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AIR QUALITY MODELLING: STATE-OF-THE-ART

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W17: AIR QUALITY MODELLING: STATE-OF-THE-ART

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Abstract

Air quality modeling is an area with a significant progress and interest during the last two decades. It covers all aspects related to pollution dispersion and impact on different ecosystems. It is very much related to the meteorological field since the atmosphere is governed by the general laws derived by the Navier-Stokes equation system. Progress in computer capabilities during the last decades has impulse substantially the research on air quality modeling in a parallel way. Air pollution modeling covers a very complex and interdisciplinary area where we include remote sensing – land use impact -, initial and boundary conditions, data assimilation techniques, chemical schemes, comparison between measured and modeled data, computer efficiency, parallel computing in air quality modeling, long-range transport impact on local air pollution, new satellite data assimilation techniques, real-time and forecasting air quality modeling and sensitivity analysis. This contribution focuses on providing a general overview of the state-of-the-art on air quality modeling, from the point of view of the "user community", i.e. policy makers, urban planners, environmental managers, etc.. It also tries to bring to the discussion key questions concerning the air quality modeling success in usage, such as, where are greatest uncertainties in emission inventories, how well do air quality models simulate urban aerosols, what are the next generation developments in models to answer new scientific questions, etc.

1. Introduction

The development of comprehensive air quality models started in the late of seventies. The Urban Airshed Model (UAM) (Morris and Meyers, 1990), followed by the Regional Oxidant Model (ROM) (Lamb, 1983a, 1983b) provided Eulerian-based models for ozone, the former for urban and the latter for regional scale. The Sulfur Transport and Emission Model (STEM) (Carmichael and Peters, 1984a, 1984b; Carmichael et al. 1991) focused on regional and continental acid deposition modeling. The CMAQ modeling system (Byun et al. 1998) is capable to process great and diverse information from complicated emission mixtures and complex distribution of sources, to modeling the complexities of atmospheric process that transport and transform these mixtures in a dynamic environment that operates in a large range of time scales covering minutes to days and weeks.

An air quality modelling system consists of a meteorological model, an emissions model, and an air quality model. The meteorological model calculates as a function of time the three-dimensional fields of wind, temperature, relative humidity, pressure, and in some cases, turbulent eddy diffusivity, clouds, and precipitation. The emissions model estimates the amount and chemical speciation of low-level (area sources) and elevated (point sources) primary pollutants based on process information (e.g., vehicle miles travelled) and day-specific meteorology (e.g., temperature). The output of the emissions and meteorological models is then input into the air quality model, which calculates the concentrations and deposition rates of gases and aerosols as a function of space and time. There are various mathematical models that can be used to simulated meteorology and air quality at the mesoscale domain. Although mathematical models differ in their treatment of meteorology or air quality, all three-dimensional models are based on a similar framework and consist of the same major components.

An air quality model typically includes:

1. a transport and diffusion component that calculates the three-dimensional motion of gases and aerosols in the gridded model domain;
2. a gas-phase chemistry component that calculates the change in gaseous concentrations due to chemical transformations;
3. an aerosol component that calculates the size distribution and chemical composition of aerosols due to chemical and physical transformations;
4. a cloud/fog component that calculates the physical characteristics of clouds and fog based on information from the meteorological model (or from observation);
5. a cloud/fog chemistry component that calculates the change in chemical concentrations in clouds and fog;
6. a wet deposition component that calculates the rates of deposition due to precipitation (and, possibly, cloud impaction and fog settling) and the corresponding change in chemical concentrations;
7. a dry deposition component that calculates the rates of dry deposition for gases and aerosols and the corresponding changes in their concentrations.

The detailed modular formation varies from model to model. It is possible, however, to formulate a general modular framework that is common to most three-dimensional modelling systems. First, the spatial and temporal resolutions of the modelling system must be defined. The spatial distribution of meteorological and chemical variables is approximated by three-dimensional gridded systems. The meteorological and the air quality models may have different grid structures over the same domain. For example, the meteorological model may use a system based on altitude (with respect to mean sea level), whereas the air quality model may use a terrain-following coordinate system. The output of the meteorological model will need to be processed to provide meteorological fields that match the gridded system of the air quality model. The emissions model uses a gridded spatial resolution that is consistent with that of the air quality model. The spatial resolution does not need to be uniform throughout the domain. In the vertical direction, meteorological and air quality models typically use a finer resolution near ground level than aloft. In addition, nesting of domains with different horizontal resolutions may be performed to accommodate the need for fine spatial resolution (e.g., on the order of 1-5 km) in critical source or receptor areas without penalizing the computational cost over the entire domain (where a larger horizontal grid size of the order of 20 km would be used).

The temporal resolution used in meteorological, emissions, and air quality models is generally 1 h. (We define temporal resolution as time averaging for model inputs and outputs, not the integration step time used in a model, which is generally on the order of seconds or minutes.) All air quality ambient standards are based on 1-h or longer averaging times. Many meteorological data are routinely available with 1-h resolution.

The three-dimensional field of meteorological variables can be constructed by a diagnostic model that uses interpolation techniques to develop a three-dimensional field based on a discrete set of data or by a dynamic (or prognostic) model that solves the fundamental equations of mass, momentum, and energy to calculate the three-dimensional field of meteorological variables. Diagnostic models are useful if:

The quality of the air pollution modelling/forecast and the Air Quality Information and Forecasting Systems (AQIFS) critically depends on:

(i) the mapping of emissions,

(ii) the air pollution (APM) and chemical transport (CTM) models, and

(iii) the meteorological fields in the considered areas.

The main problem in forecasting air quality is the prediction of episodes with high pollutant concentration in urban areas where most of the well-known methods and models, based on in-situ meteorological measurements, fail to realistically produce the meteorological input fields for the urban air pollution (UAP) models. An additional challenge for contemporary AQ models lies in the fact that the legislation on AQ targets to new categories of information, like the likelihood of hot-spot occurrence, or the number of exceedances within a year, that associate AQ forecasting capabilities with urban environment modelling demands, thus making the forecasting issue more complicated.

