ARCHIVES OF ENVIRONMENTAL PROTECTION

vol. 36 no. 1 pp. 3 - 28 2010

PL ISSN 0324-8461

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NEW CHALLENGES IN AIR QUALITY AND CLIMATE MODELING

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Keywords: Air quality, air quality models, meteorological models, chemical mechanisms, climate change, regional climate models.

Abstract: At present, when high particulate matter (PM) concentrations in ambient air cause thousands of premature deaths in Europe and global climate change is becoming the most critical issue in environmental protection, the state-of-the-science air quality and climate models constitute an essential research as well as decision support tools. Recently the great progress has been achieved in this research area. The present paper presents the goals and tools for Air Quality (AQ) Modeling, and gives overview of current challenges, including the meteorological, chemistry and climate modeling. The main emphasis is given to the regulatory and the Eulerian grid models, the latter are currently operating as so called off-line or on-line modeling systems. The issues connected with model implementation and validation is presented as well. Finally, the conclusions are drawn and recommendations for further development and integration of AQ and climate modeling in Poland are presented.

INTRODUCTION

The Earth's atmosphere is directly connected to the hydrosphere, lithosphere, kriosphere, ecosphere and biosphere. As a result, air pollution can easily be transferred to all other environmental media. Presently, the lower atmosphere over the entire globe is being polluted by both anthropogenic (industrial, transport, municipal, agricultural) and natural sources (forest fires, volcanoes releases, biological decay, dust storms). As proved in the late 1970s, most of the air pollutants are transported both through boundaries, as well as between continents (UNECE, Geneva Convention on Long-Range Transboundary Air Pollution (LRTAP), 1979). As confirmed in the 1980s, some long-lived species (CFC, halons) are transported to the stratosphere, where they catalyze the ozone destruction (UNEP, Vienna Convention for the Protection of the Ozone Layer, 1985). Since 2007, it is very likely (with probability higher than 90%) that "most of the observed increase in globally averaged temperatures since the mid-20th century is due to the observed increase in anthropogenic greenhouse gases (GHGs) concentrations" [37].

In spite of recent technological achievements in air pollution abatement, poor air quality is still a major environmental problem for many European regions. Traffic and other human activities continue to exert pressure on the state of the atmospheric environment. Currently, particulates (PM) and ozone have become a "critical pollutants" worldwide, in respect to human health. Increased levels of O_3 and fine particulates ($PM_{2.5}$) can cause severe respiratory and cardiovascular diseases and increase the risk of death.

The emission of greenhouse gases (CO_2, CH_4, ozone, CFC, N_2O) are (very likely) responsible for warming of the climate system. According to the latest IPCC Assessment Report [37], warming of the climate system is unequivocal, as is now evident from observations of increases in global average air and ocean temperatures, widespread melting of snow and ice, and rising of the global mean sea level.

Research in recent years has led to a substantial improvement of our understanding of the physicochemical behavior of the atmospheric and climate systems, as well as impacts on human health and ecosystems. Moreover, a large amount of information has been collected, and modern tools developed, that may be applied to assess both the air quality at regional and local scales, as well as global and regional climate changes.

However, several aspects of the atmospheric and climate systems are still only poorly understood. Moreover, due to the increasing knowledge of the impacts of air pollution and climate change, these effects constitute a larger global issue at present than they were in the 20^{th} century, creating a great challenge for atmospheric science community.

Thus, significant efforts has been made, both in Europe and in USA, to develoe the refined modeling tools, and establish proper databases needed for reliable multi-scale air quality and climate change assessments.

This paper presents the goals and tools for Air Quality (AQ) modeling and gives the overview of current challenges in that research area, including the meteorological, chemistry and climate modeling. The problems connected with model implementation and validations are discussed. The last chapter is dedicated to AQ and climate modeling in Poland. Finally, the conclusions and recommendations are provided. As the presented subject is extremely wide, only the most important, in author's opinion, issues, are discussed.

GOALS AND TOOLS FOR AIR QUALITY MODELING

The complexity of physical and chemical atmospheric processes results in many complexities in the atmospheric and climate systems. Since the 1950s, when the first air quality models were developed, a great progress occurred in atmospheric research. However, continually there are a lot of gaps in our knowledge and understanding, mostly due to the scale of the problem: from local, trough regional to global, as well as from the short-term episodes (1 h, 24 h) to the long-term behavior (years, decades).

The Air Quality Model (AQM) is defined as a system that quantitatively relates the concentrations (depositions) of pollutants to other parameters by mathematical methods. The AQM plays a fundamental role in both the understanding of individual processes and the whole atmospheric system, as well as in a number of regulatory, management and prognostic applications. Moreover, as presented in Figure 1, it is used in the impact assessment and in scenario analysis for decision support, as a part of the so-called Integrated Assessment Model (IAM). For the overview of the IAMs the reader is referred to [46]. Finally, AQM is an important tool in Climate Change Modeling, where it is used to study the air pollution – climate feedbacks.

The mentioned above wide range of the AQM goals resulted in developing a wide range of computational tools. There are two main AQ "modeling principles". The first one is to chose a correct model for a specified application. The second one is based on the fact that the output quality can never be better than the input quality, so the availability and

