the model's ability to simulate the atmospheric redox chemistry of Hg. The model has permitted the revaluation of the deposition to, and the emission from, the Mediterranean Sea, and results support the idea that the Mediterranean Sea represents a net source of Hg to the atmosphere and suggest that the net flux is ≈30 mg/year of elemental Hg.

Goto validated a modeling (Stretch-NICAM) for black carbon in Asia using a global-to-regional seamless aerosol transport model (Goto 2014), modifying for this purpose the Nonhydrostatic Icosahedral Atmospheric Model (NICAM) (Satoh et al. 2007). NICAM implements comprehensive physical processes for aerosols, radiation, turbulence, and cloud dynamics (Goto 2014; Goto et al. 2014).

So, various AirQ dispersion models as LUR, AERMOD, etc., are used today as tools for a refined analysis of health data in environmental epidemiological studies of predictive type, through the sophisticated categorical and statistical approach of Air Quality Health Impact Assessment (AirQ 2.2.3) software and its new version AirQ$^+$ (2016) proposed by the WHO (Liu et al. 2015a, 2015b; WHO. World Health Organization 2014) (see par. 8).

Many other models have been developed worldwide. The European Topic Centre on Air and Climate Change, which is part of the European Environment Agency (EEA), manages an online Model Documentation System (MDS) that includes descriptions and other information for almost all of the dispersion models developed by the countries of Europe. The MDS currently (August 2016) contains 142 models, mostly developed in Europe. Of those 142 models, only some were debated in this review (EIONET 2016).

Photochemical models

Photochemical models are useful tools for regulatory analysis and attainment demonstrations by assessing the effectiveness of air pollution control strategies.

These models simulate the changes of pollutant concentrations in air using the mathematical equations characterizing the chemical and physical processes in the atmosphere and can be applied at multiple spatial scales (local, regional, national, and global) (Luong 2014). Photochemical models, however, are used to carry out studies focusing on atmospheric chemistry alone.

Lagrangian (Mészáros et al. 2016) and Eulerian (both single box models and multidimensional grid-based air quality models) reference frames were used in all photochemical models.

In particular, in Eulerian photochemical models, we use a three-dimensional grid superimposed for covering the entire computational domain, and all chemical reactions are simulated in each cell at each time step. In the Lagrangian photochemical models, a single cell or a column of cells are directed according to the main wind in a way that allows an injection of the emission met with along the cell trajectory.

Most of the photochemical models are known to be very sensitive to predict the ground-level expected concentrations of pollutants (Hidy and Blanchard 2015). Most of the photochemical models used currently by scientists are of Eulerian type. Input data for photochemical models can be meteorology, emissions, topography, or atmospheric concentrations data; all inputs are specified in hourly intervals (Luong 2014), and they represent a real source of uncertainty in air models (see paragraph 9).

An important aspect in the use of air quality models is how the pollutant concentrations respond to changes in emission inputs. It is generally acknowledged that the emission inputs are one of causes of uncertainty of results of this model.

The most commonly used air photochemical models are the following:

- UAM-IV, CIT, and CALGRID for urban approach
- RADM, EURAD, NOAA, etc., for regional approach
- SAQM, MAQSIP, EURAD, UAM-V, URM, and MODELS-3/CMAQ for multilevel approach (Luong 2014)

The Urban Airshed Model® (UAM®) modeling system, developed and maintained by Systems Applications International (SAI), is the most used photochemical air quality model in the world today. Since the 1970s, the model has undergone continuous cycles of performance evaluation, update, extension, and therefore, improvement. Many other photochemical models have been developed during these 40 years, but no model today is more reliable or technically superior to UAM (Daly and Zanetti 2007).

Between the photochemical models, the Community Multi-scale Air Quality or CMAQ modeling system includes state-of-the-science capabilities for conducting a multilevel approach, by urban to regional scale simulations of multiple air quality issues, including O_3, PM, toxics, acid deposition, and visibility degradation. The Regional Modeling System for Aerosols and Deposition (REMSAD) was designed to calculate the concentrations of both inert and chemically reactive pollutants by simulating the physical and chemical processes in the atmosphere that directly influence pollutant concentrations over regional scales. It includes those processes relevant to regional haze, particulate matter, and other airborne pollutants, including soluble acidic components and mercury. Urban Airshed Model Variable Grid or UAM-V Photochemical Modeling System was a pioneering effort in photochemical air quality and has been used widely for air quality studies focusing on O_3 by 1970. It is a three-dimensional photochemical grid model developed to measure both inert and chemically reactive pollutant concentrations simulating the physical and chemical processes in the atmosphere that influence air pollutant concentrations. This model is typically applied to model for particular periods during which adverse meteorological conditions result in elevated ozone levels.

