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AIR QUALITY MODELLING

Executive Summary

5TH SEMINAR ON AIR QUALITY IN SPAIN

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Current legislation establishes that, in addition to continuous and systematic measurements by measuring stations, other technologies capable of assessing or even predicting air quality can be used. Mathematical modelling is obviously one such tool. In recent years there has been a major upsurge in the use of mathematical modelling, with the development of mathematical models addressing the simulation of meteorological conditions and dispersion (including chemical transformations) of atmospheric pollutants with a high level of accuracy. Models now cover increasingly more physical and chemical processes, more pollutants, and apply more sophisticated mathematical algorithms to solve the mathematical equations involved. Modelling techniques have also benefited from the substantial improvements in the calculation power of computers, the availability of more and better information about meteorology, emissions, etc, and by the added potential of their use in conjunction with other complementary but important tools such as geographic information systems.

However, this development in the field of modelling has resulted in only a somewhat modest implementation of these tools in the field of air quality management in Spain, which is why a common effort needs to be made involving the scientific and technical communities, end users, and air quality managers. To this end, under the aegis of the Ministry of Environment, a working group has been set up on air quality modelling that includes managers of various state and autonomous public administrations, representatives from the private sector, and research and development groups in the field of numerical air quality modelling.

The main goals towards which this group is working are: to increase our knowledge of the models that may be useful to air quality managers; to promote the use of atmospheric and dispersion models as a working tool for air quality managers; and to make it easier for managers and end users to access existing information about models and their use.

With these objectives in mind, the group considered a series of initial questions:

1. What do air quality managers expect from the models? What can the models offer?
2. What do modellers require in order to meet the needs of air quality managers?
3. How reliable are the models? What models are appropriate for each problem?
4. What models are used in Spain and in the rest of the world?
5. How should emission inventory information be used by the models?

The basic mission of the working group is to find answers to these questions, while the purpose of this document is to report on the answers obtained to date. They are the result of a labour of compilation, reflection, pooling, and discussion during 6 months including three meetings in CIEMAT and frequent debates (some of them exciting) and reviews of documents using the possibilities provided by the Internet. The document is articulated in five chapters corresponding to the aforementioned five questions. The production of these documents was assigned to specific individuals who took responsibility for them, but all the members of the working group contributed to all the articles to a greater or lesser extent, and we have tried to reflect the general, or at least the majority, opinion of the group in each question. In some cases, there have been contributions from collaborators from outside the group and they have been recognized in the document where appropriate.

The working group was made up of 14 people with a good balance (almost 50-50) between scientific-technical people and people from the public administrations. The group was coordinated by CIEMAT and the following people took part:

- Fernando Martín (CIEMAT) – Coordinator
- Maria Victoria Albizu Etxeberria (Basque Country)
- José María Baldasano (BSC)
- Roberto San José (Faculty of Computer Science - UPM)
- Rafael Borge (ETSII – UPM)
- Eloy Piernagorda (IBERINCO)
- Catina March (Balearics)
- Antonio Lozano (Andalusia)
- Susana Gil (Catalunya)
- José Luis Palau (CEAM-Valencia)
- Juan Carlos Casado (Murcia)
- Alvaro Pérez-Uría (Castilla-La Mancha)
- David Cartelle Fernández (Galicia)
- Alberto González (MMA)

What do the air quality managers expect from the models? What can the models offer?

Air quality management requires a frame of reference with mechanisms that allow possible problems to be identified and diagnosed, air quality targets to be defined, standards and control and action procedures to be established, control and monitoring strategies and action programs to be designed.

In the early days, the development of air quality management related activities was predicated by the need to address specific problems, and a dominant role was played by operational systems to monitor and control pollution, based fundamentally on the measurement of pollutants.

However, in recent decades, concerns regarding new air quality related problems, their complexity, the need to address global and cross-border issues, or the recognition that the atmospheric environment is the responsibility of society as a whole, has caused air quality management to move towards new approaches, ones in which systems must be complemented with new tools to fit the new times. Modelling may play a determinant role in these approaches.

Although a number of different definitions exist, a model can be defined as a tool that attempts to describe or reproduce the essential characteristics of a system, of the processes that form part of that system, and the results or consequences that the system produces.

In general terms, modelling is a tool that can be applied to all aspects related to atmospheric pollution, its source, and its consequences, such as: characterization of emissions, the transport, transformation, and deposition of pollutants, estimates of immission, deposition, and exposure levels, effects on ecosystems, heath and materials, and source-receptor relationships.