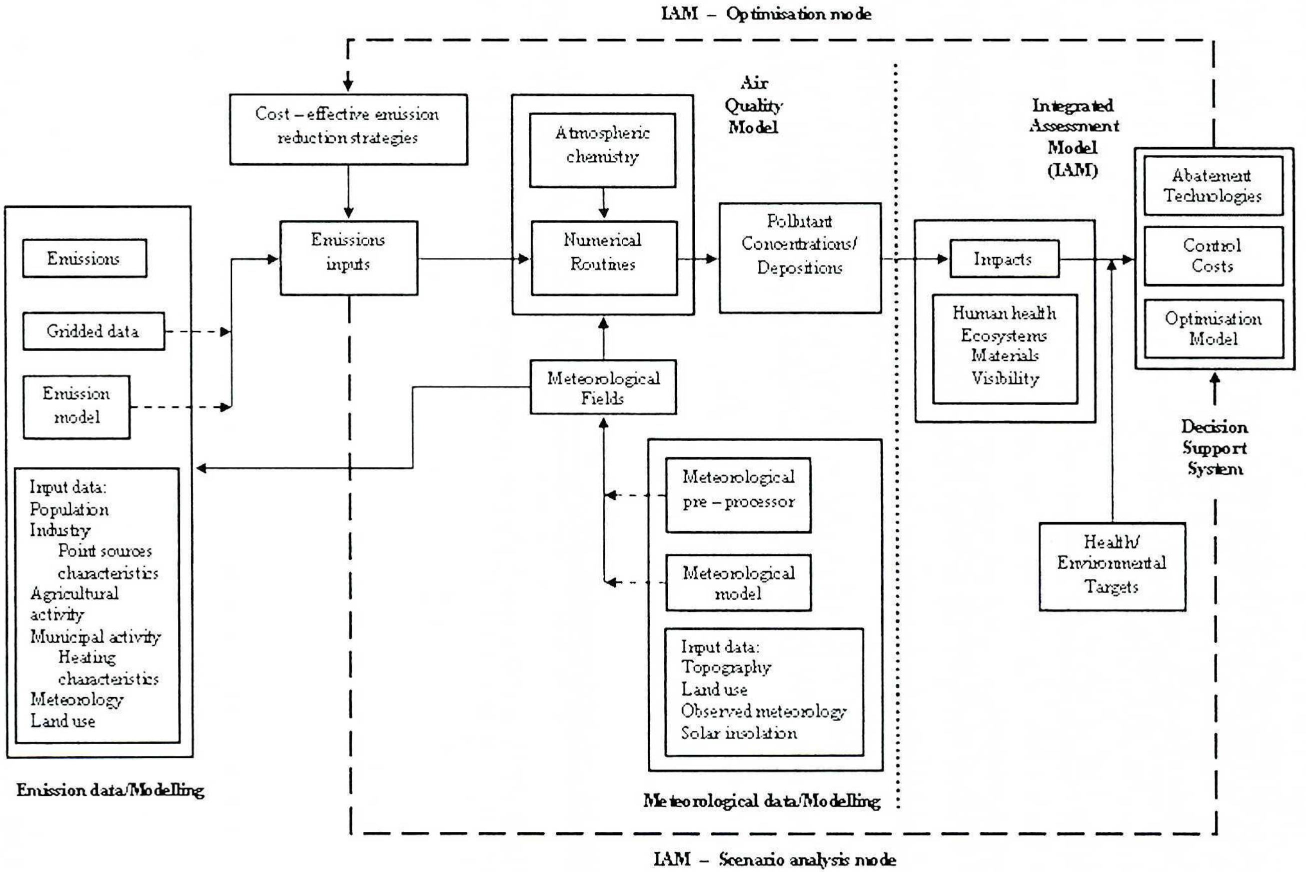

Fig. 1. Schematic of the Air Quality and the Integrated Assessment Models; the boxes with shadow represent modeling processes, thin dashed lines represent potential tools for obtaining input fields to the Air Quality Model, bold dashed lines represent scenario analysis and optimization modes of the Integrated Assessment Model (modified and extended after [67])

quality of the input data have to be ensured, before model application. The AQM varies widely from a very simple to extremely sophisticated one. Each model is a compromise between simplicity and sophistication, accuracy and practicality. The classification of AQMs has been presented by e.g. Juda-Rezler [44] and Markiewicz [56]. The main types of AQMs, which have found applications in atmospheric research, are the following:

1. Closed-form analytical – Gaussian plume/puff models.
2. Numerical models; mostly first-order closure (K-theory) models:
   - Eulerian grid,
   - Lagrangian trajectory,
   - Hybrid Lagrangian-Eulerian.
3. Stochastic models, e.g. random-walk (Monte-Carlo) trajectory particle model.
4. Statistical models.

The first two groups represent the deterministic modeling. Deterministic models calculate concentrations (and/or depositions) of selected air pollutants in space and time as related to the independent variables (emission, meteorology, chemistry), according to the solution of various equations, governing the relevant physical and chemical processes in the atmosphere. They are most suitable for air pollution calculations, although, the numerical AQMs are costly (time and storage consuming), and require a large databases. The statistical models, on the contrary, have a small computing time, however, the statistical relationships used in the models, have to be updated each time the emission or the receptor characteristics change and have to be adjusted for each area. As a consequence, they have found application mainly in prognostic modeling. In the next section only the deterministic modeling will be focused.

BASIS FOR DETERMINISTIC AIR QUALITY MODELING

The valuable reviews of various kinds of deterministic AQMs were presented by Eliassen [22] (for the long range transport modeling), Peters *et al.* [61] (for the Eulerian models), Seigneur *et al.* [69] (for the modeling of PM), Russel and Dennis [67] (for the photochemical modeling), Caputo *et al.* [11] (for the Gaussian and Lagrangian codes), Vardoulakis *et al.* [78] (for the modeling in street canyons) and, recently, by Holmes and Morawska [34] (for the modeling of PM).

For deterministic models we can write:

$$F(P,M):Q \rightarrow C,Dep \tag{1}$$

where F represents the AQ model; while P, M, Q, C and Dep denote, respectively, model's parameters, meteorology, emission, pollutant's concentration in air and pollutant's deposition on the ground. When talking about the air quality modeling, the distinction suggested by Russell and Dennis [67] seems to be most adequate: a model is a collection of mathematical relationships and algorithms that allow calculation of the evolution of pollutants, while the modeling process involves steps necessary to construct the model inputs, model development, model evaluation, analysis and use of the model results (Fig. 1).

At present, a variety of AQMs exist for different scales (street canyon, urban, regional, continental, and multi-scale). They differ from one another; however, they also share many common features. The main differences include essentially the modeling processes of emission, meteorology, and atmospheric chemistry, as well as the methods used for solving of model's equations (see dashed grids in Fig. 1). Also, the models differ in the type and number of species included (e.g. photochemical models, acidifying species models, PM models) and the grid structure applied (Eulerian, Lagrangian; mono-scale, multi-scale). The common feature is that they determine air pollution by modeling emission, transport, chemical transformation, dry and wet deposition of pollutants, and are based on the solution of a number of conservation equations. The basic conservation equation for $i = 1, \ldots, N$ species reads:

$$\frac{\partial C_i}{\partial t} = -\nabla(\vec{U} \cdot C_i) - \nabla \cdot [D_i \nabla(C_i)] + R_i(C_1, C_2, \ldots, C_N, T, t) + S_i(x, y, z, t) \tag{2}$$

where C_i is the concentration (mass/volume) of species i; $\vec{U}$ is the wind vector; D_i is the molecular diffusivity of species i; R_i is the function of concentration change of species i due to chemical reactions; T is the temperature; $S_i\ (x, y, z, t)$ is the source/sink of i at location (x, y, z). The source/sink term include emission of species and their loss due to physical processes (deposition for gases, sedimentation for particles). The way to obtain the so-called basic atmospheric diffusion equation (ADE) is to employ Reynolds' decomposition into ensemble means and turbulent fluctuating components followed by ensemble averaging, and resolving the closure problem ([44, 56, 57]). The classical approach is the first-order closure (K-theory) approximation. The resulting K-theory ADE equation for the dynamics of the averaged concentration of species i reads:

$$\frac{\partial \overline{C}_i}{\partial t} = -\nabla(\overline{\vec{U}} \cdot \overline{C}_i) - \nabla \cdot [K \nabla(\overline{C}_i)] + R_i(\overline{C}_1, \overline{C}_2, \ldots, \overline{C}_N, T, t) + \overline{S}_i(x, y, z, t) \tag{3}$$

where K is the eddy diffusivity. Equation (3) can be solved only by numerical methods, applying appropriate boundary and initial conditions. Models applying such solution are called numerical ones.

The analytical (closed-form) solving of equation 3 is possible after applying a number of simplifying assumptions. The most important of them are: a continuously emitting source, steady-state meteorological conditions, and flat underlying terrain.

The first formulation for the steady-state concentration downwind from a continuous point source was presented in 1947 by Sutton [71], and further developed by Pasquill [60] and Gifford [29] in 1961. This solution is commonly known as the Gaussian Plume Model (GPM). The concentration distribution, perpendicular to the plume axis, is assumed to be Gaussian. The plume travels with a uniform wind velocity downwind from the source. Its dimensions, perpendicular to the wind direction, are described by dispersion coefficients as a function of distance or travel time from the source. The pollutant concentration is proportional to the emission rate, and inversely proportional to the mean horizontal wind speed (the Gaussian plume formula).

The classical (first generation) GPMs are simple and based on standard meteorological input data. They can apply climatological data and the so-called Pasquill-Gifford atmospheric stability classes. However, due to assumed simplifications, their application is restricted only to homogeneous flow under steady-state conditions and mean wind speed > 1 m/s. The validity range of GPMs should therefore be limited to 10–20 km. In such distances from the source, in general, changes in the atmospheric parameters can be neglected and steady-state conditions in the concentration can be assumed.