Urban air quality information and forecasting systems

About 70% of the European population leaves in cities. A major share of anthropogenic sources of pollutants originated from conurbations. These pollutants have not only local effects (on human health, material, ecosystem), but may impact all the way to the regional (acidification, euthrophication) and global scales (atmospheric composition, climate changes). Urban areas present a challenge to atmospheric scientists, both from the experimentalist and modeller point of view as typically urban areas have high roughness elements penetrating well above the surface layer, heterogeneous distribution of surface features with wide variation in surface fluxes of heat, moisture, momentum and pollutants. Additionally the structure of the conurbation may trigger local meteorological circulations and processes (e.g., heat island, enhanced production of condensation nuclei) as well as enhanced vertical motions resulting in longer residence time of atmospheric compounds.

As model resolution is increasing towards a few kilometres or finer and various stakeholders and the public are expecting better targeted meteorological forecasts and products, it has become a necessity to be able to account for, describe and simulate urban effects and processes in various meteorological and air pollution models. On the other hand, this has brought new requirements for observations and measuring strategy in order to be able to describe, simulate and forecast meteorological and concentration fields in urban areas. Integration of these aspects will greatly benefit the development of urban air quality information and forecasting systems (UAQIFS) for a variety of applications and end-users.

Modern numerical weather prediction (NWP) and meso-meteorological models (MetM) able to resolve urban-scale processes are considered to be the main tools in future urban air pollution (UAP) forecasting and assessments because they allow for sufficiently high spatial and temporal resolution and can trace back the linkages between sources and impacts. The Cluster of European Urban Air Quality Research (CLEAR) considers improvements of meteorological data and models for urban areas as one of the targets, because most of the CLEAR projects (FUMAPEX, OSCAR, SAPPHIRE, URBAN AEROSOL, URBAN EXPOSURE, BOND, NEPAP, AIR4EU) need urban meteorological fields for their air quality studies. However, only the FUMAPEX project focuses on the evaluation and improvement of meteorological modelling and pre-processing for urban areas. This work is a logical continuation of the COST Action 715.

The following urban features can influence the atmospheric flow, microclimate, turbulence regime and, consequently, the transport, dispersion, and deposition of atmospheric pollutants within urban areas:

(1) local-scale non-homogeneities, sharp changes of roughness and heat fluxes,

(2) the building effect in reducing wind velocity,

(3) redistribution of eddies, from large to small, due to buildings,

(4) trapping of radiation in street canyons,

(5) effect of urban soil structure on diffusivities of heat and water vapour,

(6) anthropogenic heat fluxes, including the urban heat island effect,

(7) urban internal boundary layers and the urban mixing height (MH),

(8) different gas and particle deposition efficiencies for different types of the urban surfaces (walls, roofs, streets, etc.),

(9) effects of pollutants (including aerosols) on urban meteorology and climate,

(10) urban effects on clouds and precipitation.

Accordingly the following aspects of urban effects were considered by the FUMAPEX project in improved urban-scale NWP and meteorological models: higher spatial grid resolution and model downscaling, improved physiographic data and land-use classification, calculation of effective urban roughness and urban heat fluxes, urban canopy and soil sub-models, MH in urban areas.

Integrated modelling and Chemical weather forecasting

In general sense it is suggested to consider the air quality as a combination and integration at least of the following factors: air pollution, urban climate & meteorological conditions and population exposure. This is reasonable to consider them together due to the facts that:

(i) meteorology is the main source of uncertainty in UAP and emergency preparedness models,

(ii) complex and combined effects of meteorological and pollution components on human health (for example, in France in the hot summer 2003 with a large number of mortality cases),

(iii) effects of pollutants/aerosols on urban climate and meteorological events (precipitation, thunderstorms, etc.).

Quantification of the combined effect of bio-meteorological factors together with the effects of air pollution is a major issue.

In this contents two levels of the integration strategy are considered in the paper:

1. Off-line integration of Urban Meteorology, Air Pollution and Population Exposure models for urban air pollution forecast and emergency preparedness, which is the main issue e.g. in the EC FUMAPEX project.

2. On-line integration of meso-scale meteorological models and atmospheric aerosol & chemical transport models with consideration of the feedbacks of air pollution (e.g. urban aerosols) on meteorological processes and urban climate. This direction is developed by several research organisations and considered in the new COST Action 728 (http://cost.cordis.lu/src/action_detail.cfm?action=728). This will lead to a new generation of models for "chemical weather forecasting".

The following achievements are discussed in the paper:
1. Testing the quality of operational NWP systems for AQ modelling in urban areas,
2. Improvement of parameterisation of urban atmospheric processes and urban physiographic data classification,
3. Development of meteo-processor and interface between urban scale NWP and UAP models,
4. On-line integrated MetM-CTM systems for urban and meso-scale.

Air quality modelling for environment and health risk assessments

In the air quality modelling for risk assessments there is an increased interest to quantitative methods of analysis of environmental processes in combination with cost and effective methods and methods from a point of view of economic and social development.
These methods are required for analysis of environment quality, and they are connected with problems of population health. The interest is also related to methods of comparative analysis, strategy to reduce risks and expenses for practical realization of such approaches. The quantitative analysis of risks is important to reveal and identify the permitted levels of chemical, biological, radioactive agents/pollutants and etc. in the atmospheric environment and for population as well as change of climatic conditions for population's protection.

It is important for the comparative analysis of management strategy of the current behaviour of environment in order to reach the final aims and in the quantitative estimates of cumulative risks. These depend on the individual pollutants with multiple ways of impact on the environment and population health, and joint influence of multiple effects.

