Air Quality Modelling and Its Applications

Isabel Ribeiro, Joana Valente, Jorge Humberto Amorim, Ana Isabel Miranda, Myriam Lopes, Carlos Borrego, and Alexandra Monteiro

Abstract

Air quality numerical modelling systems are powerful tools for research and policy-making purposes. They describe mathematically the innumerable physical and chemical processes that characterise the atmosphere, with the aim of estimating the air quality levels over a region, ranging from the entire globe to a street, through a long- or short-term analysis. In this chapter an overview on selected air quality models is provided, with examples of numerical applications in the scope of the assessment of the air quality impacts caused by hypothetical changes on emissions, climate and other conditions.

Keywords

Atmosphere • Air quality modelling systems • Emission scenarios • Air quality assessment • Air quality forecasting

1 Introduction

The atmosphere is a complex dynamic and natural gaseous system, essential to support life on planet. Particulate matter and gaseous material emissions from both natural events (like volcanic eruptions, ground dust and salt spray from oceans, among others) and anthropogenic actions (industrial activities, transport services, etc.) may however affect the balance of the atmospheric system and cause air pollution, which could affect human health and damage plants and materials (Jacobson 1999).

The innumerable physical and chemical processes that characterise the atmosphere occur simultaneously and in interdependent ways. The dilution and dispersion of pollutants by turbulent transport, their photochemical transformation, the removing of these pollutants by clouds and precipitation and also their agglomeration and deposition via physical-chemical action on soil surface are the most important processes in the atmosphere when assessing air quality. These processes have been studied over the last decades by physicists and chemists, but a full explanation of their atmosphere behaviour is still a challenge in atmospheric sciences (Atkinson 1989; Seinfeld and Pandis 1998; Jacob and Winner 2009).

Nowadays it is possible to predict air quality through numerical air quality models, with uncertainty estimation. These air quality models describe mathematically the behaviour of the pollutants in the atmosphere taking into account the atmospheric processes.

2 Modelling Approaches

Modelling tools to assess the air quality are diverse and based on different approaches. Probably the most important challenge is to select the right model to the intended application, taking into account its main characteristics and the quality of the data available to run the simulation. In this section, an overview about the characteristics of air quality numerical models is performed.

I. Ribeiro • J. Valente • J.H. Amorim • A.I. Miranda • M. Lopes • C. Borrego • A. Monteiro (✉)
Centre for Environmental and Marine Studies (CESAM), Department of Environment and Planning, University of Aveiro, 3910-193 Aveiro, Portugal
e-mail: alexandra.monteiro@ua.pt

G. Cao and R. Orrù (eds.), *Current Environmental Issues and Challenges*,
DOI 10.1007/978-94-017-8777-2_3,

2.1 Types of Models

Several numerical models for the simulation of the dispersion of gaseous pollutants and particulate matter at different scales are currently available. These may go from simple to extremely complex, including box models, Lagrangian or Eulerian models, Gaussian models and computational fluid dynamics (CFD) models (Kumar et al. 2011).

Dispersion aerosol air quality models are usually simple. These models estimate the concentration of air pollutants at specified receptors, considering the dispersion (atmospheric transport, the turbulent atmospheric diffusion and surface wet/dry deposition) but not the chemical transformation processes. The most simple dispersion models use the Gaussian approach (Lutman et al. 2004).

Chemical transport models simulate the changes of pollutants in the atmosphere using a set of mathematical equations characterising the chemical and physical processes in the atmosphere. They became widely recognised and routinely utilised tools for regulatory analysis and attainment demonstrations by assessing the effectiveness of control strategies.

Based on the mathematical approach, models can be classified as Lagrangian or Eulerian models. Lagrangian models consider air parcels that follow a trajectory defined by the atmospheric circulation. The trajectories are normally calculated as linear segments, with the segment length and direction determined by the average wind speed and direction over the appropriate time step (Draxier and Hess 1998). Figure 1 represents the Draxler and Rolph (2011) work under the Fukushima Daiichi nuclear disaster, as an example of a Lagrangian model application (HYSPLIT4 Trajectory Model). Lagrangian models are computationally relatively simple, and they allow an easy determination of transboundary fluxes, and thus Lagrangian models are especially suitable for small number of sources or receptors. On the other hand, Eulerian models consider a mathematical approach anchored to the atmosphere surface (until few kilometres high). Eulerian models are often referred to as grid models, since the framework is a three-dimensional grid, with pollutants being emitted into the grid at the appropriate points (Fig. 2). Unlike Lagrangian models, Eulerian models can include nonlinear phenomena, especially those associated with physical and chemical processes (emissions, dispersion, transport, chemistry and deposition). Therefore, Eulerian models are computationally more demanding than Lagrangian. To simulate and integrate such processes, these models require input data provided by other models (e.g. meteorological or emission data). It is therefore more correct to refer to a system of models, rather than a model (Reid et al. 2007).

Air quality models can also be classified with respect to the scale of the phenomena they are developed to simulate. In fact, scale separation has proven to be a quite successful approach for atmospheric modelling, because different approximations and parameterisations can be applied for the different phenomena occurring at the different scales.

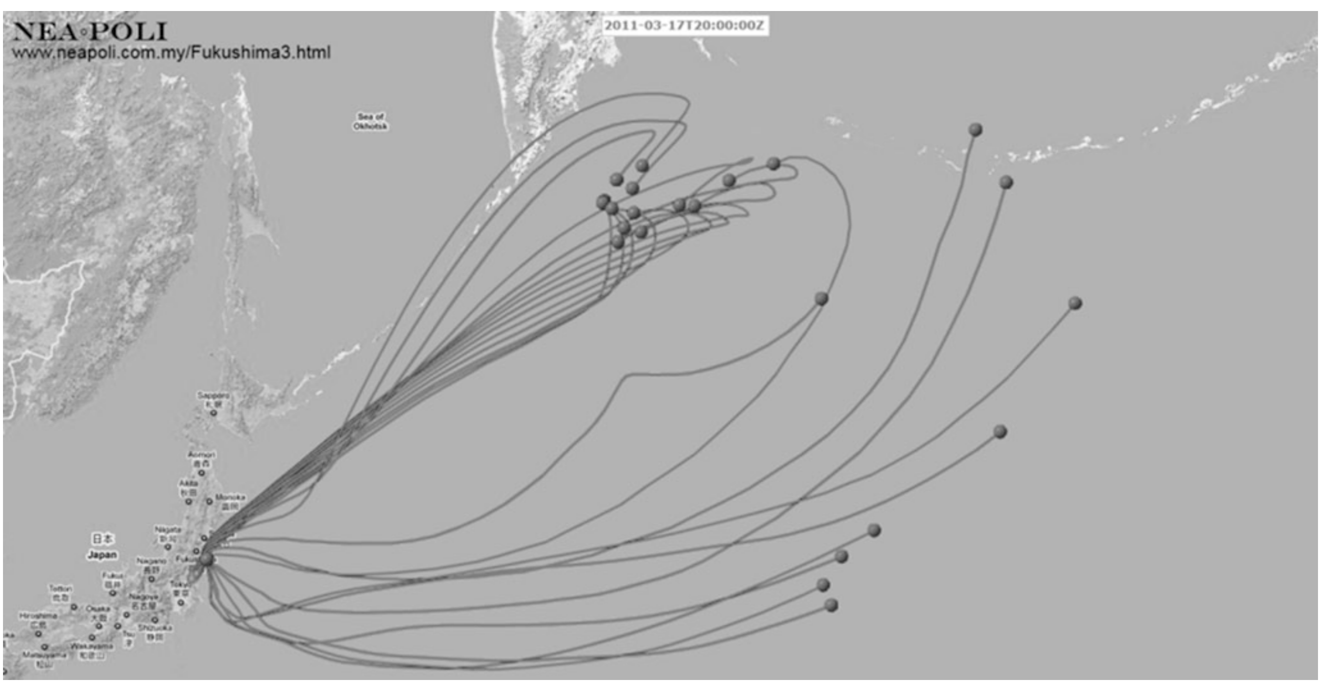

Fig. 1 Dispersion of possibly leaking radioactive substances using HYSPLIT4 Trajectory Model and 5-day forecast meteorological fields from the Global Forecast System Model (*GFM*) (From Draxler and Rolph 2011)