In contrary, the numerical models are time-dependent and can be used for a variety of applications. Among the numerical models, two types have found wide applications:
1. Eulerian grid models (EGMs), employing a coordinate system which is fixed with respect to the ground.
2. Lagrangian trajectory models (LTMs), in which coordinate system is attached to a fictitious vertical air column, which move horizontally with the adjective wind.

The Eulerian grid models solve a finite approximation to equation 3 by dividing the modeling domain into a number of grids, horizontally – for so-called 2-dimensional (2D) codes [1, 45], and also vertically – for multidimensional (3D) codes [13].

In the Lagrangian trajectory models the concentration distribution within the air column is obtained by solving equation 3 without the advection part [23]. A number of simplifying assumptions are usually employed: the vertical advection, the wind shear, and horizontal diffusion are neglected. These limit applicability of the LTM and the accuracy of the solution. The LTM found main application in long-range transport (LRT) of air pollutants. Since the beginning of the EMEP program (LRTAP Convention, Co-operative Program for Monitoring and Evaluation of the Long-range Transmission of Air Pollutants in Europe) in 1979, the Lagrangian Acid Deposition Model has been used [24]. However, recently, the 3D Eulerian, Unified EMEP Modeling System has been designed [25]. It consists of three EGMs: UNI-ACID for acidification and eutrophication, UNI-OZONE for photochemical oxidants and UNI-AERO for aerosols. Differences between the three codes are restricted to the necessary differences in chemistry and input treatment, while treatment of meteorology, emissions, transport and depositions are common in all codes.

The LTMs have same advantages over the EGMs, as they are simpler, computationally faster and have ability to more easily isolate process impacts. However, due to limitations in their formulations, the EGMs are becoming the dominant numerical AQM used in scientific studies. Simultaneously, the second-generation Gaussian plume models are the dominant tool for regulatory purposes. Therefore, in the following sections both the regulatory and the Eulerian grid models will be further discussed.

CHALLENGES IN REGULATORY AIR QUALITY MODELING

The main goal of regulatory air quality modeling is to address relevant AQ regulations in a given area. In European Union AQMs have to address the issues raised by the newly introduced Directive of 21 May 2008 *on ambient air quality and cleaner air for Europe* (2008/50/EC) and the so-called Fourth Daughter Directive (2004/107/EC) *relating to arsenic, cadmium, mercury, nickel and polycyclic aromatic hydrocarbons in ambient air*. The regulatory models are used to assess ambient air quality by calculating percentiles and establishing exceedances for pollutants under legislation (CO, SO_2, NO_2, NO_x, PM_{10}, $PM_{2.5}$, O_3, Pb, C_6H_6, As, Cd, Hg, Ni and PAH). They should be also able to calculate the so-called "source-receptor matrices" [47] and select the sources responsible for exceedances, in order to prepare the managing plans for attaining the limit values.

The classical Gaussian plume models, due to their application limitations, are not suitable to this end. Therefore, since the 1980s, the second generation GPMs that overcome most limitations of the classical ones have been developed. In contrary to the traditional approach for the boundary layer description used in the first-generation GPMs, where the atmospheric condition were classified in terms of a few stability classes, the second-generation GPMs evaluate the dispersion parameters by means of similarity relationships, based on the Monin-Obukhov similarity theory. It should be pointed out here that, unfortunately, in spite of these developments, the classical GPM, according to current legislation [62], is still a reference regulatory AQM in Poland.

In the second-generation GPM, the Gaussian plume formula is used only for the stable and the neutral conditions, while for the unstable conditions other semi-empirical formulas are applied. Also, the description of meteorological conditions is more sophisticated. Such models use meteorological pre-processors, which determinate the boundary layer parameters, and vertical profiles of several atmospheric parameters, giving as their output sequential meteorological data.

The good example of the second-generation GPM is the American Meteorology Society-Environmental Protection Agency Regulatory Model AERMOD, a steady-state plume model [76]. The AERMOD incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain. In the stable boundary layer (SBL), it assumes the concentration distribution to be Gaussian both vertically and horizontally. In the convective boundary layer (CBL), the horizontal distribution is also assumed to be Gaussian, but the vertical distribution is described with a bi-Gaussian probability density function. Dry and wet deposition of particulates and/or gases is included. The model captures the essential physical processes, while remaining fundamentally simple. The meteorological data are prepared by meteorological pre-processor AERMET.

Being the second-generation GPM, this type of a model has still some limitations of a classical one, e.g., it limits the plume length along the wind direction. A more realistic description is performed by the Gaussian segmented plumes (e.g. [11]) and the Gaussian puff models. Both types allow for simulating the evolution of pollutants in non-steady-state and non-uniform atmospheric conditions.

The best example of Gaussian puff model is the US Earth Tech., Inc. CALPUFF model [77]. It simulates continuous puffs of pollutants, emitted from a source into the ambient wind flow. As the wind flow changes from hour to hour, the pathway each puff takes, changes to the new wind flow direction. Puff diffusion is Gaussian, and concentrations are based on the contributions of each puff as it passes over or near a receptor point. The CALPUFF is a multi-layer, multi-species, non-steady-state model that simulates the effects of time- and space-varying meteorological conditions on pollution transport, transformation and removal. It also includes algorithms for subgrid scale effects (such as terrain impingement), as well as longer-range effects (such as pollutant removal due to wet scavenging and dry deposition, chemical transformation, and visibility effects of PM concentrations). The meteorological input is given by a diagnostic 3-dimensional meteorological model, CALMET. The application range of CALMET-CALPUFF is from tens to hundreds of kilometers. The implementation and application of CALMET-CALPUFF system in Poland is described by Trapp [73].

In author's opinion, both AERMET-AERMOD (for local scales) and CALMET-CALPUFF (for local to voivodeship-range scales) modeling systems should be recommended for regulatory applications in Poland, and finally replace the out-of-date classical Gaussian plume model.

DEVELOPMENTS OF REGIONAL EULERIAN GRID MODELING

Developments of the Eulerian grid models (EGMs) were initiated in the late 1970s. The first working operationally Eulerian grid model was developed by Reynolds *et al.* in 1973 [66]. It focused specifically on the prediction of urban scale ozone levels and was applied to the Los Angeles area. The first operational EGM for regional scale was the Sulphur Transport Eulerian Model (STEM-I) of Carmichael *et al.* [12].

These first generation models solved the K-theory diffusion equation (3) using meteorological fields as an external input. The main features of such models are given in Table 1.

Table 1. Main features of the first-generation Eulerian Grid Models

Model type/feature	First-generation Eulerian Grid Models
Structure	– relatively simple
Meteorological and emission data	– decoupled from the AQ model (no feedback), – meteorological fields and emission inventory prepared separate from the model as input fields, – meteorological fields obtained from objective analysis of observations
Number of species included	– few to dozen or so species included (mainly sulphur and nitrogen species)
Chemistry	– first-order
Processes parameterization	– no or simple parameterization of dry deposition, – vertical diffusion coefficient (K_z) and dry deposition velocity (v_d) parameterized based on meteorological data, – ignored cloud and precipitation processes or highly parameterized treatment (scavenging coefficients)
Numerical methods	– model equations solved using operator-splitting techniques and different numerical schemes

All numerical methods elaborated so far to solve the advection part of the differential equations (3) in the air pollution models, are impacted – to a various degree – by numerical errors connected with numerical diffusion or with generating unwanted oscillations, especially in the vicinity of point sources [47, 61]. The biggest limitation of the first-generation EGMs was substantial numerical diffusion, limited number of species included as well as very simple chemistry.