The problem to formulate such general metrics and target functionals will require additional studies which should be done in collaboration with multidisciplinary specialists. Moreover, such studies need to be done in parallel and in cooperation with research in development of mathematical models and methods of its realization required to achieve the optimal and admissible estimates.

Several approaches are considered for the tasks of risk assessment and control theory:

- First, it is the methods of the forward modelling based on analysis of ensembles of scenarios for different variants of input data and existing factors. These methods can be realized with determistic and stochastic (for example, Monte-Carlo method) algorithms.
- Second, it is the methods using the adjoint equations generated for evaluation of linear functionals such as scalar inner products defined in spaces of both the state functions of models and the weight functions with the limited supports.
- Third, it is the variational methods for linear and non-linear dynamical systems and functionals in combination with methods of the control theory, risk theory, and sensitivity theory. These methods can be realized using a combination of the forward and inverse modelling approaches taking into account the uncertainties of models, parameters, and observational data.

Air quality modelling as a natural part of the Climate change modelling

The role of greenhouse gases (such as water vapour, CO_2, O_3 and CH_4) and aerosols in climate change has been highlighted as a key area of future research (Watson et al 1997, IPCC 2001, AIRES 2001). Uncertainties in emission projections of gaseous pollutants and aerosols (especially secondary organic components) need to be addressed urgently to advance our understanding of climate forcing (Semazzi 2003). In relation to aerosols, their diverse sources, complex physicochemical characteristics and large spatial gradients make their role in climate forcing particularly challenging to quantify. In addition to primary emissions, secondary particles, such as, nitrates, sulphates and organic compounds, also result from chemical reactions involving precursor gases such as SOx, DMS, NOx, volatile organic compounds and oxidising agents including ozone. One consequence of the diverse nature of aerosols is that they exhibit negative (eg sulphates) as well as positive (eg black carbon) radiative forcing characteristics (IPCC 2001 and Jacobson 2001). Although much effort has been directed towards gaseous species, considerable uncertainties remain in size dependent aerosol compositional data, physical properties as well as processes controlling their transport and transformation, all of which affect the composition of the atmosphere (Penner et al 1998, Shine 2000, Shekar Reddy and Venkataraman 2000, Visser et al 2000, IPCC2001). Probably one of the most important sources of uncertainty relates to the indirect effect of aerosols as they also contribute to multiphase and microphysical cloud processes, which are of considerable importance to the global radiative balance (Semazzi 2003).

In addition to better parameterisation of key processes, improvements are required in regional and global scale modelling (IPCC 1996 and Semazzi 2003). Resolution of regional climate information from atmosphere-ocean general circulation models remains a limiting factor. Vertical profiles of temperature, for example, in climate and air quality models need to be better described. Such limitations hinder the prospect of reliably distinguishing between natural variability (eg due to natural forcing agents, solar irradiance and volcanic effects) and human induced changes caused by emissions of greenhouse gases and aerosols over multidecadal timescales (Semazzi 2003, NAS 2001). Consequently, the current predictions of the impact of air pollutants on climate, air quality and ecosystems or of extreme events are unreliable (eg Watson et al 1997). Therefore it very important in the future research to address all the key areas of uncertainties so as provide an improved modelling capability over regional and global scales and an improved integrated assessment methodology for formulating mitigation and adaptation strategies.

In this concern one of the important tasks is to develop a modelling instrument of coupled 'Atmospheric chemistry/Aerosol' and 'Atmospheric Dynamics/Climate' models for integrated studies (see Figure 1).

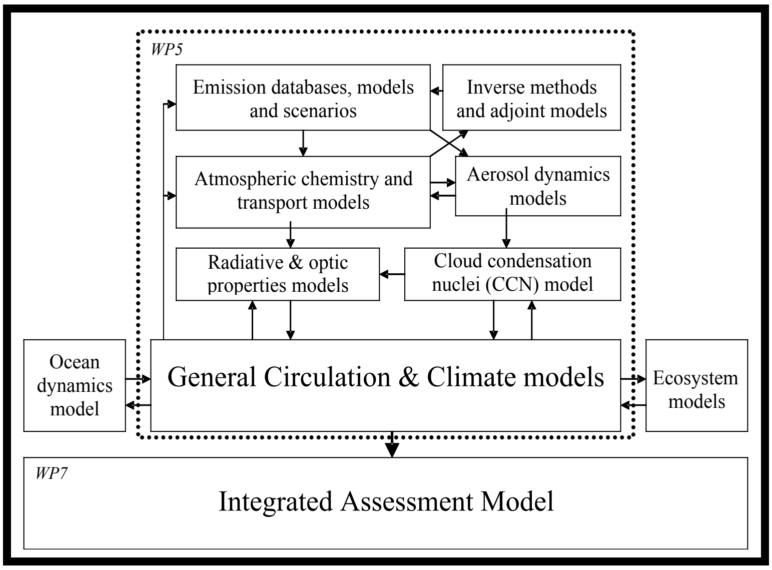


Figure 1. The integrated modelling system structure for predicting climate change and atmospheric chemical composition.

Scales of the processes/models and scale-interaction aspects

One of the important problem in air quality modelling is to develop/integrate already existing models to modelling systems that can be used to understand the impacts from aerosols and gas-phase compounds emitted from urban sources at/on the regional and global climate.
Anthropogenic pollutant and, especially, aerosol emissions are highly non-homogeneous. The formation and transformation processes of aerosols with respect to concentration of particles and precursors and the gas-phase chemistry are highly non-linear; consequently, the scale at which the emissions, formation and transformation processes are resolved in models has a significant influence on the resulting concentration fields of the aerosols and gas-phase compounds. Upscale cascade simulations can be performed using a combination of models resolving from the urban-mesoscale to the regional-global scale. The urban scale modelling is primarily intended to evaluate the source term and the role of the local processes in transformation of the primarily emitted aerosols. The mesoscale model can define intense sources like large cities and investigate the evolution of large urban plumes. These plumes are subgrid phenomena for the regional-global models that has the highest resolution (between 10km and 100km grid distances) in the zoomed areas. Therefore, the urban-mesoscale model can be applied to derive these subgrid parameterisations for the regional-global model.
To understand the impact of aerosols and gas-phase compounds emitted from local/urban sources on the regional and global processes, three scales of the integrated atmosphere-chemistry-aerosol and general circulation models have to be considered: (i) local, (ii) regional, and (iii) global.