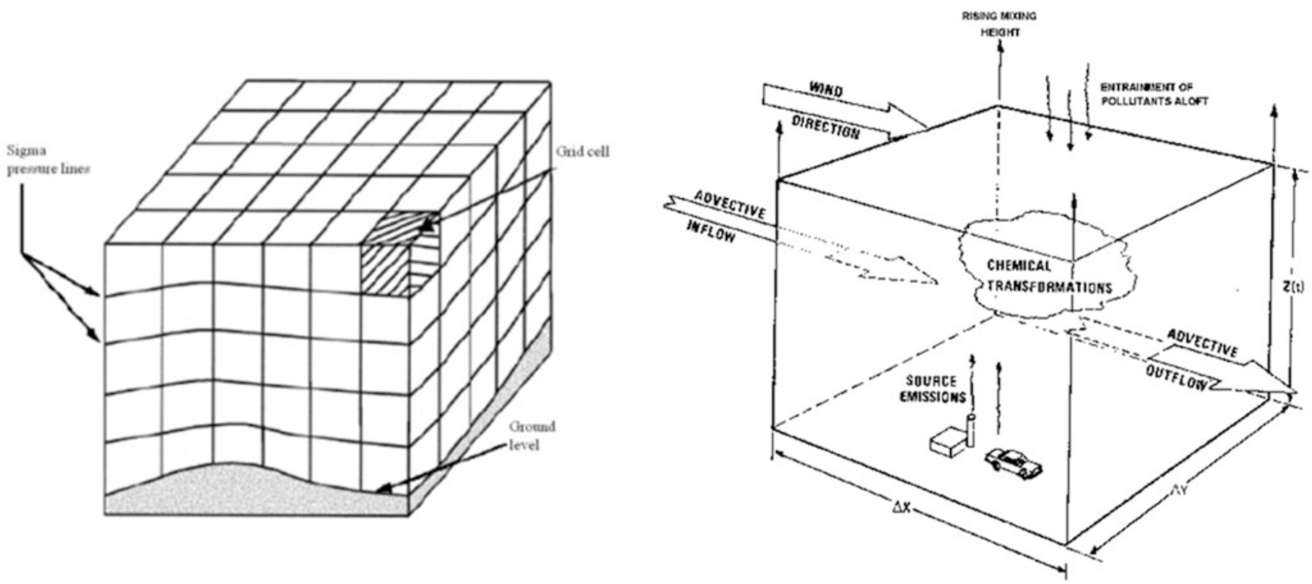

Fig. 2 Eulerian modelling framework (From Reid et al. 2007)

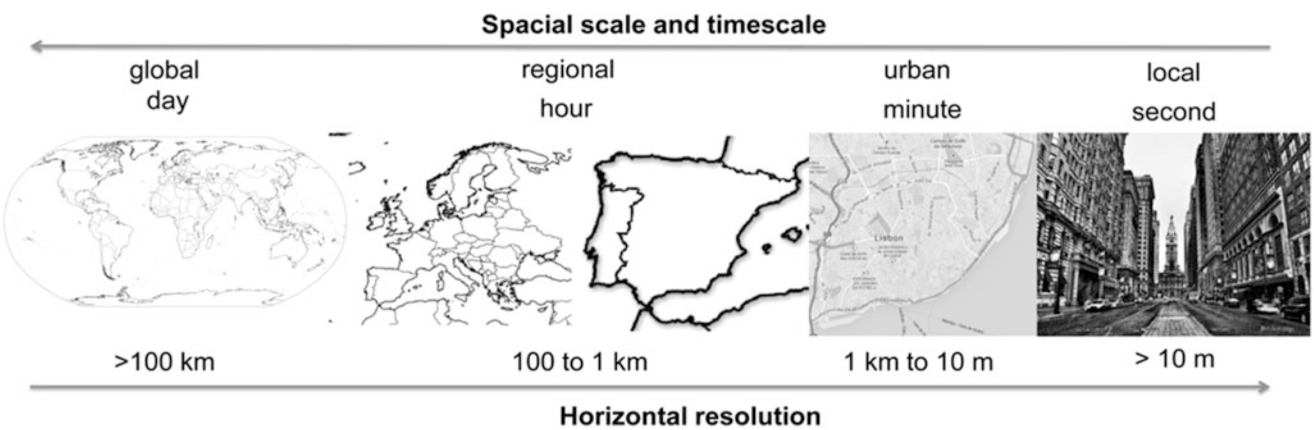

Fig. 3 Time and spatial scales regarding air quality model application

Hence, models can be classified into global, mesoscale (including regional and urban) and local (Fig. 3).

Global models consider the transport of pollutant throughout the atmosphere over the entire surface of the planet. Most global modelling has been confined to climate change issues (with carbon dioxide, CO_2, as the base) with a simplified chemical transport approach. However, expansion to other pollutants has taken place, such as gases (Horowitz et al. 2003) and aerosols (Ginoux et al. 2001), which allow a tighter description and prediction of the chemical composition and evolution of the atmosphere in a future climate. The large spatial extent of these models dictates that the spatial resolution must be relatively coarse to keep the computational demands within reasonable bounds. Mesoscale models consider spatial scales ranging from a few hundred to a few thousand kilometres. This is the spatial scale over which many of the most pressing air pollution concerns are important and is also the scale that often crosses jurisdictional boundaries. In the last years, an increasing body of scientific evidence has demonstrated that air pollution and their mitigation strategies can have significant effects, both positive and negative, on medium-term climate change at the local, regional, and global scales. Increasing evidence also shows that global warming aggravates existing air pollution problems, but most climate change mitigation efforts could have significant co-benefits for air pollution reduction, a win-win opportunity (Borrego 2013).

Local scale modelling is typically used to assess the impact of single sources, or small groups of sources, over distances ranging up to tens of kilometres. CFD modelling is a general term used to describe the analysis of systems involving fluid flow, heat transfer and associated phenomena (e.g. chemical reactions) by means of computer-based numerical methods. These models are based on a better knowledge of the

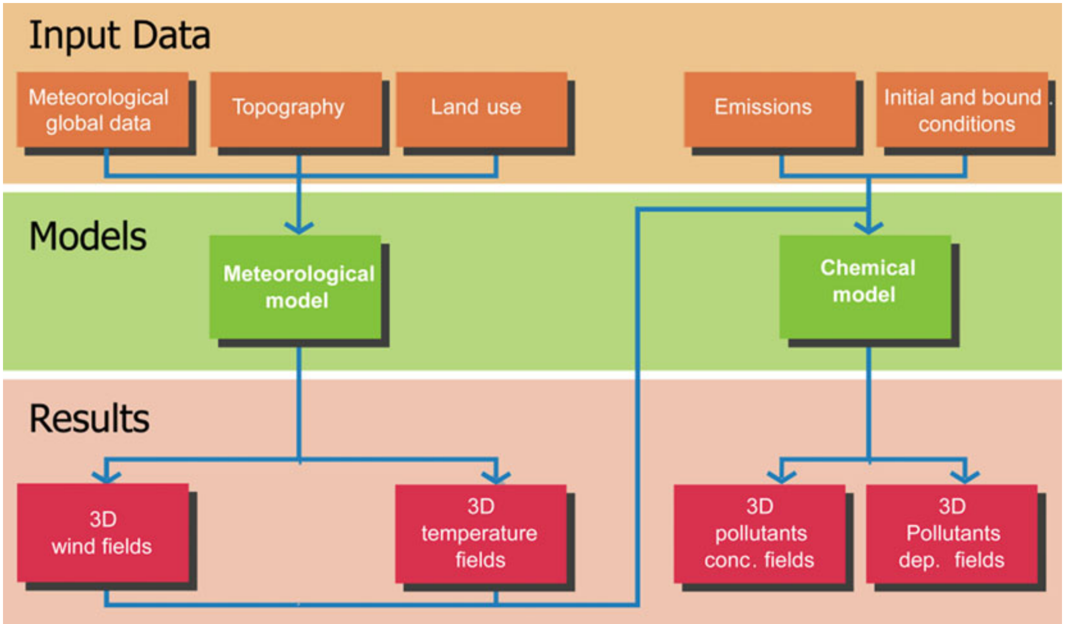

Fig. 4 Scheme of an air quality modelling system

atmosphere structure, using parameterisations of the boundary layer and solving of the Navier-Stokes equations through finite difference and finite volume methods.