In the late 1980s and the early 1990s the second-generation regional EGMs were developed, mostly in the USA, predominantly for dealing with regional acid deposition. The distinction between the first and the second generation EGMs lies mainly in a number of species included and the approaches employed for modeling of physical and chemical processes. Also, the second-generation models employ improved numerical schemes to reduce the numerical diffusion. From that time, EGMs are referred by some authors as "chemical-transport models" (CTMs). The main features of such models are given in Table 2.

Table 2. Main features of the second-generation Eulerian Grid/Chemical Transport Models

Model type/feature	Second-generation Eulerian Grid/Chemical Transport Models
Structure	– sophisticated; domain extension into lower stratosphere
Meteorological and emission data	– decoupled from the AQ model (no feedback), – meteorological fields and emission inventory prepared separate from the model as input fields, – meteorological fields usually prepared by pre-processor or diagnostic meteorological model
Number of species included	– more species included (30–60)
Chemistry	– expanded chemical mechanism – gas and aqueous-phase reactions
Parameterization	– dry and wet deposition (cloud and precipitation scavenging) included, – extensive gas- and aqueous-phase chemical mechanism
Numerical methods	– improved numerical integration schemes

The most representative CTMs are the following: RADM [16], ADOM [79], and STEM-II [13]. However, in the late 1990s, even these models appeared to be not adequate to current atmospheric modeling challenges.

CHALLENGES IN MULTI-SCALE AIR QUALITY MODELING

Air quality in a given area is a multi-scale problem. It is influenced by natural and regional background concentrations and by emissions form a given area. Therefore, current regional and/or urban modeling is generally conducted with nested or multi-scale models. Air pollution problems arising in the end of the 20th century, the great progress in the atmospheric science, as well as a huge increase of computing power; have led to development of a complex third-generation Eulerian Grid Models, called also the modeling systems, since such models form a system of several models.

The second-generation EGMs, described above, were designed to address specific air pollution issues, such as tropospheric ozone or acid deposition. Thus, their flexibility to deal with other issues, such as fine aerosols and coarse PM, heavy metals or semi-volatile organic species, was limited. The third-generation EGMs are complex 3-dimensional (3D) models, frequently including a detailed photochemical mechanism, and are the most sophisticated systems, capable of representing majority of the atmospheric processes. Usually, they are "community" models, developed by groups of research communities and distributed freely. They are much more comprehensive than the previous ones, usually designed to be applied at a continental scale, with nested grids. The horizontal domain may vary from 200 (urban) to 2000 (regional), or more kilometers. The vertical extent of the modeling domain can vary from 2000 to more than 10 000 m. Horizontally, the grid size, on a monoscale model can range from 2 to 100 or so km. Vertically, the bottom cell is generally the thinnest (20 to 100 m) in order to describe more accurately the dynamics of surface layer (where emissions and deposition occur), while the top cells are much larger [67]. The third-generation EGMs can evaluate many pollutants in a single model run, however they constitute huge computational tasks, and usually require the use of parallel computation. Moreover, the modern modeling systems are highly complex, thus requiring fairly extensive training to operate and to interpret the results accurately. The adaptation of such modeling system to a new region, with nested domains and at different resolutions, requires in-depth understanding of the limits of parameterization applicability. The real-case applications involve rigorous input data quality-checking requirements, since incorrect data can generate amplifying model errors.

The third-generation models differ in respect to applied modeling approaches of emission and meteorology, as well as applied chemical mechanisms. The challenge of the late 1990s was to develop a system that will couple emission and meteorological models with a basic AQM that includes suitable chemical mechanisms. A short summary of meteorological models and chemical mechanisms applied in third-generation AQ modeling systems will be given in next sections.

During the development of complex AQ modeling systems a number of problems arose, since AQMs and meteorological/emission models were developed independently. Therefore, the modern AQ modeling systems generally require the interface programs. If the grids of the two models are incompatible, an interpolation step is necessary to project the meteorology into the AQM's grid system. The interpolation from one grid to another can lead to a change of mass and loss of detail, especially if the original grid has greater resolution than the target grid [68].

In the USA more than six years of investment from scientists and model developers from the environmental and information communities were expended to develop the so-called Models-3 framework and the CMAQ (Community Multiscale Air Quality) modeling system [10]. Models-3 CMAQ was released to the public in 1998. In its framework, the CMAQ Chemical Transport Model (CCTM) incorporates output fields from emissions and meteorological modeling systems and several other data sources through special interface processors. Then CCTM performs chemical transport modeling for multiple pollutants on multiple scales. Currently, the Models-3 Emission Projection and Processing System (MEPPS) produce the emissions and the Dynamical Non-hydrostatic Meteorological Model, MM5 or its newer version WRF (see next section) provides the meteorological fields needed for the CCTM. They are designed to meet the present application needs for diverse air pollution problems on urban and regional scales. However, the paradigm of Models-3 CMAQ structure designation is to integrate and to test the future formulations efficiently, without development of a completely new modeling system. Thus, the emissions processing and meteorological modeling systems can be replaced with alternative processors [10].

This type of modeling system is based mainly on the "first principles" description of atmosphere, and is often referred to as "one atmosphere" modeling. While past applications focused on acid deposition and ozone, increasing attention is currently directed at integrating modeling of PM into one atmosphere modeling approaches, including all processes and all important pollutants [10, 67, 72].

Other example of such one atmosphere community system, developed also in the USA, is Comprehensive Air quality Model with eXtensions (CAMx [26]), that is driven usually also by MM5 meteorological model. As such modeling systems are very complex, their testing have been usually limited to short-duration episodes of a few days on nested grid domains covering one or a few US states. However, recently, operational, diagnostic and comparative evaluations of these two one-atmosphere regional models (CMAQ and CAMx) were performed for the full calendar year 2002 in support of regional haze regulatory applications in the eastern USA [72]. Using consistent emissions, meteorological and air quality data sets, the models were exercised on a nested 36/12 km grid system and evaluated across a broad range of time and space scales for numerous gas-phase and fine PM. The MM5 meteorological model was used to drive both AQMs. Performance by both models for speciated fine PM across the eastern USA ranged from quite good to poor. However, both CMAQ and CAMx performed comparably for most species across the two grid scales tested and across all time scales from 1 h to 1 year.

In Canada, the MC2-AQ modeling system (Mesoscale Compressible Community – Air Quality) was developed (e.g. [48]). The modeling system is based on the Canadian Mesoscale Compressible Community (MC2), a non-hydrostatic dynamical meteorological model, to which modules permitting on-line calculations of chemical transformations, anthropogenic and biogenic emissions, and deposition were added. The model system is flexible and was adapted to different scales by allowing for self-nesting.

In Europe, unfortunately, there is a lack of community based approaches. The third-generation modeling is very disparate. Different modeling groups over Europe use various approaches, based mostly on US or Canadian experiences.

Under on-going EU COST 728 Action (Enhancing Mesoscale Meteorological Modeling Capabilities for Air Pollution and Dispersion Applications) the work has been undertaken to build community AQ modeling structure for Europe. One of the main goals of that project is to develop an integration strategy of mesoscale meteorological model (MetM) and chemical transport model (CTM). The final integration system with fixed architecture (module interface structure) will have a possibility of incorporating different MetMs/NWP models and CTMs. The overall aim is to identify requirements for the unification of MetM and CTM modules and to propose recommendations for third-generation AQ modeling in Europe [18].

The next challenge in AQ modeling is to address interactions and feedbacks between atmospheric chemistry and climate. In the real atmosphere, the chemical and physical processes are effectively interacted. The chemistry can affect the meteorology, for example, through its effect on the radiation budget. Simultaneously, meteorology can strongly affect chemistry, for example, through clouds and precipitation influence on chemical transformation and removal processes. However, the up-to-date mode of operation of majority of AQMs effectively decoupled atmospheric chemistry and dynamics.