Several photochemical model applications provides the EPA including O_3, PM, and mercury for national and regional EPA policy such as the Clean Air Interstate Rule (CAIR) and the Clean Air Mercury Rule (CAMR) but does not assess which emission control strategies are cost-effective and practical to control. Detailed studies were carried out concerning the following:

– The characterization and speciation of VOC (typically, this would include hourly assessment of CO, NO, NO_2, SO_2, and various primary VOCs in the mechanism) (Jathar et al. 2014; Cheng et al. 2013)
– To assess air pollution spatial and temporal variability (Flexible Air quality Regional Model or FARM) (Di Menno di Bucchianico et al. 2014; Maurizi et al. 2013)

The major application of the photochemical model has been to assess the relative importance of VOC (Chen et al. 2010) and NO_x controls in reducing ozone levels. Most studies were found at urban level until regional scales.

For PM modeling, the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System has been recently created allowing emission data through processing methods computing sparse-matrix algorithms. The SMOKE system is currently a significant available resource for the decision-making on air emission controls finalized to both urban and regional applications, and it makes air quality forecasting possible (Luong 2014).

Photochemical processes (often evaluated through the Eulerian model type) not only bring ozone formation but can also contribute significantly to elevated particulate matter levels with several negative consequences on public health.

Receptor models

Receptor-based models utilize chemical measurements at an individual monitoring site (the receptor) to calculate the relative contributions from major sources to the pollution at that site. Receptor-based modeling is also referred to as "source apportionment" (Liao et al. 2015; Jorquera and Barraza 2012; Lowenthal et al. 2010) and allow to forecast and quantify pollutants contributing to receptors (Hu et al. 2014; Gianini et al. 2013). In contrast with dispersion models that compute the contribution of a source to a receptor as the product of the emission rate multiplied by a dispersion coefficient, receptor models start with the observation of concentrations at a receptor and attempt to apportion the measured concentrations at a sampling point among several source types. This is done based on the known and characteristic chemical composition of source and receptor materials. Receptor models are based on mass balance equations and are intrinsically statistical in the sense that they do not include a deterministic relationship between emissions and concentrations. However, mixed dispersion-receptor modeling methodologies have been developed and actually are very promising for future environmental research.

Receptor model types can be as follows:

- Chemical Mass Balance (CMB) currently endorsed by EPA (EPA, Teixeira et al. 2015; Teixeira et al. 2013; Chen and Liang 2013; Argyropoulos et al. 2012) and unmixed (Kelly et al. 2013)
- The most advanced Positive Matrix Factorization (PMF) (Tositti et al. 2014; Peng et al., 2015; Callén et al. 2014; Heo et al. 2014; Gianini et al. 2013; Jeong et al. 2011). "Source" and "receptor" are complementary and not competitive models (Luong, 2014).

These models can be applied to investigate both the sources of occasional episodes of air pollution and the emission inventory (Taiwo et al. 2014; Hackstadt and Peng 2014; Kuo et al. 2014; Tchepel et al. 2014; dos Santos et al. 2014). Most of advanced models permit the incorporation of data of wind trajectory (Inomata et al. 2013).

Stanier and Lee (2014) developed an aerosol screening model (ASM) as predictive model of vehicular ultrafine particles (less than 0.1 μm in diameter).

ASM is very important for its applications, e.g., support of evaluation for decision-making in infrastructure building and emission controls for health prevention.

A novel method called "Source Directional Apportionment" (SDA) was validated by Tian et al. (2015). The SDA method allows to forecast and quantify contributions of each source category from various directions (Koracin et al. 2011). An online source tracking method has been developed in the Nested Air Quality Prediction Modeling System (NAQPMS) coupled with cloud-process module for the first time by Ge et al. (2014).