The current computational advances allow air quality models to fully couple the meteorology within a unified modelling system (online models) with two-way interactions. However, the most common approach is still the offline system, which only allows one-way coupling from the meteorology – sampled at fixed time intervals – to the chemistry (Grell et al. 2004). This two-way interaction is important because not only can meteorology affect the chemistry through transport, precipitation and radiation processes at each time of the model simulation, but the chemical fields can also impact the meteorological variables. Therefore, online modelling systems are a very promising way for future atmospheric simulations leading to a new generation of models for environmental and chemical weather predictions (Baklanov et al. 2007).

2.1.1 Input/Output Data

Air quality models require a considerable volume of data. The specific needs reflect the methodological approach incorporated in the model, but it typically includes the following variables (Fig. 4):

- Emissions – for all sources treated by the model, the emission is required for each of the chemical species simulated by the model (including each of the species or categories used in the model chemistry), both anthropogenic and biogenic. These emissions should relate to a specific time period being studied.
- Geophysical data – information is required for a range of surface parameters, such as topography, land use and vegetation, and additional data for small-scale modelling, such as building geometry and trees.
- Meteorology – meteorological information is used to force the transport in the air quality model. This information is needed at one or several vertical levels in the atmosphere.
- Initial and boundary conditions – it is usual to specify the initial concentrations for the pollutant species in the model. These will be taken from typical or average values measured, or previously modelled, for the region of interest. It is also necessary to specify concentrations at the boundaries of the model, except for global models. It is relatively simple to estimate initial and boundary conditions at the surface based on measurements, these values are also required at higher levels in the atmosphere, where measurements are sparser. Current practice, which addresses the specification of initial and boundary conditions, is to nest the model.

Output data are usually the temporal and spatial distribution of the air pollutants concentration values.

2.1.2 Model Uncertainty Estimation

Modelling systems can represent suitable tools for air quality studies with an adequate spatial detail and the verification of the limit targets fulfilment and threshold values imposed by the legislative frameworks. Modelling approaches can provide complete spatial coverage information, but models always have uncertainties associated. According to Borrego et al. (2008), total modelling system uncertainty is defined as the sum of model uncertainty, variability and uncertainty on input data. Uncertainties associated with model formulation may be due to erroneous or incomplete representation of the dynamic and chemistry of the atmosphere, incommensurability, numerical solution techniques and choice of modelling domain and grid structure. Variability refers to stochastic atmospheric and anthropogenic processes. It contributes to uncertainties associated with emission estimation and representations of chemistry and meteorology.

The most common way to determine the total air quality modelling system uncertainty is the comparison between observations and predictions data through the application of data quality indicators that reflect the ability of a model (or modelling system) to simulate real phenomena (Borrego et al 2008). According to Chang and Hanna (2004), there are three main components for the evaluation of air quality modelling systems:

- The scientific evaluation, requiring an in-depth knowledge of the model code, examines in detail the model algorithms, physics, assumptions and codes for their accuracy, efficiency and sensitivity.
- The statistical evaluation compares model predictions to observations in order to estimate how well predictions match the observations. However, this direct comparison method may cause misleading results because uncertainties in observations and model predictions arise from different sources (Chang and Hanna 2004).
- The operational evaluation component mainly considers issues related to the user-friendliness of the model (user's guide, user interface, etc.).

However, over the last years, several workshops and papers have addressed that model evaluation criteria are dependent on the context in which models are to be applied (Steyn and Galmarini 2008). For regulatory applications, a model must be able to provide adequate description of the relationships among atmospheric processes and variables in addition to adequate quantitative estimates of species concentrations. On the other hand, under a forecasting activity, a model is judged by its ability to simulate the temporal evolution of chosen forecast variables. Therefore, Dennis et al. (2010) proposed a new framework for model evaluation to determine the suitability of a modelling system for a specific application, composed by four evaluation types:

- The operational evaluation is based on statistics to compare the magnitudes between model estimations and observations, to some selected criteria, through standard metrics (mean bias, root mean square error and correlation factor) and graphical techniques, such as Taylor diagram, time series, scatter plots and performance goal plots ("soccer plots" and "bugle" plots). This type of evaluation makes use of routine observations of ambient pollutant concentrations, emissions, meteorology and other relevant variables.
- The diagnostic evaluation examines the ability of the model to simulate each of the interacting atmospheric processes with implications on air quality. Since a change in a model input does not always lead to a linear response in the model output, diagnostic evaluations are usually complexes. Usually to ascertain whether inputs have influence on model performance issues, sensitivity tests are applied (Saltelli et al. 2004).
- The dynamic evaluation focuses on the ability of the model to predict changes on ambient air pollutant concentrations in response to changes in either source emissions or meteorological conditions. An example of dynamic evaluation would be modelling assessments of the weekday/weekend concentration differences where mobile source emissions are known to significantly change (Chow 2003).
- The probabilistic evaluation acknowledges the uncertainty in model inputs and formulation of processes by focusing on the modelled distributions of selected variables rather than individual model estimates at specific time and location. According to Foley et al. (2008), this approach provides an estimated probability distribution of pollutant concentrations at any given location and time, which can be used to estimate a range of likely concentration values or the probability of exceeding a given threshold value for a particular pollutant.

The framework for model evaluation proposed by Dennis et al. (2010) is used on the Air Quality Modelling Evaluation International Initiative (AQMEII, http://aqmeii.jrc.ec.europa.eu/). Moreover, the Forum for Air Quality Modelling (FAIRMODE activity – http://fairmode.ew.eea.europa.eu/) that aims to promote synergy between the users and exchange of relevant information is also taking into account the same framework. In this sense, a procedure for the benchmarking of air quality models has been developing in order to evaluate model performance and indicate a way to improve their use. The benchmarking model, DELTA Tool (Thunis et al. 2011), takes into account the Air Quality Directive (2008/50/EC) as well as several scientific works related to model evaluation (Hanna et al. 1993; Nappo and Essa 2001; Olesen et al. 2001; Ichikawa and Sada 2002; Pielke 2002; Delle Monache et al. 2006).

3 Applications of Air Quality Modelling

Air quality modelling approaches can successfully support research and policy-making activities, allowing to (1) assess the impacts of changes on urban planning (including green infrastructures) (e.g. Amorim et al. 2013; Borrego et al. 2006, 2011b; Martins 2012), emissions (e.g. Miranda et al. 1993; Borrego et al. 2004) and climate scenarios (e.g. Carvalho et al. 2010); (2) assess the long-term air quality (for 1 year periods, at least) (e.g. Monteiro et al. 2007; Ribeiro et al. 2013); and

(3) forecast the air quality for a short period, commonly from tomorrow to next 2 or 3 days (e.g. Borrego et al. 2011a; Kukkonen et al. 2012). Selected examples of these applications are described in this Section.

3.1 Scenario Analysis

As mentioned before, air quality modelling systems need input variables, such as emissions, meteorological parameters, land use and topography. Different input scenarios can be created to evaluate the potential impact of these changes on the air quality. This kind of application is especially useful for territory planning and policy strategies, as well as for air quality impact assessment studies. Despite the uncertainty of the scenarios, they provide alternative images of how the future might unfold.

3.1.1 Emission and Climate Scenarios

Emission scenarios describe different options for release of pollutants into the atmosphere. They may be based on assumptions about driving forces such as patterns of economic and population growth, technology development and other factors, with pollutant emissions associated. Moreover, emission scenarios drive forces to the design of climate scenarios, because climate is sensitive to greenhouse gases and other atmospheric pollutants. In fact, with a growing concern on climate change consequences in several areas of interest, including the air quality, climate scenarios became widely used.