However, such off-line methodology of coupling between the AQM and the MetM has a number of disadvantages. The most important deals with no possibility to consider chemical and dynamic feedbacks that exist in the real atmosphere. This is the most severe limitation for future applications of the off-line AQMs. They cannot be applied to investigate the current scientific questions, as e.g. the interactions between fine PM (aerosols) and clouds or aerosols and radiation [51].

The model system, allowing interactions between chemical and meteorological components, is referred to as "on-line modeling system". The on-line coupling between the AQM and the MetM gives the possibility to include feedback mechanisms, e.g. impact of changed atmospheric composition on meteorology and vice versa. Such approach may be used for studying the potential air pollutants influences on climate, as well as climate change effects on air pollution levels.

As discussed by Jacobson [38], the GATOR/MMTD model, developed between 1994 and 1997 appears to have been the first "on-line" coupled air quality-meteorological model. This model solved gas, aerosol, radiative, transport, and meteorological processes simultaneously and feedbacks of air quality and meteorological parameters in both direction. The on-line coupling is realized also in the Canadian MC2-AQ modeling system that has been implemented also in Poland [48]. Recently, a fully coupled "on-line" Weather Research and Forecasting/Chemistry (WRF/Chem) model has been developed [32]. The air quality component of the model is fully consistent with the meteorological component; both components use the same transport scheme (mass and scalar preserving), the same grid (horizontal and vertical components), and the same physics schemes for subgrid-scale transport.

METHODOLOGIES FOR GENERATING METEOROLOGICAL FIELDS

From the time when the classic GPM was the most common AQM, the methods to "fill up" AQM with meteorological data improved enormously. For GPM the routine (climatological, as wind rose) meteorological observations, usually from one station nearest to the emission source, were used. The second-generation GPM use meteorological pre-processors such as AERMET, while Gaussian puff models usually employed diagnostic meteorological models, such as CALMET. The detailed description of meteorological modeling for air-quality assessments is out of the scope of this paper; however a short explanation of different model types will be given. The reader is, however, referred to papers of Seaman [68], Łobocki [52] and Markiewicz [58], dealing specifically with that subject.

The goal of a metrological model, used to supply fields to AQM, is to produce the gridded fields, representing the key variables required by it. MetM can be grouped into three main types [68]: (1) Diagnostic (kinematic) models are those that analyze observations taken at discrete points in time and space. They are easy to operate and inexpensive. However, diagnostic MetM are based on incomplete or idealized set of equations, and thus have several disadvantages. (2) Dynamical (prognostic) models are numerical models based on the complete set of primitive equations for hydrodynamic flow. Most of dynamical MetMs, widely used in air-quality studies, were designed originally as numerical weather prognostic (NWP) models. They are further divided into hydrostatic models, that employ the simplified primitive equations, and thus are applicable for scales bigger than 10 km, and the non-hydrostatic models, applicable for scales of up to 1 km. (3) Data assimilating models are the numerical dynamical models with four-dimensional data assimilation (FDDA), intended to combine the best features of diagnostic and dynamical approaches. FDDA models introduce meteorological observations to dynamical model itself, and thus allow for reducing growth of errors in the model's solutions.

Currently, the non-hydrostatic dynamical MetMs, due to their advantages compared to diagnostic ones, have become the dominant approach used as part of AQ modeling systems. As summarized by Seaman [68], their potential for resolving regional and local-scale atmospheric circulations (at least down to scales of about 1 km) is limited only by the availability of computational resources. Also, they do not require such an extensive (and expensive) observation network to obtain products with the same resolution as diagnostic models. They usually have a nested-grid capability, terrain-following vertical coordinates, flexible resolution, and a variety of physical parameterization options. However, the dynamic MetMs are highly complex, thus much more demanding for a user, as well as more costly to operate than the diagnostic ones.

Among the non-hydrostatic dynamical MetMs, the PSU/NCAR Fifth Generation Mesoscale Model (MM5) of Grell *et al.* [31], is one of the most thoroughly tested models for air-quality studies as well as widely applied both in the USA and Europe. Recently, in some applications the NCAR Weather Research and Forecasting (WRF) model is also used (e.g. [32]). The WRF is a next-generation mesocale numerical weather prediction system, with data assimilation, designed to serve both operational forecasting and atmospheric research needs. It features multiple dynamical cores, a 3-dimensional variational (3DVAR) data assimilation system, and a software architecture allowing for computational parallelism and system extensibility. The WRF is suitable for a broad spectrum of applications across scales ranging from meters to thousands of kilometers. As mentioned in the previous section, recently the WRF model was fully coupled "on-line" with AQ model (WRF/Chem).

GLOBAL AND REGIONAL CLIMATE MODELS

A General Circulation Models (GCMs), referred also as a Global Climate Models, use the same equations of motion as a NWP global models, but the purpose is different. While the global NWP models are used to predict the weather in a short and medium time range, GCMs are used to simulate long-term changes of climate as a result of slow changes in some boundary conditions or anthropogenically driven changes, such as the GHGs concentrations. To simulate climate changes in a statistical sense (i.e. the means and variability), GCM's are run for much longer periods (years, decades). The state-of-the-art GCMs are coupled with atmosphere-ocean models, i.e. models simulating the surface and deep-ocean circulations. Also, the GCMs can further be coupled to dynamic models of sea ice and conditions on land [59].

Most climate models are large dynamical deterministic systems involving a million variables on huge computers. They can reproduce reasonably well climate features on large scales (global and continental), but their accuracy decreases when proceeding from continental to regional and local scales because of the lack of resolution [27]. This is especially true for surface fields, such as precipitation and surface air temperature, which are critically affected by topography and land use. However, in many applications, particularly related to the assessment of climate-change impacts, the information on surface climate change at regional to local scale is fundamental. To bridge the gap between the climate information provided by GCMs and that needed in impact studies, several approaches have been developed, commonly called downscaling or regionalization techniques [30]. The most popular approaches are: (1) statistical downscaling, i.e., the identification of statistical relationships between large-scale fields and local surface climate elements, and (2) dynamical downscaling, i.e., nesting of a fine scale limited area model (or Regional Climate Model, RCM) within the GCM. The latter approach is more correct from a physical point of view, but is much more demanding on computer resources. Another way to increase resolution is to use GCMs with a variable horizontal resolution [19]. The availability of different methodologies giving often different results implies that a full assessment of the uncertainties in the regional climate change simulations may require the use of multiple techniques. This approach is currently being implemented in the on-going CECILIA project (6 EU Framework Program), that is dedicated to climate change impacts in the Central and Eastern Europe. In this region, the need for high resolution studies is particularly important, as it is characterized by the northern flanks of the Alps, the long arc of the Carpathians, and smaller mountain chains and highlands in the Czech Republic, Slovakia, Poland, Romania and Bulgaria that significantly affect the local climate conditions. A resolution, sufficient to capture the effects of these topographical and associated land-use features, is necessary.

During the last decade, Regional Climate Models have been increasingly used to examine climate variations at scales that are not resolved by global models. The RCMs are adapted from MetM numerical models or NWP models. Boundary conditions are provided by large scale analyses or GCMs. At higher spatial resolutions, RCMs capture climate features related to regional forcing as orography, lakes, complex coastlines, and heterogeneous land use. To the extent that they produce realistic climate simulations, such models can be powerful tools in the study of regional climate impacts.