Various studies have applied different AirQ models (Park et al. 2014; Irwin 2014; Pokorná et al. 2013; Chung et al. 2012; Koracin et al. 2011; Sahu et al. 2011; Friend et al. 2011; Kong et al. 2010), and several works have examined emerging air pollutants. Some investigations have found that no threshold of effect can be identified for the common air pollutants at the population level, involving that an impact (Hu et al. 2014) can be observed in some individuals even at low exposure level (Li and Jia 2014). For instance, no threshold is used for $PM_{2.5}$, and the exposure-response relationship for mortality is not significantly different from linear. Li and Jia have applied a similar approach for their modeling research on the gas/particulate partitioning behavior for PBDEs in air.

Liu et al. (2015a, 2015b) for the first time investigated the sources and contributions of PAHs using three receptor models (principal component analysis (PCA), PMF, and Multilinear Engine 2 (ME2)); thanks to results obtained, for the first time the cancer risks for each identified source were quantitatively calculated by combining the incremental lifetime cancer risk (ILCR) values with the estimated source contributions.

Callén et al. (2014), using a PMF model, assessed the ILCR related to source apportionment of PM2.5-bound polycyclic aromatic hydrocarbons (Callén et al. 2014).

Clarke et al. (2014) used the CMB model, applying it for the first time to solve odor signature issues. In fact, the olfactory annoyance caused by industrial emissions perceived at receptor level is often the result of a combination of different smells. The olfactory annoyance represents a true emerging industrial hygiene problem. Heo et al. (2014) assessed the relationship between fine particle air pollution and mortality using a PMF model in Seoul, Korea.

Gariazzo et al. have developed the EXPAH model. A model to estimate PAH and $PM_{2.5}$ exposure in children and elderly people in Rome (Italy) has been developed and applied using data from the EXPAH project. Unlike the approach of epidemiological studies, which estimate exposure using ambient data from representative sites, this new model assesses exposure by taking into account variables such as indoor concentrations in different living environments estimated based on outdoor air and the daily time spent in each of these environments. Application of the method to a city, starting from the map of ambient air pollutants, allows obtaining an exposure map by applying the exposure formula over the model cells. However, the approach assumes that the individuals studied spend most of their time in the vicinity of their homes, which according to various statistical surveys is particularly true of elderly subjects and children. It should also be considered that they suffer more often from severe health outcomes due to air pollution; the approach is therefore sound also from the scientific standpoint. The pollutant concentration in each microenvironment studied (home, school, work, other indoor sites, walking, commuting, and other outdoor areas) was used to develop an infiltration model to calculate exposure. Based on data provided by the monitoring campaigns carried out in the framework of the EXPAH project (action 3.3), indoor/outdoor infiltration factors were obtained for the main microenvironments identified, by applying a linear best fit procedure that assumes a direct link between indoor and outdoor concentrations. Results demonstrate a good correlation between the two concentrations, pointing at an outdoor origin of the indoor pollutants and demonstrating the applicability of an infiltration factor to estimate indoor concentrations. Starting from the ambient air concentrations estimated by a

Chemical Transport Model over the study area, indoor concentrations were calculated by applying the infiltration factors.

The historical city center was found to be the most exposed, with PAH and BaP concentrations up to 2 and 0.6 ng/m^3, respectively; concentrations declined approaching the outskirts, reaching values as low as 0.4 and 0.12 ng/m^3 on a yearly basis for PAHs and BaP, respectively. The Total Toxicity Equivalent Concentration (TTEC) was also evaluated using the same data, to take into account the toxicity of each PAH compound. Annual average TTECT values of 0.48 ng/m^3 were estimated for children and the elderly. As regards $PM_{2.5}$, yearly average concentrations up to 16 μg/m^3 were calculated in the downtown area. The $PM_{2.5}$ exposure maps showed a more uniform diffusion, with a less marked decline in the outskirts compared with PAHs. No differences were found between PAH and BaP exposure for children and the elderly, whereas small differences were found for $PM_{2.5}$. This is mainly due to the predominance of home and other indoor microenvironments in the daily activities data used for these two groups, which show similar occupancy times. Seasonality was a strong variable in overall exposure. For children, an average exposure to PAHs and BaP up to 4.0 and 1.1 ng/m^3, respectively, was estimated in the winter, and exposures lower than 0.6 and 0.15 ng/m^3, respectively, during the warm season. These data highlight the inability of current legal PAH limits to represent the actual annual average exposure of the population.

Performance of Air Quality models and evaluation of their real-world limitations

The extent to which a specific air quality model is suitable for the assessment of source impacts depends upon several factors as topographic and meteorological complexities of the area; accuracy of emissions inventory, meteorological data, air quality data; and complexities of atmospheric processes.