Numerical aspects of the model down-scaling, different nesting techniques …

……

Real-time air quality modelling

Air quality modelling and air quality models (AQMs) predict air quality, based on surrounding air quality based on weather, topography, and other factors. To do this, air quality models imitate the physical and chemical processes that take place in the atmosphere. The term "air quality modelling" is a fairly generic term, and often includes studies of ozone levels, concentrations of particulate matter (PM), acid rain deposition, and the like. Most often, however, air quality models seem to be concerned with ozone concentrations and the very real problem of regulatory compliance.

It is important to understand where AQMs stand in the "larger scheme" of things. Figure 2 shows in flowchart form the air pollution system, which includes the science and the public policy/legislative components. Notice that the modelling part is only one component of the overall air quality analysis picture. **The specific purpose of air quality modelling is to determine the best control strategy by which air quality can be improved in some geographical area**. If there is anything missing from this chart, it is any direct mention of the economic implications of control measures, but that is perhaps incorporated under "Legislation". You should recognize that there is considerable politics between the boxes "Control strategy options" and "Control measures". Evidence of that is the recent Supreme Court case in US regarding new air quality standards for atmospheric pollutants.

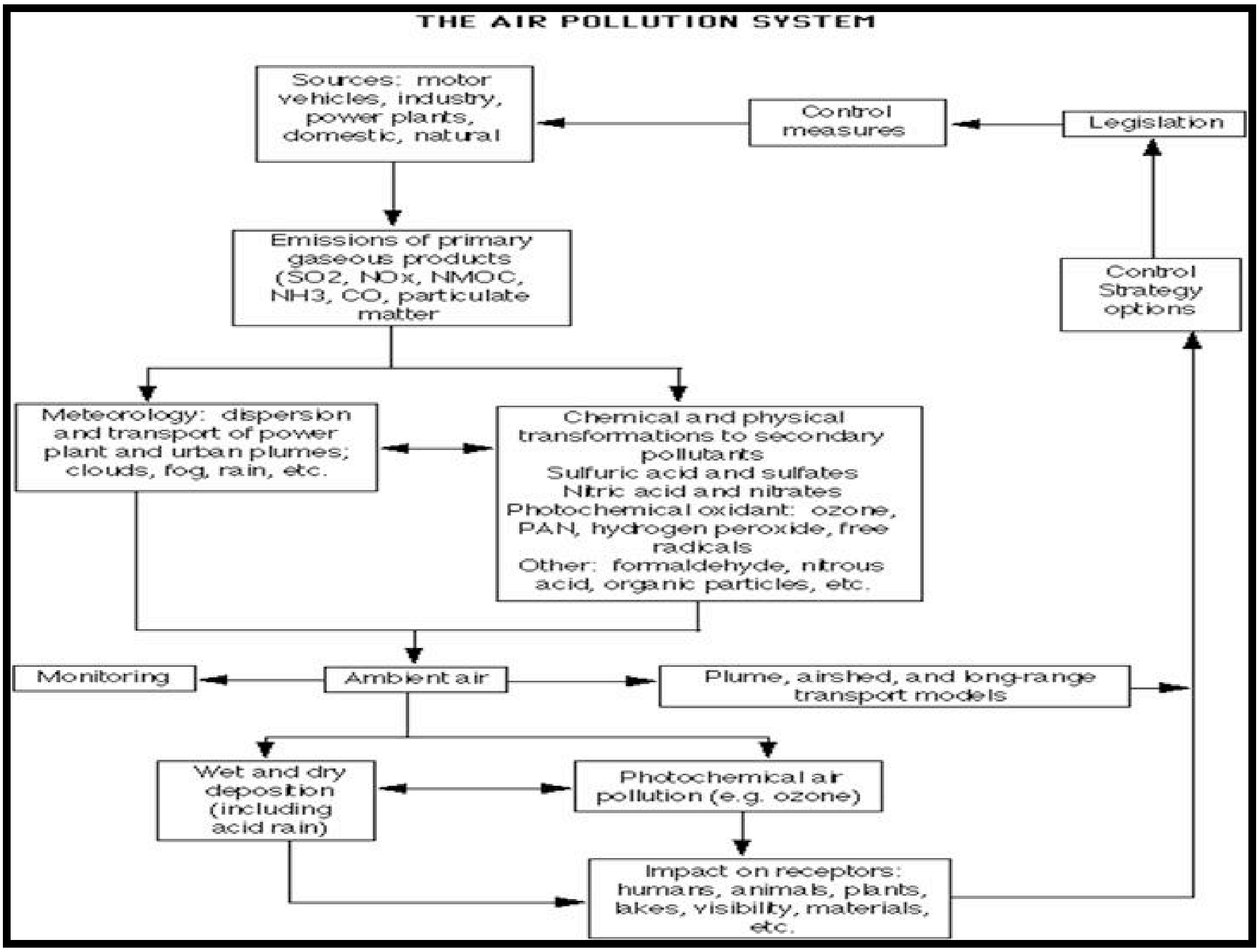


Figure 2 The air pollution system.

A complete understanding of the air pollution system diagram above is essential for success in any part of air quality work. The Figure 3 shows a general scheme for air quality models. In this graphic, meteorological and emissions data, combined with the users control strategies, all combine to provide input to the air quality model, resulting in some type of dataset as a result.