The skill of RCMs in simulating climate variability of 50 km and 25 km resolutions has been evaluated so far. Under CECILIA project emphasis is given to adapt some of the RCMs, i.e.: RegCM (ICTP, Trieste) and ALADIN-Climate (Meteo-France) for very high (10 km) resolution simulations over selected sub-domains of the region. One of the key issues is to study the impact of climate change on AQ and health. To exploit the sensitivity of air-pollution levels to the potential climate change, RCMs will be used to drive the off-line AQMs. The modeling system is built with two RCMs as "meteorological drivers": RegCM [65] and ALADIN-Climat [9] and two AQMs: CAMx and CMAQ. Six modeling groups from five countries are involved in these activities. Polish group, working at Warsaw University of Technology (WUT), implemented RegCM-CAMx modeling system for the sub-European domain established over Poland.

CHEMISTRY

Atmospheric chemistry module is an important part of AQ model (Fig. 1). Since the development of the first-generation EGMs, that involved simple first-order sulphur-species reactions, there has been an enormous growth in understanding of the atmospheric chemistry, as well as in developing chemical mechanisms for AQ modeling. As discussed by Dodge [20], a fully explicit mechanism for representing gas-phase atmospheric chemistry would contain up to 20 000 reactions and several thousand species. There is no need, however, nor computational feasibility to incorporate such a huge number of components into AQM. As discussed by Peters *et al.* [61], the compromises between the need of accurate and general chemical description, restrictions imposed by computational considerations (the integration of the chemistry rate equations consumes the majority of the AQM computing time), uncertainty and availability associated with the supporting data (each species and reaction included in the chemical mechanism have to be supported by a large amount of input data: reaction rate constants, activation energies, yields, products, ambient observations, emission rates of primary species etc.), remain critical in formulation of chemical mechanisms.

In the third generation EGMs, which are "one-atmosphere" modeling systems, the considered chemical mechanism have to be able to handle the most important issues of the real atmosphere chemistry, in particular, sulphur-nitrogen chemistry, photochemical oxidant cycle as well as secondary particulates ($PM_{2.5}$) chemistry, including hydrocarbons, elemental carbon and sulphate.

The existing gas-phase chemistry mechanisms differ in respect to [50]: (1) formulation of the reaction mechanism, (2) rate constants for the reactions and their temperature and pressure dependencies, and (3) temporal integration of the reaction rates by the chemical solver. For inorganic species, however, the reactions included in different chemical mechanisms are nearly identical, as inorganic chemistry is reasonably well understood. In contrary, for organic species, the existing mechanisms differ in respect to the number and types of hydrocarbon species included, as well as to details, in which their chemistry is represented. The common attribute of different chemical mechanisms is that they have to reduce the number of organic species carried in model calculations. This is done by "lumping" hydrocarbon compounds into groups of similar structure and/or reactivities (e.g. alkanes, alkenes, aromatics, and carbonyls). Some of organic species are included explicitly (usually formaldehyde, isoprene, ethane and toluene), while other are represented by carbon surrogates, and/or molecular surrogates.

The chemical mechanisms, most widely used in research and regulatory AQMs, are: (1) a lumped structure mechanism, known as the Carbon Bond Mechanism (CBM), in which n-bounded carbon atoms, regardless of the molecule in which they appear, are represented using n-carbon atom surrogate, (2) a lumped species mechanism, called the SAPRC mechanism, (3) a lumped species mechanism, the RADM/RACM mechanism. The CBM-IV mechanism of Gery *et al.* [28] contains 33 species represented in 81 reactions, while the updated SAPRC-07 mechanism [14], consists of 72 species in 198 reactions. The RACM [70] that is a revised version of the RADM2 mechanism includes 77 species in 237 reactions.

A review and an evaluation of chemical mechanisms currently used in AQ models are presented in [50] and [20], where a description of the chamber data available for their development and evaluation is also given. Recently, a comparison of photochemical mechanisms for air quality modeling has also been discussed in [39].

In addition, aqueous-phase chemical mechanisms have been implemented in those AQ models, which focus on acid deposition and/or on evolution of aerosols. Operational multi-dimensional models, which include aqueous phase chemistry, contain from 5 to 100 additional species and 10 to 200 additional reactions [67]. In most cases, the emphasis is placed on sulphur oxidation routes, and relatively small mechanisms are added (e.g. CBM-IV with sulphur).

IMPLEMENTATION AND VALIDATION OF AIR QUALITY AND CLIMATE MODELS

As discussed before, the modern meteorological, air quality and climate models are highly complex modeling systems, developed by the communities of atmospheric and information scientists. Most of such models (e.g. MM5, WRF, CAMx, CMAQ, RegCM) are freely available for interested users. However, it should be pointed out, that adaptation of such modeling systems to a new region (implementation) is a huge and demanding task. It requires in-depth understanding of atmospheric processes and of the limits of parameterization applicability, as well as extensive modeling experience. Moreover, a reasonably widespread training to operate such systems and to interpret the results correctly is required.

The model results often influence decisions that have large economic, health and environmental consequences. Therefore, modeling systems have to be methodically evaluated before their predictions can be used with confidence. Uncertainty in the model results is due to: (1) the errors in the input data, (2) the simplification of atmospheric processes adopted in model formulation, and (3) the randomness of these processes. Thus, the quality of input data has to be always ensured, as incorrect data can generate amplifying model errors. However, because of the effects of uncertainty and its inherent randomness, it is not possible for any AQ or climate model to ever be "perfect", and there is always a base amount of scatter that cannot be removed [15, 44].

Evaluation of AQMs can be performed in three modes: (1) scientific, (2) statistical, and (3) operational [15]. In a scientific evaluation, the model algorithms, physics, assumptions and codes are examined in detail for their accuracy, efficiency and sensitivity. This evaluation is performed by model developers before the model became available for other users. The statistical evaluation deals with examination of model predictions against observations and has to be performed each time when model is implemented to a new region. The operational evaluation considers the user-friendliness of the model.

The statistical evaluation of AQMs performance focuses on assessing the accuracy of the model predictions relative to observations. Several scientists, also in Poland, carried out discussion on the evaluation methods and criteria. The reader is referred to e.g. Willmott [83], Madany [54], Brandt *et al.* [5], Juda-Rezler [43–45], Markiewicz [56], Chang and Hanna [15]. However, standard evaluation procedures and performance standards still do not exist. Recently, Borrego *et al.* [4] presented systematic description of the modeling uncertainty analysis methodologies as well as proposal of guidelines for uncertainty estimation.

The present EU legislation defines the requirements of Quality Assurance/Quality Control (QA/QC) procedures for AQ modeling, defining Quality Objectives as an acceptability measure, to guarantee they indicate a good model performance and reliable modeling results for decision makers. However, as it was concluded by Borrego *et al.* [4] the quality indicators defined by EU directives are ambiguous and inadequate in several aspects, mainly in what concerns the error measures for hourly and daily indicators based on the highest observed concentration.

During validation process of the EGMs, the observed values of point measurements at a station are compared against predicted values averaged for the grid cell area. Therefore, not all existing station data could be used for model validation purposes. Stations chosen for validation should be representative of the grid area climatic conditions (i.e. stations situated in specific conditions, for example sites of a high elevation, should be excluded) as well as of average air quality within the grid area (i.e. station should not be influenced by local sources). Moreover, the usual requirement of temporal data completeness should be met as well as the requirement of a statistically sufficient number of stations, covering the entire area of interest [45].

In the formulas given below, the following notation is used: C_o and C_p are the concentration observed and predicted by a model, σ_o and σ_p are the standard deviation of observations and predictions, N is the total number of monitoring stations, $\overline{C}_0$ and $\overline{C}_p$ are the mean values of observations and predictions, respectively, and $\hat{C}_{pi}$ is the conditional mean value of C_p on a given C_o.