Meteorological conditions are broadly representative, and air quality model projections are not further complicated if related to areas spatially uniform. Indeed, areas subject to major topographic influences experience meteorological complexities that are often difficult to measure and simulate. Models with adequate performance are available for increasingly complex environments.

The monitoring of the impact of point sources on the ambient air quality is still a difficult task, in particular for elevated sources. The difficulty is linked to the complexity and unpredictability of meteorological elements that control the dispersion of air pollutants. It should be noted that because of the high variability of the wind direction, the sites of maximum pollution are not predictable. In fact, the elevated point sources emit well above the ground and, in case of temperature inversion, frequently above the inversion layer. The meteorological conditions observed during "normal" conditions, instead, generally ensure a good dispersion of the pollutants. Under very turbulent atmospheric conditions characterized by thermal instability of the atmosphere associated with strong insolation and weak winds, the plume of the point sources of medium elevation may reach the ground in the vicinity of the source, giving rise to exceedances of short-term limit values.

Such complexities and related challenges for the air quality simulation should be considered when selecting the most appropriate air quality model for an application. Another important aspect of air quality models is how the pollutant concentrations respond to changes in emission inputs. It is generally acknowledged that the emission inputs are one of causes of uncertainty of results of models.

The operational evaluations of different air quality models have yielded an array of statistical metrics that are so diverse and numerous that it is difficult to judge the overall performance of all air models.

For US EPA (2015), the air quality models are accompanied by several sources of uncertainty. An "irreducible" uncertainty stems from the "unknown" conditions as the turbulent velocity field which may not be correctly counted for in the model. So, there are deviations than the observed concentrations in individual events due to variations in the "unknown" conditions.

We can synthesize the uncertainties in the following:

1. Uncertainties in the input conditions (emission characteristics and meteorological data are an example)
2. Errors in the measured concentrations
3. Inadequate model physics and formulation

The main meteorological parameters that affect negatively the accuracy of air quality models predictions are therefore

- Boundary layer depth
- Surface and boundary layer wind speed and direction
- Surface and boundary layer temperatures
- Turbulence
- Surface parameters
- Cloud cover and solar radiation
- Cloud microphysics
- Precipitation

Errors in meteorology are still a major source of error in all air quality models. If the model wind does not affect air pollutants correctly, then all models will not predict the observed pollution episodes, irrespective of the air quality modeling system used.

For example, the deposition episodes during rain events represent a very difficult condition to model accurately because not only wind speeds and directions must be accurately predicted but also the occurrence and magnitude of rainfall.

Competent and experienced atmospheric scientists, meteorologists, and physical and software analysts are an essential prerequisite to the successful application of air quality models. The need for such specialists is critical when the more sophisticated models are used or the area being investigated has very complicated meteorological or topographic features. In fact, it is important to note that a model applied improperly or with inappropriate data can lead to serious errors regarding the source impact or the effectiveness of a control strategy.

Suitability of Air Quality models

Gaussian plume models use a "steady-state" approximation, which assumes that over the model time step, the emissions, meteorology, and other model inputs are constant throughout the model domain, resulting in a resolved plume with the emissions distributed throughout the plume according to a Gaussian distribution. However, this formulation allows for only relatively inert pollutants, with very limited considerations of transformation and removal (e.g., deposition), and further limits the domain for which the model may be used. Thus, Gaussian models may not be appropriate if model inputs are changing sharply.

Lagrangian puff models, instead, are non-steady-state and assume that model input conditions are changing over the time step. Lagrangian models can also be used to determine near- and far-field impacts from a limited number of sources with a high resolution. Generally, Lagrangian models have been used for relatively inert pollutants but are more complex than Gaussian models. Some Lagrangian models treat in-plume gas and particulate chemistry. Photochemical Eulerian models assume that emissions are spread evenly throughout each model grid cell. Typically, Eulerian models have difficulty with fine-scale resolution of individual plumes. However, these types of models can be appropriately applied for assessment of near-field and regional-scale reactive pollutant impacts from specific sources or all sources.

In a proposed rule, the US EPA (2015) reports a list of AirQ Models useful both for any air pollution prevision and classical contaminants.