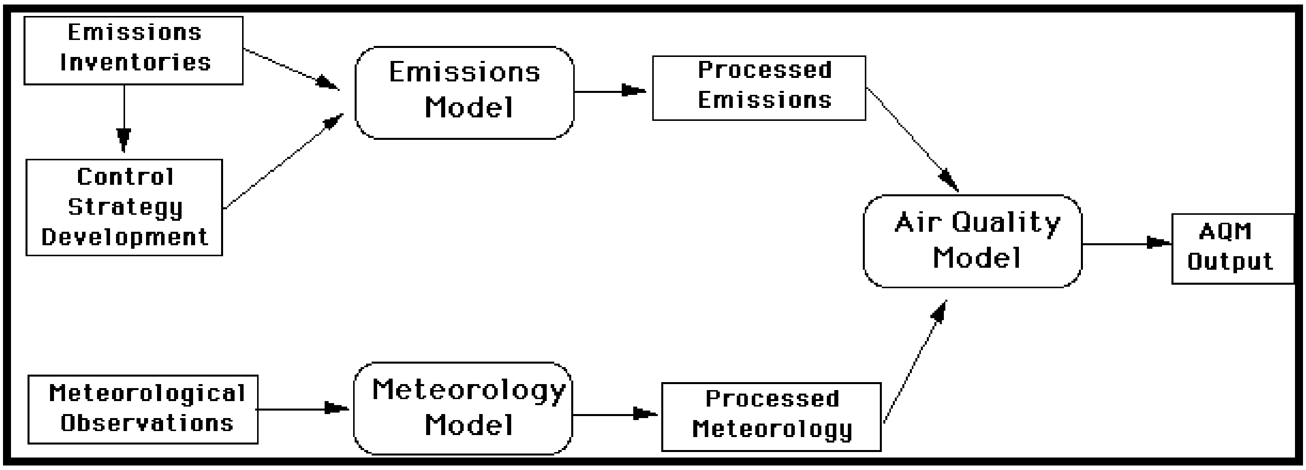


Figure 3 Emission modelling system.

In many air quality models, the meteorological data is approximated, collected in the field, or both, while the emissions inventories are often predicted using an emissions model. Emissions models typically use the principle of mass balance, and assume that emissions from a particular source for a specific pollutant in a specified time frame are equal to the product of the activity of the source in the unit activity. Most air quality models, require the analyst to be able to deal with the majority of the areas listed below:

- Meteorology and atmospheric physics
- Atmospheric chemistry
- Emissions inventories
- Computer Science (and computational science), which includes numerical analysis
- Regulatory Issues and Processes

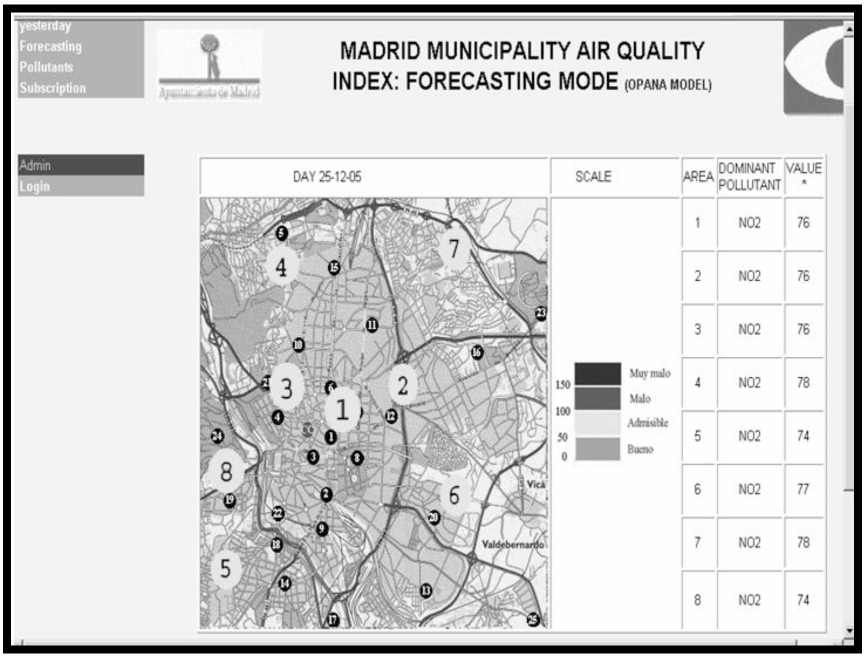
Computer capabilities have increased substantially during the last decade. Cluster platforms or parallel systems are used more often due to the fact that single processor capabilities are reaching their limits with actual architectures. Important efforts are made on developing software parallel applications which can parallel complex air quality models to optimize the performance on these platforms. Because of these advances, real-time air quality forecasting systems have started to be developed using complex 4D grid systems which include also reliable, robust and efficient chemical carbon mechanism. Real-time air quality modelling requires specific characteristics on modelling tools. A proper combination on data assimilation techniques, computer capabilities, parallel options and visualization techniques is required to perform a consistent, robust, efficient and reliable real-time air quality modelling system. Internet technology also is an essential technical element not only to disseminate the air quality forecasting information but also to access to the produced data in real-time in an efficient way.

Real-time air quality models require a reliable and robust chemical information related to the initial and boundary conditions (Stensrud et al. 2000) on our limited or mesoscale air quality models. Ideally, real-time mesoscale air quality models should be nested to real-time global chemical models which will produce proper initial and boundary condition for our mesoscale and urban and local scale applications. Real-time air quality applications can be designed in several ways depending on the specific type of application we are going to carry on. Typically for a European real-time air quality modelling system, a mother domain of about 6000 x 6000 km should be prepared. The spatial resolution should be as high as possible but resolutions on about 80 – 25 km can be applied depending on the computer capabilities we are having. If we do not have access to real-time global chemical model results, prescribed profiles can be used based on averaged values obtained from historical global chemical model runs.