The currently widely used statistical measures can be divided into five groups.

1. Measures of difference: Mean Bias (MB), Normalized Mean Bias (NMB) and Fractional Bias (FB). If bias is calculated as difference between observed (C_o) and predicted (C_p) values, a negative value of bias indicates that the model is over predicting the observations. Unbiased models will have small bias and also a value of FB close to zero.

$$MB = \frac{1}{N}\sum_{i=1}^{N}(C_{oi} - C_{pi}) \tag{4}$$

$$NMB = \frac{\sum_{i=1}^{N}(C_{oi} - C_{pi})}{\sum_{i=1}^{N}(C_{oi})} \tag{5}$$

$$FB = \frac{\overline{C}_o - \overline{C}_p}{0.5(\overline{C}_o + \overline{C}_p)} = \frac{MB}{0.5(\overline{C}_o + \overline{C}_p)} \tag{6}$$

2. Measures of model error: Root Mean Squared Error (RMSE), with its systematic ($RMSE_s$), and unsystematic ($RMSE_u$) part and Normalized Mean Square Error (NMSE), low value of which indicates less scattered model predictions. A perfect model will have $RMSE_s$ equal to zero and $RMSE_u$ equal to RMSE.

$$RMSE = \sqrt{\frac{1}{N}\sum_{1}^{N}(C_{oi} - C_{pi})^2} \tag{7}$$

$$RMSE_s = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(C_{oi} - \hat{C}_{pi})^2} \tag{8}$$

$$RMSE_u = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(C_{pi} - \hat{C}_{pi})^2} \tag{9}$$

$$NMSE = \frac{\frac{1}{N}\cdot\sum_{i=1}^{N}(C_{oi} - C_{pi})^2}{\overline{C}_o \cdot \overline{C}_p} \tag{10}$$

3. Measures of standard deviations: ratio of standard deviations (F), Fractional Standard Deviation (FSD). A model that gives a good estimation of the spread of the measurements will have a value of F close to one and a value of FSD close to zero.

$$F = \left(\frac{\sigma_p}{\sigma_o}\right)^2 \tag{11}$$

$$FSD = \frac{2\cdot(\sigma_o^2 - \sigma_p^2)}{(\sigma_o^2 + \sigma_p^2)} \tag{12}$$

4. Measures of correlation: correlation coefficient (r), index of agreement (IA). IA, which is both a relative and bounded measure, was proposed by Willmott [86] as an alternative to r. A model that gives a perfect agreement between the measured and predicted values will have a value of r and IA equal to one.

$$r = \frac{\sum_{i=1}^{N}\left(C_{oi}-\overline{C}_{o}\right)\cdot\left(C_{pi}-\overline{C}_{p}\right)}{\sqrt{\sum_{i=1}^{N}\left(C_{oi}-\overline{C}_{o}\right)^{2}\cdot\sum_{i=1}^{N}\left(C_{pi}-\overline{C}_{p}\right)^{2}}} \tag{13}$$

$$IA = 1-\frac{\sum_{i=1}^{N}\left(C_{oi}-C_{pi}\right)^{2}}{\sum_{i=1}^{N}\left(\left|C_{pi}-\overline{C}_{o}\right|+\left|C_{oi}-\overline{C}_{o}\right|\right)^{2}} \tag{14}$$

5. Measures of variance: Explained variance (EXV), proposed in atmospheric modeling by Juda-Rezler [43, 44] which is a measure of how much of the observed variance is explained by the model. If the MSE is equal to zero, EXV is equal to one. For a good model, the EXV should be greater than 0.3.

$$EXV = \frac{\left[\sum_{i=1}^{N}\left(C_{oi}-\overline{C}_{o}\right)^{2}-\sum_{i=1}^{N}\left(C_{oi}-C_{pi}\right)^{2}\right]}{\left[\sum_{i=1}^{N}\left(C_{oi}-\overline{C}_{o}\right)^{2}\right]} \tag{15}$$

6. Predictions within factor 2 of the observations (*FAC2*).

FAC2 = fraction of the data for which

$$0.5 \le \frac{C_p}{C_o} \le 2 \tag{16}$$

Although all listed indices are important for model performance evaluation, it is possible to recommend a subset of them able to characterize the general uncertainties estimation. From the author's application experience ([43–45]), these are: r (eq. 13), *FB* (eq. 6), *RMSE* (eq. 7), $RMSE_s$ (eq. 8), $RMSE_u$ (eq. 9), *NMSE* (eq. 10), *EXV* (eq. 15) and *FAC2* (eq. 16).

Global and regional climate models are used for future climate predictions. As these predictions are connected with required emission reductions, which in the case of CO_2 are extremely difficult and costly, climate models performance should also be carefully evaluated. This is done by simulating the so called present climate (1961–1990) using reanalysis of observations for GCM/RCM forcing. In Europe, the common approach is to use the ERA-40 reanalysis fields from ECMWF (Reading, UK) for GCM/RCM forcing and observed data from CRU (Norwich, UK) for model validation. Unfortunately, also for climate models (as for AQMs), the consistent procedure for the uncertainty evaluation, was not adopted so far.

AIR QUALITY AND CLIMATE MODELING IN POLAND

In Poland, AQ modeling research was started by Juda and Budziński [40], as early as in 1961, when the first Polish AQM was developed on the basis of Sutton formula [71]. The model was then used to formulate first Polish guidelines for AQ modeling, edited in 1968 [41]. The methodology of calculating concentration percentiles, developed for the model, was at that time unique on a world scale. In 1976 the next model, based on Pasquill formula [60], was developed by the same team of professor Juda from Warsaw University of Technology [42], followed by the second guidelines edited in 1981 [17].These developments placed Poland in the head of AQ modeling groups in the world at that time.

Unfortunately, since then, the development of regulatory AQ models stopped in Poland, placing it currently at the tail end in Europe. In spite of huge progress achieved in this field internationally, the classical GPM, according to current legislation [62], is still a reference regulatory AQM in Poland. Although a few second-generation GPMs have been developed (e.g. [55]), such up-to-date approach was not implemented to the existing AQ legislation. Moreover, the obligatory version of GPM model, only slightly differs from the version of GPM from 1981.

However, during fifty years of AQ modeling in Poland, a few modeling groups have been established and different types of non-regulatory models have been developed or implemented. In 1995 Madany and Bartochowska [53] presented the review of Polish AQMs, based on an inquiry. The inquiry resulted from collection of twenty nine AQ models from twelve institutions. Majority of these models are first generation GPMs, moreover, most of the presented models have not been verified nor published in the scientific literature. The newer catalogue of Polish AQMs does not exist. Among the most important published modeling approaches are:

- the urban scale SO_2 modeling by 3D EGM [43];
- the regional scale (for entire Polish area) SO_x and NO_x modeling by 2D EGM [1, 45];
- the regional scale 3D hybrid Eulerian-Lagrangian modeling of gaseous pollutants [74], with implementation for the Black Triangle area [75];
- the regional and long range heavy metals modeling by 3D EGM [2];
- the urban/regional scale SO_2 modeling by 3D EGM [35, 36];
- and a multi-scale oxidants modeling by MC2-AQ modeling system [48].

The currently ongoing researches include modeling by the use of:

- national scale atmospheric transport model FRAME (Fine Resolution Atmospheric Multi-pollutant Exchange), the segmented-plume Gaussian model originally developed for the United Kingdom [49];
- CALMET-CALPUFF modeling system [73];
- GEM-AQ modeling system for short-term simulation over Poland (WUT);
- RegCM-CAMx modeling system for short and long-term simulation over Poland (WUT).