The impact of climate change on the air quality over Europe was illustrated by Carvalho et al. (2010), using a reference year (1990) and the IPCC SRES A2 year (2100) (Fig. 5). The modelling results suggest that the O_3 and PM10 levels in the atmosphere levels will be deeply impacted, depending on the region and the month. The Western and Central Europe will be the most affected areas: the predictions from this study point out that the variations of O_3 monthly mean surface concentration may reach an increase of 50 $\mu g{\cdot}m^{-3}$ in July 2010. Regarding PM10 monthly mean surface concentration, the biggest variation predicted is on October (almost 30 $\mu g{\cdot}m^{-3}$). Also in accordance with Carvalho et al. (2010), the changes in the boundary layer height, relative humidity, temperature, solar radiation, wind speed and precipitation may be responsible for significant differences in pollutant concentration patterns. In this sense, it is important to understand how future air quality will be under future climate scenarios and therefore contribute to the definition of adaptation and mitigation measures (Jacob and Winner 2009; Dawson and Winner 2012).

3.1.2 Plans and Programmes

In order to reduce and control the effects of air pollution on human health and in the environment, the European Air Quality Directive (Directive 2008/50/EC) established the obligations of the member states to elaborate and implement plans and programmes (PP) to improve air quality when the air quality standards are not met. The implementation of PP to air quality improvement should be based on the design of measures to reduce the pollutant atmospheric concentrations and meet the legal limits. In other words, PP are a set of scenarios developed to reduce atmospheric emissions and, consequently, improve air quality over a specific region.

These emission reduction scenarios can imply, for instance, the replacement of technologies in industrial sources or in residential combustion fireplaces (Borrego et al. 2012a) or decrease of heavy-duty vehicles circulating in city centres and the implementation of washing and sweeping city street actions (Borrego et al. 2012b). The efficiencies of the PP are assessed through the application of an air quality modelling system in order to identify the most adequate measures to be adopted. Figure 6 illustrates two examples of the implementation of PP to reduce PM10 concentrations through the emission reduction from traffic, industry and residential combustion sectors (Fig. 6a) and to reduce NO_2 concentrations reducing emissions from traffic (Fig. 6b) over the northern region of Portugal (Borrego et al. 2012a, b).

3.1.3 Urban Planning

Despite the progress made in controlling local air pollution, urban areas still show increasing signs of environmental stress, and air quality is one of the major concerns. The findings of several studies (e.g. Minnery 1992) provide evidence that the shape of a city and the land use distribution determine the location of emission sources and the pattern of urban traffic, ultimately affecting urban air quality. Urban sprawl is altering the landscape, with current trends pointing to further changes in land use that will, in turn, lead to changes in population, energy consumption, atmospheric emissions and air quality. Urban planners have debated on the most sustainable urban structure, with arguments in favour and against urban compaction and dispersion (Martins 2012). In this sense, air quality models can be a helpful tool for urban planners aiming to develop successful urban growth strategies to a city while tackling the multivariate dimensions of sustainability (Borrego et al. 2006). In this sense, these advanced tools can provide information to better select the most adequate location for new communication routes and industry, residential or recreational areas.

As an example of the role of green infrastructures on air quality, Amorim et al. (2013) evaluated the impact of trees over the dispersion of carbon monoxide (CO) emitted by

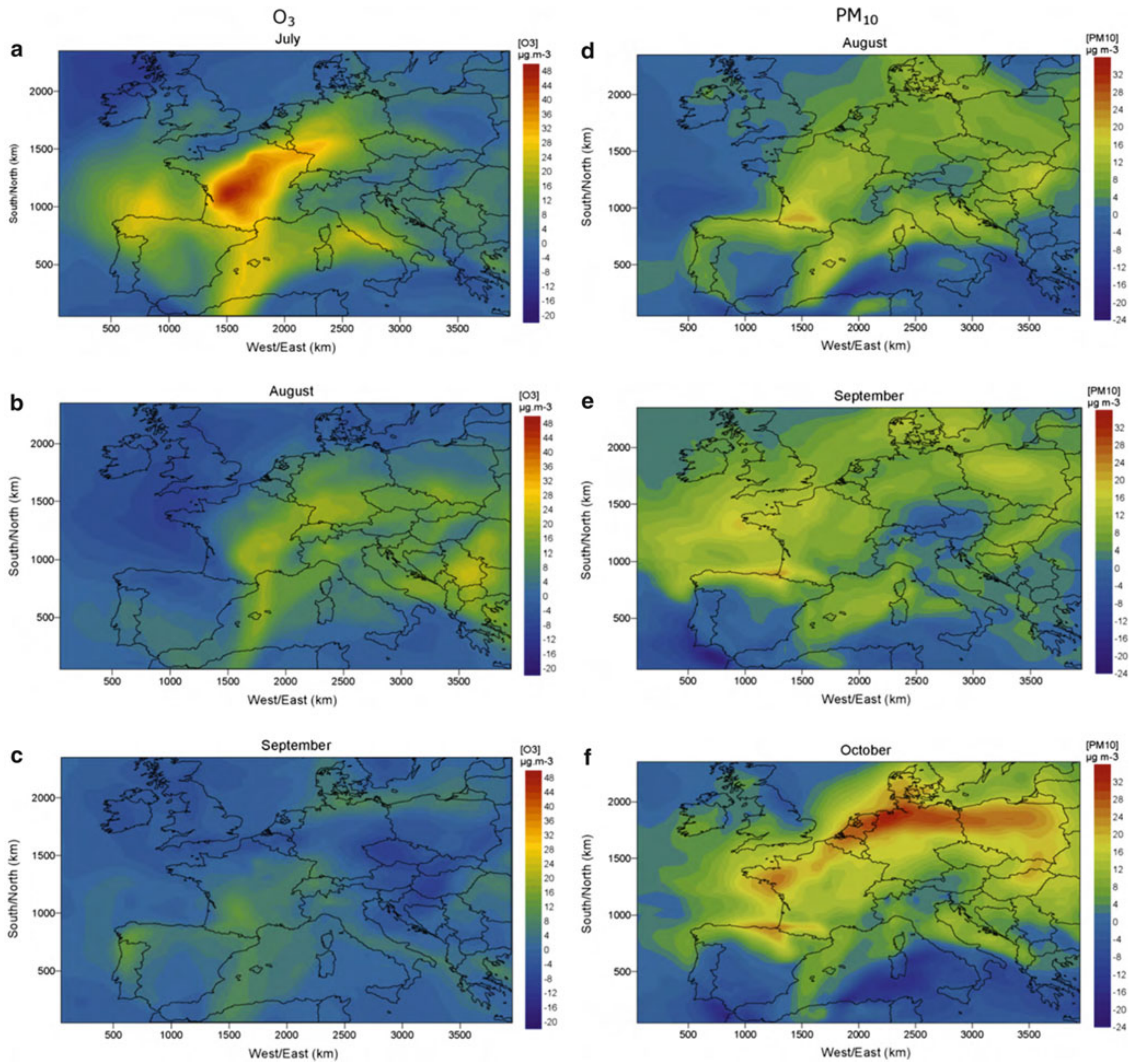

Fig. 5 Monthly mean surface O_3 (**a–c**) and PM10 (**d–f**) concentration changes ($\mu g \cdot m^{-3}$) simulated across Europe, only considering climate change from July to October (1990–2010) (From Carvalho et al. 2010)

road traffic in the city centre of two Portuguese cities (Fig. 7). The results indicated that the effect of the urban canopy on the dispersion of road traffic emitted air pollutants is highly complex and very spatially dependent. These conclusions support the importance of integrating the knowledge provided by the application of CFD models when defining strategies to optimise the role of green areas on human comfort and health.