The real-time emission module is another essential element of our system. The emissions should be calculated in a consistent way such as the nesting domains and mother domain should keep a full mass balance. This is important since much of the GIS techniques are not keeping this consistency and care should be taken into account to perform such activity. On the other hand, traffic, industrial and biogenic emissions are clearly depended on the weather variables such as temperature. This fact obliges us to link the weather forecasting system with the “emission forecasting system” since forecasting emissions are required to the forecasting period with our prescribed simulation period.

The temporal design of the real-time air quality forecasting system is done in two periods, the first period uses data assimilation technique – typically a 4DVAR – which assimilated meteorological and – if available – chemical monitoring data. This process is important since the maximum quality on these data is obliged otherwise important deviations between forecasted and measured data will be found. New non direct monitored data coming from satellite probes is starting to be available in real-time although much more work is necessary on this aspect. The advantage of satellite information is that it can cover large spatial domains – perfectly applicable to mother air quality model domains – with a good spatial resolution but the limitations on cloud covering and vertical resolution makes it an area still with a lot of research to be done.

There are different types or real-time air quality modelling tools. There are tools which can be applied to forecast the air concentrations at urban and regional domains which are applicable over cities and/or regions. These types of systems have been applied in the past over large cities and/or regions. Different examples have been applied in the past for Madrid City and Bilbao (Spain) (San José et al., 1997, 1999, 2000) under several EU projects such as EMMA, APNEE and APNEE-TU. (see Figure 4). These models were using limited area domains such as REMEST mesoscale meteorological model (based on the MEMO model, University of Karlsruhe, 1995) and SMVGEAR (Jacobson and Turco, 1994) with CBM-IV. Nowadays, European real-time air quality forecasts are produced under daily basis by our Laboratory (Environmental Software and Modelling Group, UPM, 2006) by using MM5 and CMAQ (OPANA V3) which can be used as boundary conditions for urban and regional high spatial resolution real-time air quality forecasting systems. (see Figures 5 and 6). Plans to implement a National Air Quality Forecasting System which includes chemical data assimilation and a 72 hour time horizon with 5 km spatial resolution for U.S. has been recently approved by NOAA (December, 6, 2005) for 2008.

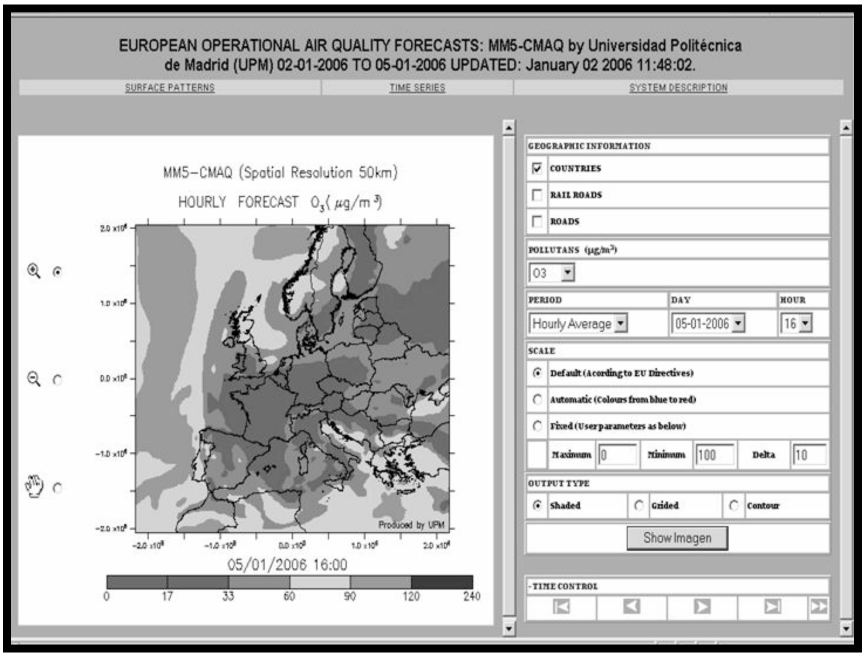


MADRID MUNICIPALITY AIR QUALITY
INDEX: FORECASTING MODE (OPANA MODEL)

DAY 25-12-05

AREA	DOMINANT POLLUTANT	VALUE *
1	NO2	76
2	NO2	76
3	NO2	76
4	NO2	78
5	NO2	74
6	NO2	77
7	NO2	78
8	NO2	74

Figure 4 Air Quality Forecasting System for Madrid City as developed for APNEE EU (IST) project (2000-2002) by using OPANA V2.


EUROPEAN OPERATIONAL AIR QUALITY FORECASTS: MM5-CMAQ by Universidad Politécnica de Madrid (UPM) 02-01-2006 TO 05-01-2006 UPDATED: January 02 2006 11:48:02.