A procedure for air quality models benchmarking was defined in EU by SubGroup4 of WG2 in Forum for Air quality Modelling in Europe (FAIRMODE) (Thunis et al. 2011). WG2 is involved in the benchmarking of emission inventories in selected cities. The proposed procedure was meant as a support to both model users and model developers. The benchmarking procedure was finalized to support modeling groups in their application of AirQ models in the frame of the European Air Quality Directive (2008). This procedure is based mainly on already existing technical aids: the evaluation tools developed in the CityDelta (CD) and EuroDelta (ED) of European projects (the advantages of using this tool is that every group will use the same scale and also a decent level of harmonization will be reached across EU) and the ENSEMBLE European systems (a web-based platform developed for multipurpose model application that allows on-line model inter-comparison and evaluation). These tools can be properly adapted and renewed taking into account the experience gathered worldwide on air quality model evaluations and available software. Some of the most known ones include the Model Validation Kit of the Harmonization initiative which contains the BOOT software (Chang and Hanna 2004), the ASTM Guidance (ASTM 2000), the USA-EPA AMET (Appel and Gilliam 2008) package, and the VERDI tool.

The added value of the proposed procedure by the European Council derives from the fact that all AirQ models used for regulatory purposes will be evaluated with a single model tool and will have a common place where to compare, assess, and experiment each other's case study, both on past or present, using the online web facility; furthermore, the data relevant to various types of analysis will be available from a single source point.

AirQ software

Recently, several sophisticated approaches have been used in environmental epidemiological studies to refine the spatial resolution of monitoring data by applying geographic information systems (GIS)-based interpolation methods. Also, LUR models are available in modern epidemiological literature for the analysis of cohort study health data. LUR models, in fact, integrate some landscape characteristics such as proximity to roadways and other outdoor sources of air pollution. So today, it is very easy to come across approaches that use air quality models (e.g., AERMOD, etc.) and micro-environmental personal exposure modeling tools to support air pollution exposure and health studies. Some studies have also used results from atmospheric dispersion models for a refined analysis of health data (Isakov et al. 2009; Callén et al. 2014; Liu et al. 2015a, 2015b).

The WHO European Center for Environment and Health (WHO 2014) has proposed AirQ software model 2.2 as a valid and reliable tool to estimate the potential health effects of air pollution, to assign score points to criteria pollutants, and to enable assessment of scenarios characterized by varied pollutants.

AirQ software is a Windows software that collects, manages, and displays results from air quality information data and noise levels. It is designed to calculate the magnitude of the impacts of air pollution on health in a given population. AirQ software 2.2.3 and the new version AirQ+1.0 software

(WHO 2016) can be applied for any city, country, or region of the world to reply to important epidemiological and ecological questions such as the following: How much of a particular health outcome is attributable to selected air pollutants? or Compared to the current scenario, what would be the change in health effects if air pollution levels changed in the future?

The program keeps a searchable database of results, so data can be picked out by sample, location, and date. It can plot linear graphs of readings with time, or polar ones against wind direction. The approach proposed by the WHO can be classified into categorical and statistical groups (WHO. World Health Organization 2014). The approach was based on the Air Quality Health Impact Assessment (AirQ 2.2.3) software developed by the WHO European Centre for Environment and Health, Bilthoven Division. The software was used to estimate the impact of short-term exposure to six classic atmospheric pollutants (O_3, CO, NO_x, SO_x, PM_{10}, and $PM_{2.5}$) on the health of residents living in a certain period and area.

The program is designed to evaluate the following:

- The impact of exposure to atmospheric pollutants on mortality and morbidity (both chronic and acute diseases)
- Impacts on health caused by long-term exposure, assuming that the pollution level remains constant during the simulation years

The health impact is measured by the following:

- Reduction in life for certain classes of age
- Years of life lost (Yoll) in the first year of the simulation
- Years of life lost in the subsequent 10 years (Fattore 2008)

The assessment is based on the attributable proportion (AP), defined as the fraction of the health outcome in a certain population attributable to exposure to a given atmospheric pollutant. The AP is calculated by a general formula:

$$\mathrm{AP} = \sum\{(\mathrm{RR(c)}-1) \times \mathrm{P(c)}\} \Big/ \sum(\mathrm{RR(c)} \times \mathrm{P(c)})$$

where AP is the attributable proportion of the health outcome, RR is the relative risk for a given health outcome, and P(c) is the amount of the population in category "c" of exposure. If the baseline frequency of the health outcome in the population being investigated is known, the rate attributable to the exposure can be calculated as

$$\mathrm{IE} = \mathrm{I} \times \mathrm{AP}$$

where IE is the rate of the health outcome attributable to the exposure and I is the baseline frequency of the health outcome in the population under investigation.