As another example of the role of city planning on urban sustainability, Borrego et al. (2011b) applied an advanced Gaussian dispersion model (URBAIR) to previously selected intervention areas in three European cities with distinct characteristics: Helsinki, Athens (Fig. 8) and Gliwice (González et al. 2013). The model simulated the impact of different traffic management options on air quality, reinforcing that distinct urban planning options strongly influence local air pollutant levels. This work showed that the model used is capable of providing guidelines to urban planners and policy decision makers, on different traffic management strategies and their resultant air quality levels, supporting the decision processes on urban planning.

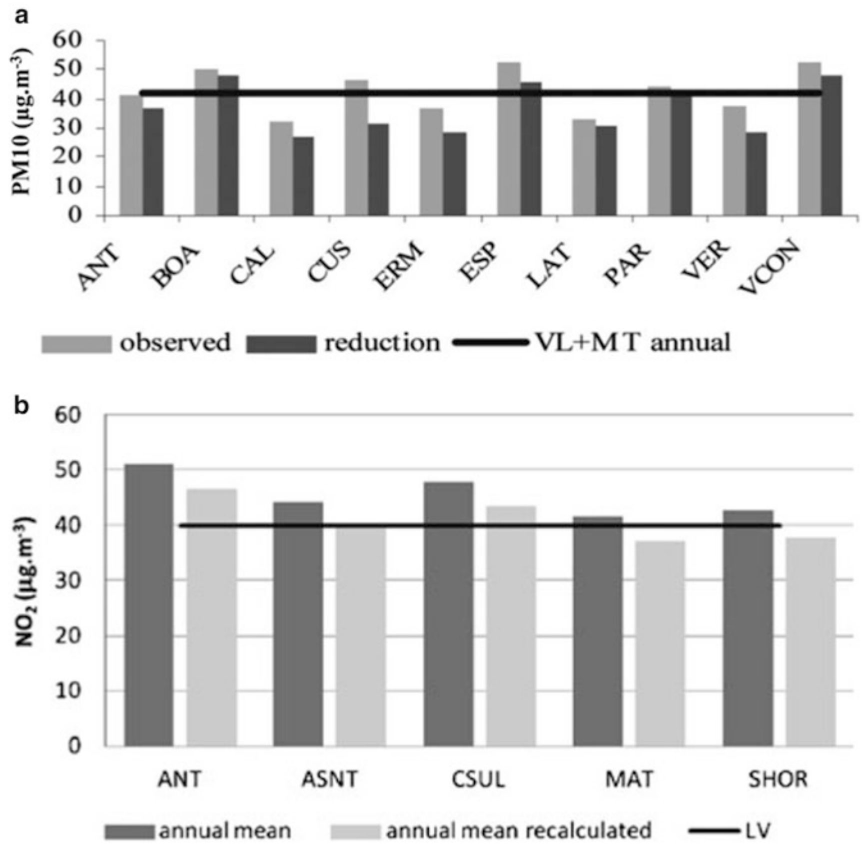

Fig. 6 Annual mean concentrations before and after the implementation of plans and programmes and limit value plus margin of tolerance (LV + MT) over the northern region of Portugal: (**a**) to reduce PM10 emissions from traffic, industry and residential combustion sectors (From Borrego et al. 2012a) and (**b**) to reduce NO_2 emissions from traffic (From Borrego et al. 2012b)

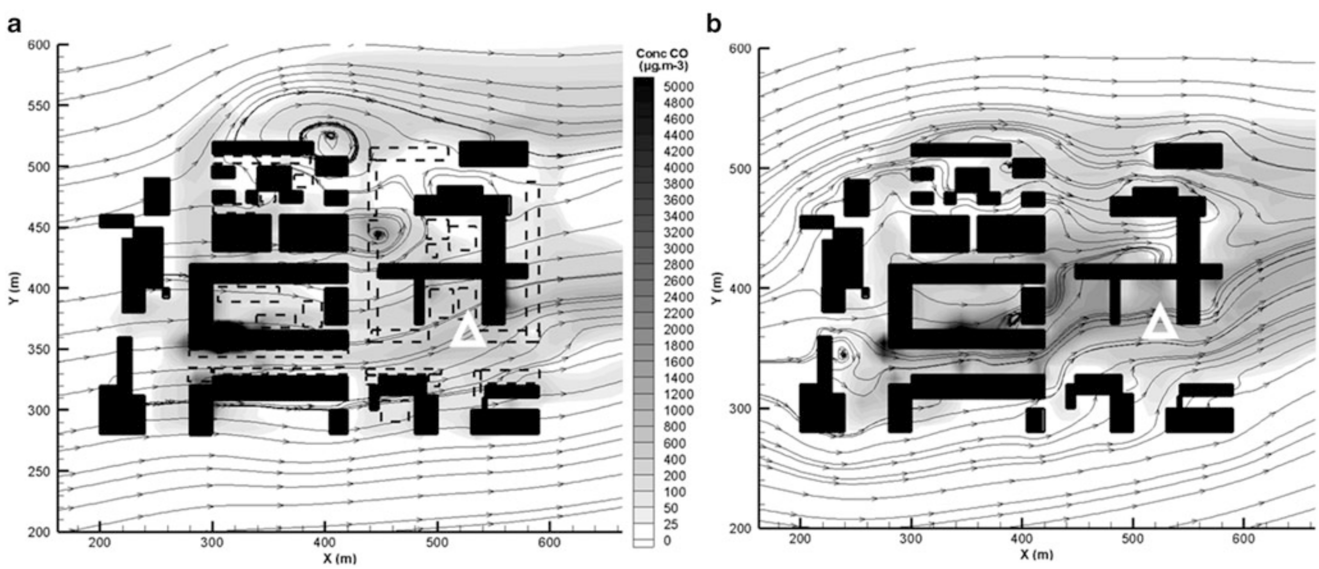

Fig. 7 Horizontal streamlines (3 m high) and CO concentration field with (**a**) and without (**b**) the effect of trees at the Aveiro city centre (in Portugal) between 10 and 11 a.m. *Unfilled rectangles* indicate tree blocks and the *white triangle* is the AQS location (From Amorim et al. 2013)

3.2 Long-Term Assessment

Especially in Europe and North America, air quality assessment is regularly based on the long-term application of modelling systems (van Loon et al. 2007; Thunis et al. 2011; Zhang et al. 2011; Emery et al. 2012; Solazzo et al. 2012). One of the main objectives of long-term air quality assessment is the verification of both limit targets and threshold values fulfilment imposed by legislation with respect to relevant pollutants in order to minimise the impacts on human health and natural ecosystems.