By air quality model, we usually mean a calculation tool that can provide an estimate of immission levels caused by the emission of pollutants, under certain conditions, over a previously defined geographic area.

There are different types of air quality models, although in the field of atmospheric environment perhaps the most commonly used are those based on mathematical algorithms. However, the use of these models requires certain data to be collected. Some of this data can be collected prior to the use of the air quality model, such as meteorological characterization or modelling, and emission data, including spatial distribution and temporal evolution. Meanwhile other types of information are needed in order to process the results of the model and to provide additional information of interest (economic assessment of pollution abatement strategies, new technologies, blame and liability analysis, etc).

In general, the principal purpose of using models is to provide air quality managers with objective, numerical information that is as real and accurate as possible, to be used as an element of valuation, assessment, or decision support within the framework of air quality plans, programmes, control and monitoring strategies, etc. In chapter 1 of the document, we show several examples of the usefulness of these tools.

When faced with a problem for which modelling can provide solutions, the air quality manager can choose between developing a specific solution and adapting an existing tool. Before making the choice, it is advisable to conduct a technical-economic analysis. Whatever the choice, using a model must always involve a process of development, adaptation, setup, and validation to ensure that the model is able to fulfil its purpose. And when it is in operation a model must be subject to an ongoing process of verification and improvement.

For models to be a useful tool for air quality managers, they must be sure that the results of applying the model really do provide an added value to their work, while also facilitating or even simplifying their work. Chapter 1 sets out some requirements that managers consider to be important if models are to be of use to them.

The use of modelling tools can provide important benefits to air quality managers. But in order to do so, we must first make sure that we have a clear understanding of the conceptual bases that underpin these tools, their range of validity or application, and the characteristics of the products that they provide, and take into account their limitations (models are not the real world but only an approximation).

The text of the first draft of the new Air Quality Law states that there are a number of concepts or issues whose clarification, definition, estimation, or operation in general may require or advocate the use of models, thereby complementing existing measurement networks, on a national, regional, and local scale. These are: the design, development, and monitoring of plans and programmes; the assessment and prediction of air quality; evaluation systems; and the monitoring and prevention of pollution. The main activities in which the complementary use of modelling could be required are summarized in appendix 1 of the first chapter of this document. However, this law also raises important issues regarding the implementation of air quality models. Among these are the issues of scope of competency (state, autonomous communities, city councils) and administrative boundaries (the atmosphere does not recognize political borders), the need for qualified personnel and economic resources, and the existence of a great variety of available tools or models (the need for harmonization). Finally, it could be interesting to reflect on whether or not there should be *Entidades Colaboradores de la Administración* (Collaborating Government Agencies) for modelling, such as those commonly found in other similar fields like emissions measurement or control.

What do modellers require in order to meet the needs of air quality managers?

There are a considerable number of air quality modelling tools from which to choose. The last 10 years has seen a significant development of air quality models. Since the early 70's, when Gaussian models were developed, until the present day, the progress and evolution of tools for air quality modelling has been constant and substantial. Today there are models that are capable of handling the physical and chemical processes affecting the atmosphere and pollutants in considerable detail.

The development of air quality models has been positively influenced by the increase in computer power. Air quality models have developed in parallel with meteorological models. These have been gradually adapting to the needs of air quality models, providing the information they require for their input. There are several different types of meteorological and air quality models of widely varying complexity and applicability. The models employed to analyse photochemical pollution and from aerosols are especially important.

Also, many models nowadays are able to simulate processes over several spatial and temporal scales, obtaining a representation which is more complete and closer to reality, by means of nesting techniques that allow models to reproduce atmospheric processes in a large spatial domain (hemispherical or continental) and progressively narrow the domain to smaller areas (national, regional and local).

There are also data assimilation techniques whereby models can assimilate the observed meteorological and air quality information, thereby increasing their capacity to reproduce reality by damping possible deviations in predictions. This technique is highly developed in the field of meteorology, whereas it is still under development in the field of air quality.

It is important to experimentally identify the processes involved before choosing, configuring, and applying the appropriate models. We also believe that it is necessary to continue researching into the processes associated with pollution episodes on a number of different scales. Although they may be well enough known on a synoptic scale, there are nevertheless gaps in our knowledge of the interaction between the different scales and of long-range transport.