Finally, when the size of the population is known, the number of cases attributable to the exposure can be estimated as

$$\mathrm{NE} = \mathrm{IE} \times N$$

where NE is the number of cases attributable to the exposure and N is the size of the population studied.

The approach proposed by the WHO has not been widely adopted; in fact, only five papers are found in Medline (Ghozikali et al. 2015; Gholampour et al. 2014; Naddafi et al. 2012). Of these, four were published between 2011 and 2014: three are Iranian studies and one is an Italian study. The Iranian scientists are very interested in this application because of the poor air quality of Iranian cities. If one considers all the papers published worldwide, the total is about 10. In particular, Fattore et al. 2011 assessed the outcomes of $PM_{2.5}$ exposure and found that short-term exposure was the most significant health impact on 24,000 inhabitants of two Italian cities. This study showed that O_3 and NO_2 each caused about three excess cases of total mortality.

In Iran, Ghozikali and colleagues (2016) have examined the associations between O_3, NO_2, and SO_2 concentrations and hospitalizations for COPD among the residents of Tabriz and found that for every 10 μg/m^3 increase in their concentrations, the risk of hospitalization increased by about 0.58, 0.38, and 0.44%, respectively.

Miri et al. (2016) have studied the effect (total mortality, cardiovascular and respiratory mortality, hospitalization due to cardiovascular and respiratory diseases, chronic obstructive pulmonary disease, and acute myocardial infarction) of PM_{10}, $PM_{2.5}$, NO_2, SO_2, and O_3 pollutants on people's health of Mashhad city. Miri et al. report that for each 10 μg/m^3, a relative risk rate of pollutant concentration for total mortality due to PM_{10}, $PM_{2.5}$, SO_2, NO_2, and O_3 was increased by 0.6, 1.5, 0.4, 0.3, and 0.46%, respectively, and the attributable proportion of total mortality attributed to these pollutants was equal to 4.24, 4.57, 0.99, 2.21, 2.08, and 1.61% (CI 95%), respectively, of the total mortality (correct for the non-accident) that occurred in the year of study.

Gholampour et al. 2014 have studied outdoor PM exposure and health impacts in two urban and industrial areas in Tabriz. The deaths associated with TSP, PM_{10}, and $PM_{2.5}$ concentrations were 327, 363, and 360, respectively; cardiovascular mortality for TSP and PM_{10} was 202 and 227, respectively; and mortality due to respiratory disease was 99 (TSP) and 67 (PM_{10}). The study by Naddafi and co-workers was performed in Tehran and examined PM_{10}, SO_2, NO_2, and O_3 concentrations to assess human exposure and health impacts in terms of attributable proportion of the health outcome, annual number of excess cases of mortality for all causes, and cardiovascular and respiratory diseases. The annual average concentrations of PM_{10}, SO_2, NO_2, and O_3 were 90.58, 89.16, 85, and

68.82 μg/m^3, respectively. The short-term effects of PM_{10} had the highest health impact on the 8,700,000 inhabitants, causing an excess of total mortality of 2194 out of 47,284 in a year. In contrast, SO_2, NO_2, and O_3 concentrations caused approximately 1458, 1050, and 819 excess cases of total mortality, respectively.

Skotak and Swiatczak (2008) studied the adverse health effect associated with the PM10 exposure in some areas in Poland, and they showed ill-health's endpoints in polluted industrial regions in the southern part of Poland.

Boldo and the Air Pollution and Health: a European Information System (APHEIS) group (2006) have quantified the public health impact of long-term exposure to $PM_{2.5}$ in terms of attributable number of deaths and the potential gain in life expectancy in 23 European cities. Results show 16,926 premature deaths from all causes, including 11,612 cardiopulmonary deaths and 1901 lung-cancer deaths. These deaths would have been prevented annually if long-term exposure to $PM_{2.5}$ levels were reduced to 15 μg/m^3 in each city. So, this reduction would increase life expectancy at age 30 by a range between 1 month and more than 2 years in the APHEIS cities.