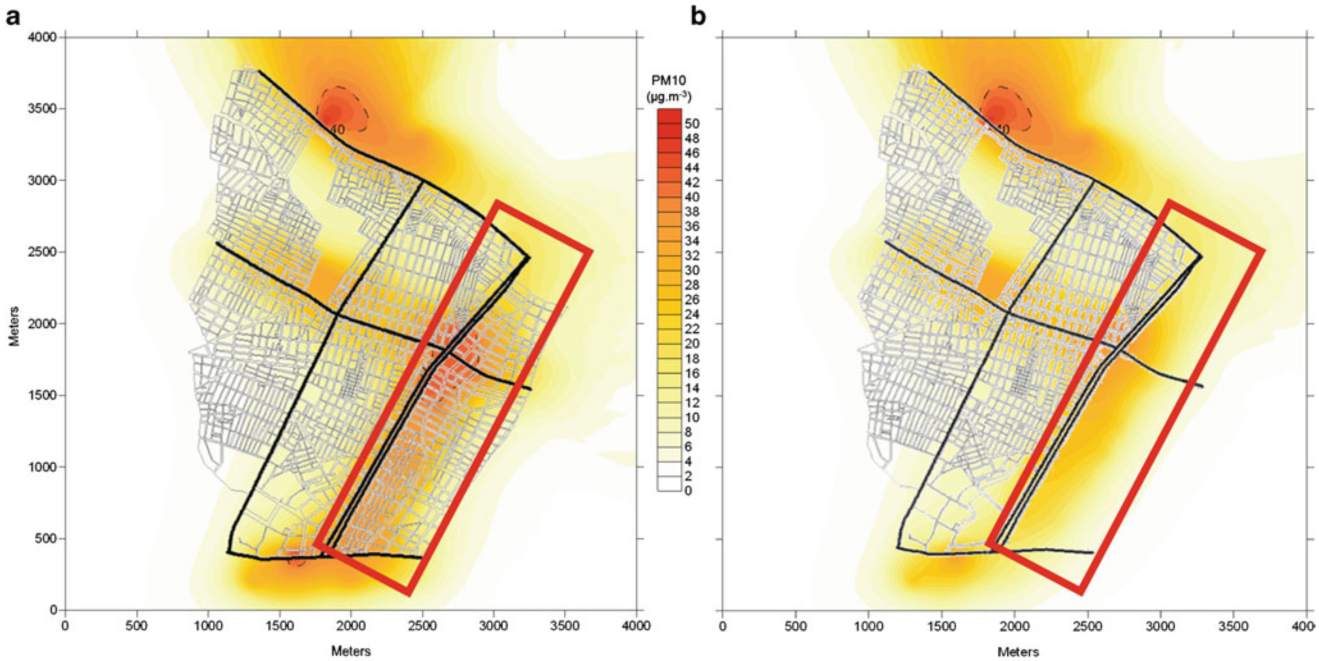

Fig. 8 Comparison of 1.5 m-high horizontal annual average PM10 concentration fields in Athens domain for two different intervention strategies in Western Athens. The planning alternative shown in image (**a**) consists on the construction of new residential buildings, while (**b**) corresponds to the conversion into a green area. The *red rectangle* indicates the intervention area, located at an industrial degraded area in the municipality of Egaleo (From Borrego et al. 2011b)

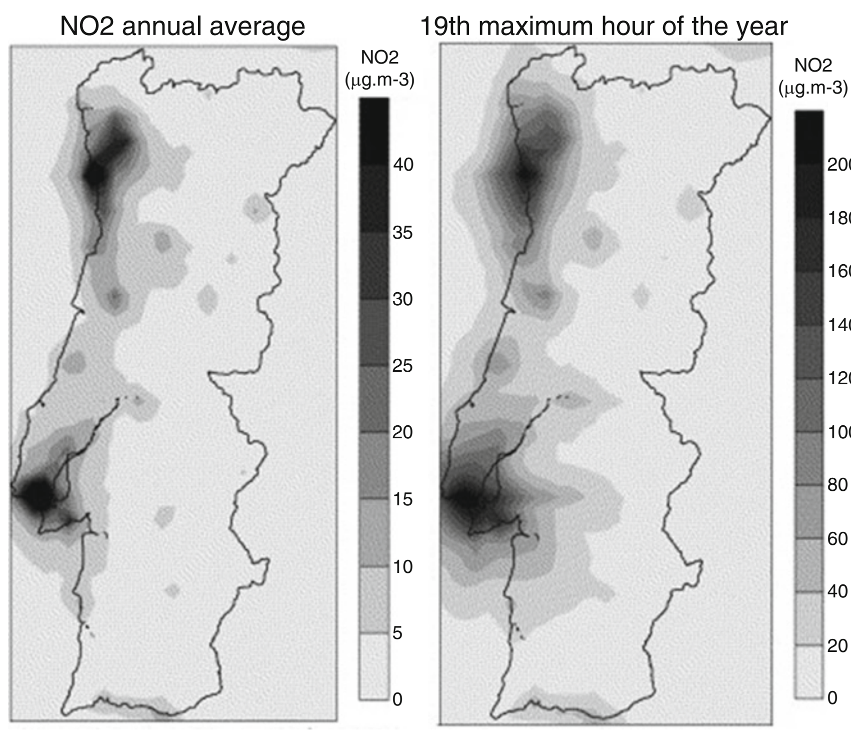

Fig. 9 Modelling results for NO_2 considering human health protection limit values (Directive 1999/30/EC) for the year 2001 (From Monteiro et al. 2007)

The European Union Member States must report annually the air quality assessment. Traditionally, this report has been based on monitored data, but due to sparse or non-existent fixed monitoring stations, this assessment has some limitations. Modelling approaches can contribute to this assessment by providing air quality concentration fields and thus the spatial distribution of pollutants (Fig. 9) (Monteiro et al. 2007), allowing the crossing of this information with other type of information such as the population density (Ribeiro et al. 2013).

The long-term air quality assessment based on modelling application could also be useful to study the representativeness and spatial coverage of the monitoring network, improving air quality assessment activities (Monteiro et al. 2005).

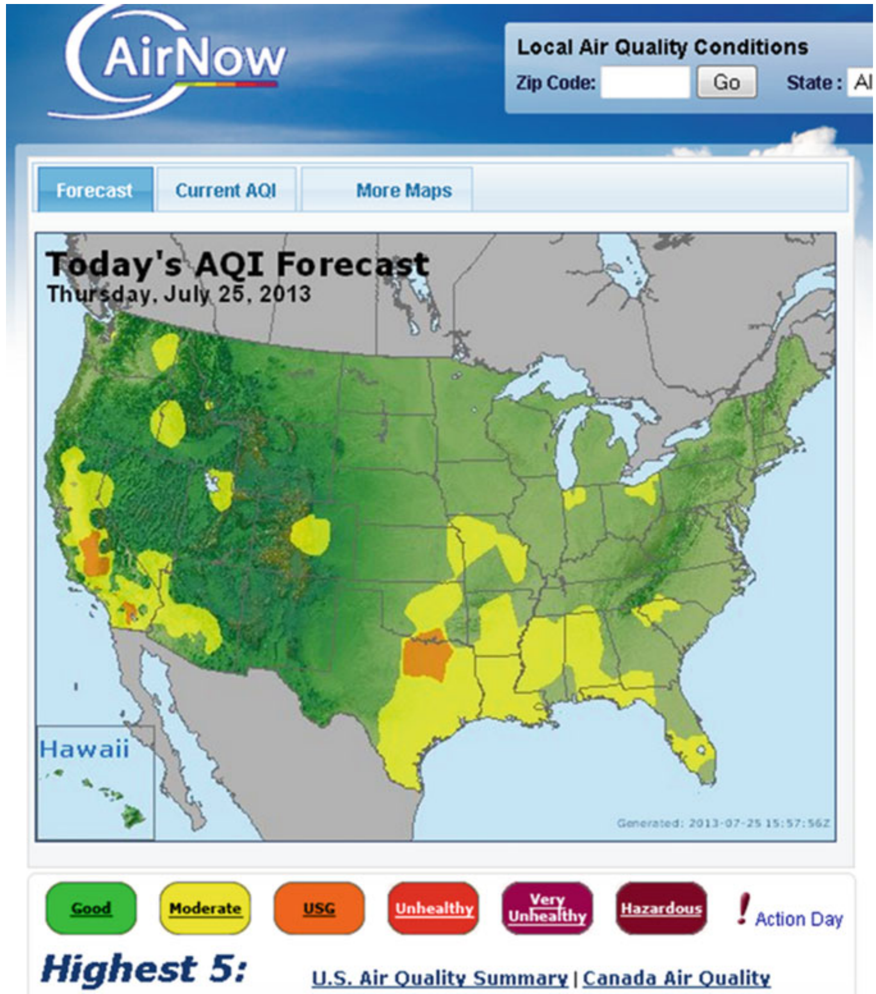

Fig. 10 Air quality index forecast for July 25, 2013, over the USA (From http://www.airnow.gov/)

3.3 Air Quality Forecast

Air quality forecasting is both a challenge and a scientific problem which has recently emerged as a major priority in many urbanised and industrialised countries due to increasing consciousness of the effect of airborne pollutant emissions on health and the environment. The goals of reliable air quality forecasts are evident: exposure of the population can be more efficiently reduced and better protection can be ensured by means of information and short-term action plans. For this purpose, European legislation has set ambient air quality standards for acceptable levels of air pollutants (like O_3, NO_2, SO_2, PM2.5 and PM10) and has also recommended the use of modelling tools to assess and forecast air quality in order to develop emission abatement plans and to alert the population when health-related issues occur (Borrego et al. 2011a).