GEOGRAPHIC INFORMATION
☑ COUNTRIES
☐ RAIL ROADS
☐ ROADS

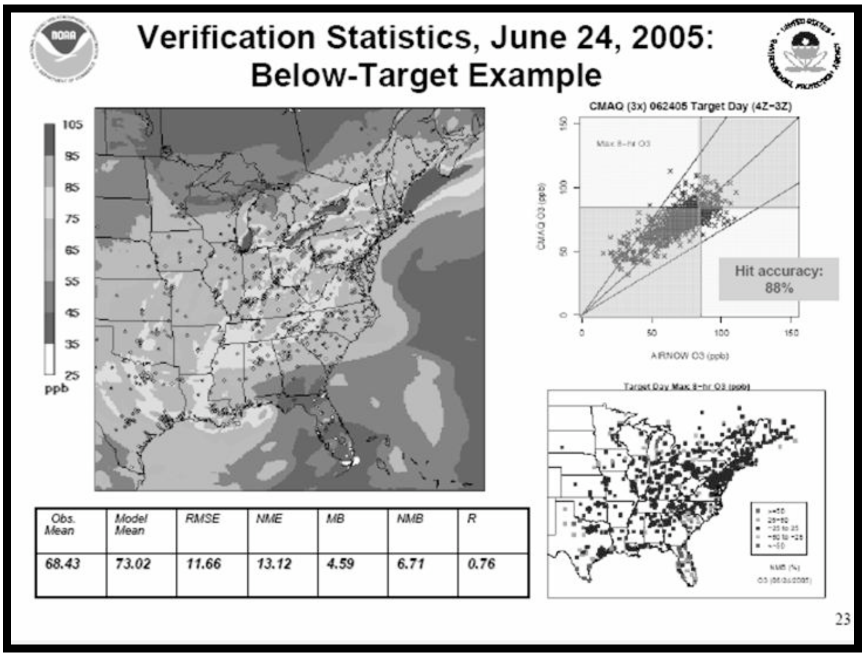
POLLUTANS (µg/m³): O3

PERIOD: Hourly Average
DAY: 05-01-2006
HOUR: 16

SCALE
● Default (Acording to EU Directives)
○ Automatic (Colours from blue to red)
○ Fixed (User parameters as below)
Maximum: 0 Minimum: 100 Delta: 10

OUTPUT TYPE
● Shaded ○ Grided ○ Contour

Figura 5 European Operational Air Quality Forecasts by using OPANA V3 (MM5-CMAQ) for January, 5, 2006 at 16:00 for Ozone concentrations.


Verification Statistics, June 24, 2005: Below-Target Example

Obs. Mean	Model Mean	RMSE	NME	MB	NMB	R
68.43	73.02	11.66	13.12	4.59	6.71	0.76

Figure 6 Verification statistics for a nationwide air quality forecasting system by using the MM5-CMAQ air quality modelling system to be in operation in US on Summer 2008.

Internet and information technologies for AQM

Environmental degradation (and thus air quality problems) may be linked to imbalance in interrelations between humans and natural world, and is thus systemic. From the “users point of view”, air quality models pose the typical characteristics of environmental applications concerning data management, i.e (Günther, 1998)

❑The amount of data to be processed is unusually large.

❑Data management is usually highly distributed.

❑Data management is extremely heterogeneous.

❑Environmental data objects frequently have a complex internal structure.

❑Environmental data objects are often spatio-temporal.

❑Environmental data is frequently uncertain.

❑The processing of user queries may require complex logical connections and joins.

Thus, urban air quality management may be considered among the central themes of the life cycle of environmental quality information within an urban domain, as represented in Figure 7 (Karatzas, 2005). While the environment, as a system “produces” data, the environment-related legislative framework specifies procedures, methods and terms under which environmental monitoring and modelling should take place for regulatory purposes. In addition to that, urban environment management actions are defined, by which environmental quality related goals should be reached in an area of interest. Thus, AQM may be considered as an environmental information “generator” within this context.

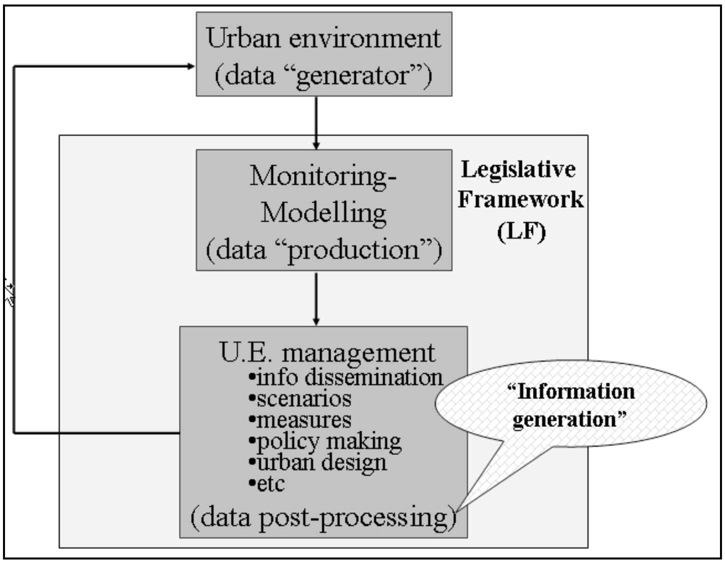


***Figure** 7*. Environmental Information Life Cycle.

Focusing on air quality, is should be noted that it is one of the more advanced environmental fields regarding the European Union legal framework developed. The first EU legislation concerning air quality information exchange and availability was Dir. 82/459, which was replaced by Dir. 97/101 which established a reciprocal exchange of information and data from networks and individual stations measuring ambient air pollution within the Member States. The 96/62 directive on ambient air quality assessment and management, also called “framework directive for air quality”, which was adopted by the European Council in September 1996, and the Daughter Directives issued thereinafter, stress the need of model application as a supplementary assessment method for reporting of monitoring data and for managing and policy making support (European Commission, 2002; van den Hout, 2002). The usage of AQM on the basis of legislative-regulatory terms and purposes is the case in USA, Japan, and many other countries.

Due to this reason, there is a need for countries to build upon the scientific expertise and experiences of each other and to harmonise model development in some respects. This need has been specified in Europe, with the aid of a number of scientific initiatives in this area, like the EUROTRAC-2 subproject SATURN (URL 1) and the European Initiative on "Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes" (URL 2). Yet, one of the main problems still existing is that the use of an air quality (AQ) model is considered to be (and it is in a vast degree) a dedicated tasks, that needs to be supported by experts. In addition to that, information and data required for an effective or operational application of AQM usually call for on-line, real or near real time accessibility, and have as a prerequisite the need for complicated pre-processing. Thus, the space and time distribution of input data, which is a characteristic that reflects the organisational structure of authorities responsible for their collection and archiving, is among the most pronounced difficulties one has to face when applying an AQM system for a certain area. In addition to that, some of these models require considerable computational resources to be made available, which may not be the case for a single application site, regardless of the diminishing cost of PC clusters, which are becoming more and more popular within the modelling society.