Tominz evaluated, in Trieste city, the possible health benefits by exposure reduction of PM_{10} to values not over 60, 50, 40, 30, 20, and 10 μg/m^3, using PM10 data of the year 2002. Tominz found that 1.8% (CI 95% 0.6%; 2.9%) of natural deaths, 2.2% (CI 95% 0.6%; 3.7%) of cardiovascular deaths, 2.5% (CI 95% 0; 7.3%) of respiratory deaths, 1.5% (CI 95% 0.6; 2.4%) of cardiovascular admissions, and 1.6% (CI 95% 0; 3.3%) of respiratory admissions were attributable to PM_{10} concentrations over 20 μg/m^3.

The findings of these very few studies are crucial to improve air pollution management; in fact, the magnitude of certain health impacts underscores the need for urgent action to reduce the health outcomes of air pollution.

AirQ$^+$ is the WHO update version of AirQ software developed in May 2016. Both long- and short-term exposure to ambient air pollution from several pollutants can be studied. All calculations performed by AirQ$^+$ software are based on methodologies and concentration-response functions well established by epidemiological studies. Additionally, AirQ+ can estimate also the effects of household air pollution related to solid fuel use (SFU). Researchers have the possibility to use values for a pollutant not included in AirQ+ database if RRs and other input data are available. However, in this case, it is highly recommended to use results from a meta-analysis rather than from a single local study. The concentration-response functions used in the software are based on the systematic review of all studies available until 2013 and their meta-analysis.

Discussion and conclusion

This brief review highlights that air pollution is still a critical public health issue and that further studies for a better correlation of air quality and population health are required. The AirQ model is intended for exposure assessment, risk assessment, epidemiological and geographical information systems, and other applications. Several approaches can provide useful information for toxicity evaluation of various pollutant categories and to add a new tool of environmental epidemiology. An understanding of air pollutant source transport is crucial, and it is a basic mechanism in determining the fate of air pollutants and their effects on human health. Assessment of the health effects of air pollution requires detailed exposure estimates. However, combining the data from different air monitoring stations appears to underestimate individual exposure. Although most health outcomes are not limited to a single pollutant, nearly all studies focus on the risks related to single pollutants and do not consider their mixtures. There is a clear need to develop methods for evaluating and managing the effects of air pollution through a multipollutant approach. In fact, as the link between air pollution and several illnesses has been established by a long time, air quality forecast will play a very important role in mitigating health risk. If predictions show exceeding pollution levels with respect to legal guidelines, local authorities can take several preventive measures or better manage the risks (e.g., encouraging car drivers to lower their speed, reducing emission from main sources of pollution as industries and home warming, etc.) (Fig. 1).

The knowledge of several public health figures should therefore be harnessed and exploited, and chemists and biologists should work in team with engineers, physicists, and

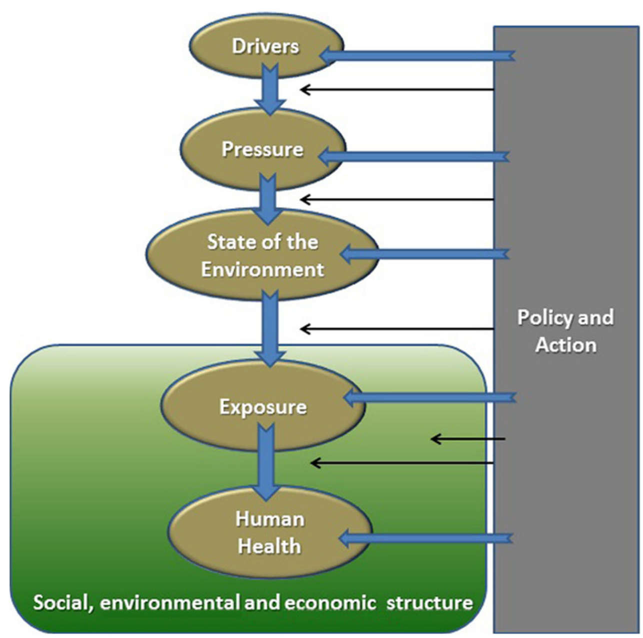

Fig. 1 DEPSEEA flowchart

software scientists, who are becoming increasingly essential, to support population health studies.

Public health is already based on contributions from several disciplines, including engineering, industrial design, and statistics, but today a multidisciplinary training is urgently needed, especially for environmental doctors, whose knowledge is objectively insufficient to apply critically the new tools. The future of public health and of environmental epidemiology therefore needs to be entrusted to a multidisciplinary team that has a deeper knowledge of the new available statistic tools.

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