There are currently several air quality modelling forecasting systems on a local, regional and continental scale in Europe and worldwide (see http://www.chemicalweather.eu for Europe and http://www.airnow.gov/ for the USA). Their forecast maps usually show the predicted Air Quality Index (AQI) (Fig. 10), which is an indicator/classification used to communicate to the public how polluted the air is currently or how polluted it is forecast to become. This will allow the authorities to take actions to prevent or reduce the adverse effects of the exposure of the population through early warnings and to implement alert systems for the population when exceedances of air quality targets are predicted.

4 Final Remarks

The atmosphere is a complex and natural gaseous system, which balance may be affected by the introduction of gaseous or particulate compounds emitted by natural and/or anthropogenic sources and affecting human health and causing damage to plants and materials. Focused on these concerns, atmospheric sciences have been moving forwards. Nowadays, the air quality prediction, for an area ranging from the entire globe to a street, is possible through numerical models, describing mathematically the behaviour of the pollutants in the atmosphere taking into account the atmospheric processes. For that, the models require diverse input information, such as meteorological fields, terrain characterisation (topography, land use or roughness), atmospheric pollutant emissions and boundary conditions.

There are several numerical modelling tools to predict the air quality based on different approaches. To select the right model to the intended application and taking into account its main characteristics is the first and, probably, the most important step on air quality prediction activity.

Air quality models are considered as powerful tools in research and policy-making activities, allowing the assessment of the impacts from emission, climate or other type of variable scenarios. This kind of application provides appropriate information to analyse how driving forces may influence air quality outcomes. Thus, it is especially useful for environmental impact assessment studies, urban planning and to structure policy strategies. The scenario analysis provides alternative images of how the future might unfold, in spite of the high uncertainty associated with the scenario development.

Especially in North America and Europe, public administrations and environmental authorities are mandated to control and manage air quality in order to minimise air pollution effects on human health and natural ecosystems. In this sense, long-term air quality assessment should be performed annually verifying the fulfilment of the limit targets and threshold values imposed by legislation with respect to the relevant pollutants. This kind of assessment application based on an air quality modelling system also contributes to the identification of air quality problems and causes and therefore to the development and implementation of measures to reduce air pollution levels (plans and programmes). Moreover, there are tens of air quality forecasting systems providing predictions of air pollution concentration fields for the next 2 or 3 days, allowing the authorities to take actions to prevent or reduce the adverse effects of the exposure of the population through early warnings and to implement alert systems for the population when exceedances of air quality targets are predicted.

In spite of the uncertainty associated with the air quality models and the required input data, air quality modelling can provide, with enough accuracy, useful information to decision-making support techniques that may assist in moving towards more sustainable practices, ensuring a better quality of life for the citizens from global to local scale.

Acknowledgements The authors acknowledge the Portuguese Science Foundation for the financing of BIOGAIR project (PTDC/AAC-AMB/103866/2008; FCOMP-01-0124-FEDER-008587), for the Ph.D. grant of Isabel Ribeiro (SFRH/BD/60370/2009) and the post doc grants of Alexandra Monteiro (SFRH/BPD/63796/2009), Joana Valente (SFRH/BPD/78933/2011) and Jorge Humberto Amorim (SFRH/BPD/48121/2008). Thanks are extended to the Portuguese Agency for the Environment for supporting the air quality assessment and forecasting over Portugal and the "Comissão de Coordenação e Desenvolvimento Regional do Norte" for the coordination and responsibility of the plans and programmes.

References

Amorim, J.H., Rodrigues, V., Tavares, R., Valente, J., Borrego, C.: CFD modelling of the aerodynamic effect of trees on urban air pollution dispersion. Sci. Total Environ. **461–462**, 541–551 (2013)

Atkinson, B.W.: Meso-scale atmospheric circulations, 495 p. Academic, London (1989)

Baklanov, A., Fay, B., Kaminski, J., (eds.): Overview of existing integrated (offline and online) mesoscale systems in Europe; COST 728 D2.1 report, p 108, April (2007)

Borrego, C.: Air pollution and climate change: two slides of the same coin. In: EuNetAir Newsletter COST action TD1105. **Iss. 2**, June. http://www.eunetair.it/cost/newsletter/Newsletter_EuNetAir-Issue2_June2013.pdf (2013)

Borrego, C., Martins, H., Carvalho, A., Carvalho, A.C., Lopes, M., Valente, J., Miranda, A.I.: Portuguese power plants impact on air quality. In: Air Pollution 2004, 30 June – 2 July, Rhodes, Greece (2004)

Borrego, C., Martins, H., Tchepel, O., Salmim, L., Monteiro, A., Miranda, A.I.: How urban structure can affect city sustainability from an air quality perspective. Urb. Air Qual. Model. **21**(4), 461–467 (2006)

Borrego, C., Monteiro, A., Ferreira, J., Costa, A.M., Carvalho, A.C., Lopes, M.: Procedures for estimation of modelling uncertainty in air quality assessment. Environ. Int. **34**, 613–620 (2008)

Borrego, C., Monteiro, A., Pay, M.T., Ribeiro, I., Miranda, A.I., Basart, S., Baldasano, J.M.: How bias-correction can improve air quality forecast over Portugal. Atmos. Environ. **45**, 6629–6641 (2011a)

Borrego, C., Cascão, P., Lopes, M., Amorim, J.H., Tavares, R., Rodrigues, V., Martins, J., Miranda, A.I., Chrysoulakis, N.: Impact of urban planning alternatives on air quality: URBAIR model application. In: Brebbia, C.A., Longhurst, J.W.S. (eds.) XIX International Conference on Modelling, Monitoring and Management of Air Pollution. WIT Transactions on Ecology and the Environment, vol. 147, p. 12. WIT, Southampton (2011b)

Borrego, C., Sá, E., Carvalho, A., Sousa, S., Miranda, A.I.: Plans and programmes to improve air quality over Portugal: A numerical modelling approach. Int. J. Environ. Pollut. **48**(1–4), 60–68 (2012a)

Borrego, C., Monteiro, A., Sa, E., Carvalho, A., Coelho, D., Dias, D., Miranda, A.I.: Reducing NO_2 pollution over urban areas: Air quality modelling as a fundamental management tool. Water Air Soil Pollut. **223**(8), 5307–5320 (2012b)

Carvalho, A., Monteiro, A., Solman, S., Miranda, A.I., Borrego, C.: Climate-driven changes in air quality over Europe by the end of the 21st century, with special reference to Portugal. Environ. Sci. Policy **13**, 445–458 (2010)

Chang, J.C., Hanna, S.R.: Air quality model performance evaluation. Meteorol. Atmos. Phys. **87**, 167–196 (2004)

Chow, J.C.: Introduction to special topic: Weekend and weekday differences in ozone levels. J. Air Waste Manage. Assoc. **53**, 771 (2003)

Dawson, J.P., Winner, D.A.: New directions: Adapting air quality management to climate change: A must for planning. Atmos. Environ. **50**, 387–389 (2012)

Delle Monache, L., Deng, X., Zhou, Y., Stull, R.: Ozone ensemble forecasts: 1. A new ensemble design. J. Geophys. Res. **111**(D05307) (2006)