With regard to the data required by air quality models, there are also some important considerations that would help us to make better and easier use of models:

- Meteorological Information. It must be robust, accurate, and reliable in terms of the requirements of air quality models (document EPA-454/R-05-002 of October, 2005 and published by EPA in November, 2006). It must also be appropriate to the type of photochemical modelling or air quality study that is to be performed. There are many sources of meteorological information, but there is no standardization regarding its collection and use. Therefore guidelines should be drawn up concerning the information requirements of different types of models. Accessibility to meteorological information by the scientific community, government bodies, and companies should also be improved.
- Pollutant emissions. Emission data of primary pollutants for air quality modelling should be disaggregated in space and time. In the case of volatile organic compounds, these emissions should be broken down into a number of representative groups or species. Emissions of pollutants should also be disaggregated spatially and temporally, and by source. All possible sources of pollutants should be considered, including nature itself (biogenic emission, dust resuspension, etc). A national inventory is needed together with several regional ones (compatible between one another). They must be easy to update, include more pollutants (e.g. particles of natural origin), with a better spatial and temporal resolution. It is also important for good emission models to be developed to run in predictive mode; that is, they should be able to predict emissions so as to be able to predict immissions
- Land use and topography. Land use and topography data are also fundamental for a correct modelling of air quality. Different classifications of land use will be employed in the same model depending on the specific application (biogenic emission, meteorology, pollutant deposition). With regard to availability of information, digital models of land and land use data are available from the European Environment Agency and the USGS in the USA, among others.

In conclusion, we can say that:

- There needs to be much more research into the different atmospheric processes in Spain, especially into the interaction between the different scales.
- There needs to be easier access to meteorological information over the Internet, especially for scientific uses and for public authorities.
- The national emission inventory must be extended to meet the needs of air quality models; for example, a greater spatial (1 Km) and temporal (1 hour) disaggregation. Regional inventories compatible with the national one should produced, and all these improvements should be implemented for emission forecasting as well.
- It is necessary to know the estimated spatial representation of the information measured in the various air quality networks in order to attempt to make the results obtained by modern models more compatible with the observed values.
- It would seem to be necessary to have a place where the information can be accessible to citizens in situ and over the Internet, but with uniform formats.
- It is necessary to organize more congresses, conferences, seminars, workshops, working groups, thematic networks, etc. to facilitate dialogue among researchers, environmental authorities – at every level - and the public. An air quality modelling website would be ideal.
- Special care must be taken in the validation of concentration data from stations, since in some cases wrongly validated data has been detected.
- Meteorological scenarios should be used as a relative reference because many episodes of air pollution cannot be associated to a specific type of meteorological scenario.
- Long-term simulations using meteorological models should be carried out.
- A great deal of emphasis should be placed on developing good predictive emission models.

How reliable are the models? What models are appropriate for each problem?

A large number of models are used to simulate meteorology and pollutant dispersion and they have a more or less limited range of application, according to the type of pollutant, the meteorology and, more specifically, the type of air flows, all of which will be greatly influenced by the geographical characteristics of the area to be modelled.

Spain has an extraordinarily diverse geography: abrupt Mediterranean, Cantabrian, and Atlantic coasts; flat Atlantic and Mediterranean coasts; Mediterranean and Atlantic islands with complex topographies; large valleys, plateaus, and some very mountainous areas. There is also considerable climate diversity, with a marked difference between Wet and Dry Spain.

Considering the geographical particularities and their influences on air flows, in areas of flat and uniform terrain (without major changes in land uses), simple models (Gaussian plume models) can be applied with reasonable reliability. They are easy to use by feeding them with meteorological information from at least one meteorological tower, and they have very low computational requirements.

In flat coastal areas the presence of the sea results in a marked heterogeneity, causing cyclical atmospheric circulations such as breezes. In this case, more complex models (mass-consistent, 3D models are required together with a good amount of meteorological data from several different towers, or hydrostatic models) in order to provide a more accurate representation of the three-dimensional nature the air flows.

In the case of areas with gentle hills, similar models can be applied as in the previous cases. Dispersion models have to be more complex, either Lagrangian models (the pollutant is simulated using a large set of elements - clouds or particles – that are dispersed independently from one another) or Eulerian models (these simulate the dispersion of pollutants using a calculation grid covering the area of interest).

Areas of complex topography produce air flows of a thermal origin (the warming and cooling of slopes), such as mountain-valley breezes, and mechanical disturbances from large scale winds (synoptic winds) because the mountains act as obstacles. These are the most unfavourable cases, where more complex models (non-hydrostatic models) are needed involving the need for more input information, better spatial resolution and, therefore, more computational cost and user experience. Dispersion models will also be of the more complex kind (Lagrangian or Eulerian models).