It is interesting to note that contemporary developments concerning modern Problem Solving Environments, the semantic grid and the semantic web, suggest that web-based management of environmental simulation tasks is one of the principal ways to follow concerning air quality simulations and modelling. Yet, before a holistic, effective, and wide-spread semantic grid and web platform is available, small-scale, but still multi-scale and effective solutions are required, for supporting web-based environmental simulation. Such solutions should be able to communicate and collaborate with existing modelling systems, while allowing for integration in the emerging grid community, if required.

Environmental information availability is thus supported by the development of the appropriate environment. Formation infrastructure (Saarenmaa et. al., 2002), that include access, processing and visualization of distributed AQ information (http://datafed.net/), an approach is supported by recent publications (Abramson et. al., 2002, Mineter et. al., 2005), Informatics developments and internet technologies maturation and spreading have resulted in the fact that for both scientific computing and for decision making and information providence, contemporary World Wide Web related technologies are able to play a key role.

Application category examples

1) Web-based integration

The need for the integration of a number of information resources in an efficient way for AQM purposes was underlined already in the frame of a number of research projects conducted with the support of the European Union in the 90ties, in the frame of the Informatics for the Environment umbrella. One of the most advanced projects at that time was ECOSIM, that suggested a client-server architecture, based on TCP/IP and http (URL 3; system architecture description and details available via Fedra, 1999). The main components were model servers, where the different simulation models were executed (for different environmental domains of interest, like air quality, coastal and ground water quality), and data base servers including the on-line connection to monitoring networks. The main server coordinated the various information resources and provided the elements of the user interface: graphical display, GIS, and an embedded expert system that supports users with the definition of scenarios for analysis.

2) Web-based wizards

A wizard is basically a series of screens or dialogue boxes that users follow through the completion of a task. Generally, each wizard screen asks users to enter information, either by making selections, or filling in fields. In the case of environmental-AQ simulations, the web-based wizard application helps the user in going through the whole AQ simulation process by providing a workflow scenario to be followed, accompanied by logical checks and support functions. To this end, wizards should be considered application services which are designed in such a way that they (a) help the user to apply a state-of-the-art AQ modelling tool in an easy, step-wise way, (b) . "save" time by remembering user's previous actions and choices/decisions and (c) explain every step needed to continue until the final objective is accomplished. An example of a wizard application is the Model User's Interface, which is a generalised, wizard-based, interface application, which allows for remote workflow management of scientific simulation tasks, and has already been applied in air quality modelling (Karatzas, 2005) (see Figure 8), and in non-destructive testing calculations (Karatzas et. al., 2005) alike. The implementation of the MUI is based on Java Web Start technologies for the client and Tomcat4 servlet container for the server. Thus, the platform used for development is J2SDK1.4 (http://java.sun.com). The client is a Java2 Swing application that makes use of Java Web Start technology to enable remote application invocation. The server is currently built on Java Servlet2.3 technology and the development environment was a GNU/Linux system with Tomcat4.1 servlet container and PostgreSQL7.3 database. The user may, thus, invoke the graphical interface of the application, and be guided though the appropriate selection of variables, upload of necessary data files and execution of batch jobs of models that are originally written in languages like Fortran (a schematic architecture of the application is provided in Figure 1).

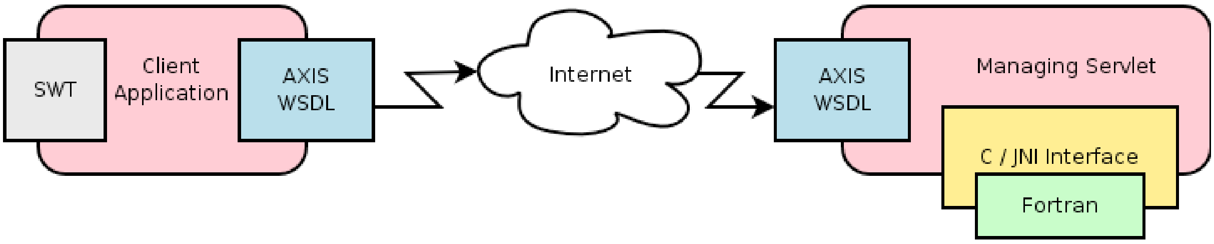


Figure 8: Basic architecture of the model user's interface wizard application.

The simulation may be executed in a remote, dedicated server, while the results may be downloaded and forwarded to the necessary post-processing upon finishing. It should be noted that the application is fully parameterised, user-tailored and localised (now supporting multilingual environments), easily adaptable to any type of AQ model.

3) Web services

According to Parikh and Pradhan (2003)," Augmented Web services are the next generation process aware services that enable meaningful end-to-end interactions in an application agnostic ecosystem. These Web services represent evolving open standards initiatives driven by standards bodies such as OASIS, W3C, JCP, etc. Thus, Web services may be considered as true software components or *artifacts* that lend themselves well to modeling techniques." This is not the only reason why web services are considered to be an appropriate technology for the support of scientific simulations, and more specifically for AQM. The application of web services technologies in the environmental sector has been reported for both data and processes (Radetzki et. al., 2002), and is already being standardized is various engineering disciplines (ASHRAE, 2004). Contemporary

AQM require for input resulting from heterogeneous sources (spanning from land use satellite data to upper troposphere boundary and initial conditions and earth based emission observations), while they include modules that should be invoked only when they are required and not at all times, in operational basis (aerosol modules, cloud modules, photochemistry etc). This heterogeneity concerning both information and simulation resources formulates the "ideal" environment of web service applications, which seem to be one of the main drives towards the future of scientific simulations, in general (Muetzelfeldt, 2004), leading to an advanced AQM environment (Miniwater et al., 2005)

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