Dennis, R., Fox, T., Fuentes, M., Gilliland, A., Hanna, S., Hogrefe, C., Irwin, J., Rao, S.T., Scheffe, R., Schere, K., Steyn, D., Venkatram, A.: A framework for evaluating of regional-scale numerical

photochemical modeling systems. Environ. Fluid Mech. **10**(4), 471–489 (2010)
Draxier, R., Hess, G.D.: An overview of the HYSPLIT_4 modelling system for trajectories, dispersion and deposition. Aust Meteorol. Mag. **47**(4), 295–308 (1998)
Draxler, R.R., Rolph, G.D.: HYSPLIT (HYbrid Single-Particle Lagrangian Integrated Trajectory) Model access via NOAA ARL READY website (http://ready.arl.noaa.gov/HYSPLIT.php). NOAA Air Resources Laboratory, Silver Spring, MD (2011)
Emery, C., Jung, J., Downey, N., Johnson, J., Jimenez, M., Yarwood, G., Morris, R.: Regional and global modeling estimates of policy relevant background ozone over the United States. Atmos. Environ. **47**, 206–217 (2012)
Foley, K., Pinder, R., Napelonak, S.: New directions in air quality model evaluation: probabilistic model evaluation. Poster presented at the CMAS conference; Chapel Hill, NC. http://www.cmascenter.org/conference/2008/agenda.cfm (2008)
Ginoux, P., Chin, M., Tegen, I., Prospero, J.M., Holben, B., Dubovik, O., Lin, S.J.: Sources and distributions of dust aerosols simulated with the GOCART model. J. Geophys. Res. **106**, 20255–20273 (2001)
González, A., Donnelly, A., Jones, M., Chrysoulakis, N., Lopes, M.: A decision-support system for sustainable urban metabolism in Europe. Environ. Impact Asses. Rev. **38**, 109–119 (2013)
Grell, G., Knoche, R., Peckham, S.E., McKeen, S.A.: Online versus offline air quality modeling on cloud-resolving scales. Geophys. Res. Lett. **31**, L16117 (2004)
Hanna, S.R., Chang, J.C., Strimaitis, D.G.: Hazardous gas model evaluation with field observations. Atmos. Environ. **27A**, 2265–2285 (1993)
Horowitz, L., Walters, S., Mauzeralles, D., Emmonds, L., Rash, P., Granier, C., Tie, X., Lamarque, J., Schultz, M., Tyndall, G., Orlando, J., Brasseur, G.: A global simulation of tropospheric ozone and related tracers: Description and evaluation of MOZART, version 2. J. Geophys. Res. **108**(D24), 4784 (2003)
Ichikawa, Y., Sada, K.: An atmospheric dispersion model for the environment impact assessment of thermal power plants in Japan – a method for evaluating topographical effects. J. Air Waste Manage. Assoc. **52**, 313 (2002)
Jacob, D.J., Winner, D.A.: Effect of climate change on air quality. Atmos. Environ. **43**, 51–63 (2009)
Jacobson, M.Z.: Fundamentals of atmospheric modelling. Cambridge University Press, Cambridge, UK (1999)
Kukkonen, J., Balk, T., Scultz, M., Baklanov, A., Klein, T., Miranda, A. I., Monteiro, A., Hirtl, M., Tarvainen, V., Boy, M., Peuch, V.-H., Poupkou, A., Kioutsioukis, I., Finardi, S., Sofiev, M., Sokhi, R., Lehtinen, K., Karatzas, K., San José, R., Astitha, M., Kallos, G., Schaap, M., Reimer, E., Jakobs, H., Eben, K.: A review of operational, regional-scale, chemical weather forecasting models in Europe. Atmos. Chem. Phy. **12**, 1–87 (2012)
Kumar, P., Ketzel, M., Vardoulakis, S., Pirjola, L., Britter, R.: Dynamics and dispersion modelling of nanoparticles from road traffic in the urban atmospheric environment – a review. J. Aerosol. Sci. **42**(9), 580–603 (2011)
Lutman, E.R., Jones, S.R., Hill, R.A., McDonald, P., Lambers, B.: Comparison between the predictions of a Gaussian plume model and a Lagrangian particle dispersion model for annual average calculations of long-range dispersion of radionuclides. J. Environ. Radioact. **75**, 339–355 (2004)
Martins, H.: Urban compaction or dispersion? An air quality modelling study. Atmos. Environ. **54**, 60–72 (2012)
Minnery, J.: Urban Form and Development Strategies: Equity, Environmental and Economic Implications. The National Housing Strategy Background, Paper 7. AGPS, Canberra (1992)
Miranda, A.I., Conceição, M.S., Borrego, C.: A contribution to the air quality impact assessment of a roadway in Lisbon. The air quality model APOLO. Sci. Total Environ. **134**(1–3), 1–7 (1993)
Monteiro, A., Vautard, R., Borrego, C., Miranda, A.I.: Long-term simulations of photo oxidant pollution over Portugal using the CHIMERE model. Atmos. Environ. **39**, 3089–3101 (2005)
Monteiro, A., Miranda, A.I., Borrego, C., Vautard, R., Ferreira, J., Perez, A.T.: Long-term assessment of particulate matter using CHIMERE model. Atmos. Environ. **41**, 7726–7738 (2007)
Nappo, C.J., Essa, K.S.M.: Modeling dispersion from near-surface tracer releases at Cape Canaveral. Atmos. Environ. **35**, 3999–4010 (2001)
Olesen, H.R.: Ten years of harmonisation activities: past, present and future. In: 7th International Conference on Harmonisation Within Atmospheric Dispersion Modelling for Regulatory Purposes. European Commission, Joint Research Centre (2001)
Pielke, R.A.: Mesoscale meteorological modeling. Academic, San Diego (2002)
Reid, N., Misra, P.K., Amman, M., Hales, J.: Air quality modeling for policy development. J. Toxicol. Environ. Health **70A**(3–4), 295–310 (2007)
Ribeiro I., Monteiro A., Fernandes A.P., Monteiro A.C., Lopes M., Borrego C., Miranda A.I.: Air quality modelling as a supplementary assessment method in the framework of the European air quality Directive. In: 15th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, 6–9 May 2013, Madrid, Spain (2013)
Saltelli, A., Tarantola, S., Campolongo, F., Ratto, M.: Sensitivity Analysis in Practice. A Guide to Assessing Scientific Models. Wiley, Chichester (2004)
Seinfeld, J.H., Pandis, S.N.: Atmospheric Chemistry and Physics: From Air Pollution to Climate Change. Wiley, New York (1998). ISBN 9780471178163
Solazzo, E., Bianconi, R., Vautard, R., Appel, K.W., Moran, M.D., Hogrefe, C., Bessagnet, B., Brandt, J., Christensen, J.H., Chemel, C., Coll, I., van der Gon, H.D., Ferreira, J., Forkel, R., Francis, X.V., Grell, G., Grossi, P., Hansen, A.B., Jeričević, A., Kraljević, L., Miranda, A.I., Nopmongcol, U., Pirovano, G., Prank, M., Riccio, A., Sartelet, K.N., Schaap, M., Silver, J.D., Sokhi, R.S., Vira, J., Werhahn, J., Wolke, R., Yarwood, G., Zhang, J., Rao, S.T., Galmarini, S.: Model evaluation and ensemble modelling of surface-level ozone in Europe and North America in the context of AQMEII. Atmos. Environ. **53**, 60–74 (2012)
Steyn, D.G., Galmarini, S.: Evaluating the predictive and explanatory value of atmospheric numerical models: Between relativism and objectivism. Open Atmos. Sci. J. **2**, 38–45 (2008)
Thunis, P., Georgieva, E., Pederzoli, A., Pernigotti, D.: "The DELTA Tool and Benchmarking Report Template", Concepts and User's Guide, p. 31. Join Research Centre, Ispra (2011)
van Loon, M., Vautard, R., Schaap, M., Bergström, R., Bessagnet, B., Brandt, J., Builtjes, P.J.H., Christensen, J.H., Cuvelier, C., Graff, A., Jonson, J.E., Krol, M., Langner, J., Roberts, P., Rouil, L., Stern, R., Tarrasón, L., Thunis, P., Vignati, E., White, L., Wind, P.: Evaluation of long-term ozone simulations from seven regional air quality models and their ensemble. Atmos. Environ. **41**(10), 2083–2097 (2007)
Zhang, L., Jacob, D.J., Downey, N.V., Wood, D.A., Blewitt, D., van Carouge, C.C., Donkelaar, A., Jones, D.B.A., Murray, L.T., Wang, Y.: Improved estimate of the policy-relevant background ozone in the United States using the GEOS-Chem global model with $1/2^\circ \times 2/3^\circ$ horizontal resolution over North America. Atmos. Environ. **45**(37), 6769–6776 (2011)