The input information needed by air quality models is basically:

- Emission data; generally provided by an emission inventory model. The accuracy of such data is fundamental to the model. Information about the pollutants that the chemical mechanism of the dispersion model requires should be provided and should be temporally and spatially disaggregated.

- Meteorological information and 3D meteorological fields (wind, temperature, humidity, parameters relative to turbulence and dispersion, etc), and 2D meteorological fields (solar radiation, mixing layer height, rain, etc). This highly detailed information is generally provided by means of meteorological models, which in turn use information from stations.
- Others: latitude, day of the year, deposition velocities, photolysis parameters (very important for atmospheric chemistry), orography of the area, land use, initial conditions (what initial pollution there is) and boundary conditions (what pollution enters our calculation domain from outside), etc.

For model validation, experimental information is required from several air quality networks (such as EMEP, Autonomous Communities, etc.), other automatic stations, ozone soundings, and satellite data, in addition to other information already validated by the corresponding environmental authorities, and complementary meteorological information, databases from the experimental campaigns of various projects, etc.

The current trend in the use of air quality models for regulatory applications is mainly focused on the production of use guidelines for air quality models rather than designating official models, since current models are still under development whereas the official models may have become obsolete and limited. The guides for using air quality models must be dynamic documents subject to continuous review by users and modellers in order to meet the needs and requirements of air quality problems as they arise. They are also to report on how the results of models and other measurements should be used to meet the acceptance requirements of the air quality models, and how the air quality models should be used to ensure compliance with those acceptance requirements.

The US Environmental Protection Agency () has developed a series of guidelines (US EPA, 2005), based on the 1991 guidelines (US EPA, 1991) for the use of a series of statistical measurements in model evaluation for those areas where data from monitoring stations is sufficiently dense. These measurements are mean normalized bias error (MNBE), mean normalized gross error (MNGE), and unpaired peak prediction accuracy (UPA). Informal goodness-of-fit criteria or performance standard criteria have been evolving for more than ten years so that today we have a framework of study for assessing the performance of air quality models. The accepted criteria are: MNBE = ±5 to ±15%; MNGE = +30 to +35%; and UPA = ±15 to ±20%. It is accepted that a model works under these statistical values once the influence of initial and boundary conditions is eliminated.

Meanwhile, Spanish legislation derived from European regulations establishes the uncertainty levels that models must conform to for each pollutant. Modelling uncertainty is defined as the maximum deviation from the relevant threshold of measured and calculated concentration levels over the calculation period, without taking into account the chronology of events. When evaluating models, the uncertainty levels established by Spanish legislation and those stipulated by the EPA should be taken into account.

The design of a model validation system must be focused on determining how accurately the model can predict when limit values and public information and alert thresholds will be exceeded, and how the models fits the observed time series of pollutant concentrations using the available measured data (air quality stations, meteorological data, satellite information, etc). The operational validation system should have two levels: a level of simplified and routine interaction (level 1) based on a number of classical discrete (categorical) statistical data or ability indexes, following air quality criteria from the EU; and another non-routine level (level 2) that focuses on the components of the forecasting tool, is based on the available complementary information, and depends on specific scenarios. It is essential that the validation system is not a static system, but that it is continuously improving its capacity and, therefore, the quality of its predictions.

What models are used in Spain and in the rest of the world?

A great many different models are being developed and used worldwide in the field of air quality. This is due to the diversity of pollutants, spatial and temporal scales, and physical and chemical processes, along with the need to produce the information required for the dispersion models (meteorology and emission). The degree of complexity also varies greatly, as does the range of applicability of each model.

There are dispersion models for pollutants without chemical complex reactions such as CALPUFF, MELPUFF, CTDMPLUS, ISC3, FLEXPART, HYPACT, etc. Models focused on the simulation of atmospheric photochemistry include CMAQ, CAMX, CHIMERE, MARS, CALGRID, OPANA, etc. Others, like BSC-DREAM, are specific to simulating the long range transport of particulate matter. There are models, like OSPM, that are designed to evaluate pollution in the streets, and models to simulate the behaviour of denser-than-air gases (toxic clouds emitted in industrial accidents), like SLAB.

In addition to these dispersion models per se, we should add the meteorological models required to provide the weather data needed by the dispersion models). The most commonly used are MM5 and WRF, although RAMS and CALMET, among others, are also worthy of mention.

Emission models are another very important and necessary group to provide the estimated pollutant emission data required by dispersion models. Some of them are focused on a specific type of source, as is the case of MOBILE6, MACTRA-MICTRA or COPERTIII for traffic emissions, or WBEIS for biogenic emissions, or MECH for mechanical resuspension of particles. Others, however, can handle a wide range of sources of pollution (SMOKE, EMICAT2000, and EMIMO).

The EPA establishes a series of recommended models to address different air quality problems. The selection process for recommended models is very rigorous, albeit slow, given that all models are subjected to exhaustive tests to verify their ability to reproduce atmospheric processes (validation against field experiment data) and validity against other models (intercomparison model). In spite of the fact that these models are not usually the most up to date and therefore have probably been superseded by other more recent models, they can nevertheless be said to have proven reliability. These EPA recommended models are available on their website at http: // www.epa.gov/ttn/scram/.

Meanwhile, through its European Topic Centre on Air and Climate Change, the European Environment Agency has developed a database of models applied to various aspects of air quality called the Model Documentation System (http://air-climate.eionet.eu.int/databases/MDS/index_html). Its aim is to provide a guide to users of models to help them choose the most suitable models for each specific application.

Also, as part of European COST actions 728 and 732, an inventory of atmospheric models has been produced. These models, intended both for meteorology and for dispersion and chemistry, have been developed and/or used by various research groups, companies, and administrations in a number of different European countries(http: // www.mi.uni-hamburg.de/index.php? Id=539).

In Spain, the use of models has been growing considerably in the last decade. There is a small but significant number of groups dedicated to the modelling of air quality, not only in the academic and research area, but also in the consulting sector and, to a lesser extent, in the government sector. An appendix to this document contains some tables summarizing the activity of various modelling groups, the models they use, and the kind of studies and applications they have conducted.

In Spain other studies have been carried out using mathematical techniques based on neuronal networks and statistical models, or techniques involving the combination of measurements, modelling, and geographic information systems.

Modelling activities could be better coordinated if there were a website on air pollution modelling where all the relevant information about models, description, applications, results of simulations at a national level for air quality assessment, predictions, news, courses, congresses, links to others web, etc. could be found. Such a website could be oriented towards creating a "collaborative environment" accessible by members of the community of modellers and users, in which free software, updated documents, experiences, forum of debate, etc. could be posted

At CIEMAT, work is underway on the design and structure of the content of such a website, and on the preparation of written and graphical material. This web will have several different sections:

1. Introduction to atmospheric models.
2. Types of models, providing detailed explanations of their basic features.
3. Atmospheric models used in Spain. To include a list of the models used in Spain both for universities and research centres, and for companies and local, autonomous, and national governments. The models will be described together with the type of problem, studies, and/or application they are being used for.
4. Links of interest, allowing users to have a ready access to other websites: specific subjects, atmospheric modelling research groups, institutions, projects, and programs, and other modelling-related information of interest.
5. Meteorological and air quality predictions (links to web pages with this information).
6. Results of the use of models in the annual assessment of air quality in Spain with the option of downloading information.
7. Information and documentation regarding news, courses, publications, and congresses on this topic. The possibility of conducting online courses using e-learning technology is also being considered.

How should emission inventory information be used by the models?

An important topic in modelling is emission inventory; that is, information about how much pollutant is emitted, and where, when, how, etc. This information has to be very accurate if it is to be used in air quality modelling, because emission errors lead directly to errors in concentration calculations. Also, emission data must cover the same number of pollutants as those we wish to study and which are included in the chemical mechanism of the dispersion model, it must give information on how the emissions change over time and how they are spatially distributed, for both point-specific sources and mobile or area-specific sources, in accordance with the requirements of the case in question and the model system used. To illustrate all these aspects, an example of the adaptation of a macro-scale inventory with total annual emissions to the requirements of a dispersion model, Coal Bond IV, based on photochemical mechanism, is shown in the document.

Final remarks

We believe that the work of this group has only just begun, since very important issues have been addressed but other aspects are still left unexplored. We believe this more than justifies the continuity of the Working Group on Air Quality Modelling after the 5th Seminar on Air Quality in Spain has been held. This group can act as a forum for modellers, researchers, and air quality managers. On such a forum, they could jointly discuss the latest advances and innovations in this subject and establish specific research priorities and needs. They could develop guidelines and methodologies for a better selection and use of models in response to the eternal question of why there is not one or several official models in Spain. A forum could support the Ministry of Environment on some legislative aspects in which modelling could play an important role, especially in view of the latest European directives and national legislation. There could also be an associated website on air quality modelling which would be a vehicle of communication and information transfer among modellers, air quality managers and the public, as well as an instrument of education, training, and consultation for non-experts.