Regional Climate simulations are currently performed by two institutions in Poland: (1) the Institute of Meteorology and Water Management in Warsaw, and (2) the WUT. Both groups are using the RegCM model. At WUT the RegCM model adapted for very high (10 km) resolution was implemented for the domain centered over Poland (52 N, 19.3 E; 120 x 109 grid pints, in x and y directions, respectively). The model, driven by ERA40 reanalysis fields, was positively tested for the domain and the high resolution RegCM simulations for 1991–2000, driven by the ECHAM5 global climate model, were completed. The high resolution AQ simulations by the coupled RCM-AQ models (RegCM-CAMx) have been started. Validation of the test run results indicated a satisfactory model performance. Currently, the high resolution photochemical simulations for control run (1990–2000) and future climate projection by ECHAM5–RegCM–CAMx have been started. That system of models is a first modeling tool of such class, which works operationally for long-term simulations in Poland.

CONCLUSIONS AND RECOMMENDATIONS

The current directions and development in the AQ and climate modeling, including Polish experiences, were discussed in the present paper. In spite of recent huge progress achieved in that research area, there are still many modeling uncertainties as well as shortcomings, forming a challenge to atmospheric science community.

The challenge of the late 1990s was to develop a comprehensive third-generation Chemical-Transport Models, that couple emission and meteorological models with a basic AQM comprising suitable chemical mechanism. Such a comprehensive modeling systems are currently used by the majority of leading modeling groups all over the world (also in Poland). A few third generation AQMs became freely available for interested users. However, it has to be underlined, that the implementation and operation of such modeling systems in a new region is a huge and demanding task that should be realized by specialized and experienced teams.

During the last ten years the development of on-line modeling systems, allowing interactions between chemical and meteorological components, was initiated. Such highly complex approaches are used for studying the potential air pollutants influences on climate (e.g. aerosols), as well as climate change effects on air pollution levels. Further development of such methodology is the AQ/climate modeling challenge in coming years.

The AQ/Climate model results influence decisions of large economic, health and environmental consequences. Hence, modeling systems have to be methodically evaluated before their predictions can be used with confidence. However, there is still lack of a consistent procedure for the uncertainty evaluation of both AQ and climate models. Consequently, the development and acceptation of a reliable evaluation procedure is still a challenge to the scientific community. The subset of statistical parameters for the AQM uncertainties estimation is proposed in present paper, comprising the correlation coefficient, the fractional bias, the root mean square error with its systematic and unsystematic parts, the normalized mean square error, explained variance and predictions within factor 2 of the observations.

For any of the current AQ modeling tools, the main uncertainty is related to the emission input data. There is still lack of reliable emission databases for Europe. The existing models usually applying EMEP/LRTAP databases; however, these are aggregated data for 50 km x 50 km grid squares. This shortcoming is severely limiting the quality of the European AQ assessments. Therefore, the development of the reliable European emission database is a great challenge to the adequate EU bodies and scientific communities, also to Polish scientists and decision-makers.

The main uncertainties in Climate Models are caused by surface boundary and initial conditions, model parameterization and applied approximations by simplified or neglected physical processes. Research towards reducing these uncertainties will be a great challenge in coming years. In the last decade Regional Climate Models were progressively more used to study climate variations on scales that are not resolved by global models. Up to now, the skill of RCMs in simulating climate variability of 50 km and 25 km resolutions has been evaluated. The next challenge is to adopt the RCMs for higher (10 km) resolution simulations. This task is currently realized under ongoing EU CECILIA project (also by Polish scientists from the WUT).

In Poland, the AQ modeling research started 50 years ago, when Poland was a leading country in that field. Since then approximately thirty AQMs have been developed/implemented, though most of them are out-of-date first generation Gaussian plume models. Moreover, most of Polish AQMs have not been verified with observations nor published in scientific literature. The current modeling activities in the country are only partly linked, with almost lack of co-operation and experience exchange. The existing AQ modeling for regulatory purposes is absolutely out-of-date. For the last 27 years almost the same classical GPM acts as obligatory AQM in Poland. On the other hand, two state-of-the-arts, complex modeling systems have been recently adopted for Polish area: the RegCM-CAMx and MC2/GEM-AQ. Both systems have been implemented and are operating at Warsaw University of Technology. Unfortunately, there is no interest among decision-makers to support this activity.

Substantial work has still to be done concerning AQ and Climate modeling in Poland, facing a huge challenge to decision-makers and scientific community. The most important recommendations may be summarized as follows.

First of all, there is an urgent need for introduction of the second-generation GPM as a regulatory AQM in Poland. It is recommended to use AERMET-AERMOD for local scale applications and CALMET-CALPUFF for local to voivodeship-range scale applications. Secondly, further development of multi-scale AQ modeling is needed. The advantage of experience gained in that field so far by the modeling group from WUT could be taken. Thirty, there is an urgent need for the development of national Integrated Assessment Model (schematic of which is given in this paper, Fig. 1), in order to support AQ policy in the country. However, it is a huge and demanding task, for which considerable financing is needed. Finally, due to the complexity of atmospheric system, further developments can be achieved only by co-operation effort of various Polish research groups. These should end, ultimately, with creation of Polish AQ and climate research community.

Acknowledgements

This work was supported by the EC 6. Framework Program, Project CECILIA (Central and Eastern Europe Climate Change Impact and Vulnerability Assessment), Contract No GOCE 037005 (http://www.cecilia-eu.org).

LIST OF ACRONYMS

AERMOD	Second generation regulatory Gaussian Plume Model (US EPA)
ADE	Atmospheric Diffusion Equation
AQ	Air Quality
AQM	Air Quality Model

CALPUFF	Second generation Gaussian puff model (US Earth Tech., Inc.)
CAMx	Third generation Comprehensive Air quality Model with eXtensions (ENVIRON Int. Corp., California, USA)
CBL	Convective Boundary Layer
CBM	Carbon Bond Mechanism
CRU	Climate Research Unit (University of East Anglia, Norwich, UK)
CTM	Chemical-Transport Model
CMAQ	Third generation Community Multiscale Air Quality model (US EPA)
ECMWF	European Centre for Medium-Range Weather Forecasts (Reading, UK)
EEA	European Environmental Agency
EGM	Eulerian Grid Model
EMEP	Co-operative Program for Monitoring and Evaluation of the Long-range Transmission of Air Pollutants in Europe operating under LRTAP Convention
FDDA	Four-Dimensional Data Assimilation
GCM	General Circulation Model/Global Climate Model
GHG	GreenHouse Gas
GPM	Gaussian Plume Model
IAM	Integrated Assessment Model
IPCC	Intergovernmental Panel of Climate Change
LRT	Long-Range Transport
LRTAP	UNECE, Geneva Convention on Long-Range Transboundary Air Pollution
LTM	Lagrangian Trajectory Model
MC2/GEM	Mesoscale Compressible Community/Global Environmental Multiscale model (Canadian Meteorological Service/ York University, Canada)
MetM	Mesoscale Meteorological Model
MM5	Fifth Generation Mesoscale Meteorological model (PSU/NCAR, USA)
NWP	Numerical Weather Prognostic model
PM	Particulate Matter
PM_X	Particulate Matter of so called surrogate diameter below X μm
RCM	Regional Climate Model
RegCM	RCM developed at The Abdus Salam International Centre for Theoretical Physics (Trieste, Italy)
SBL	Stable Boundary Layer
WRF	Weather Research and Forecasting model (NCAR, USA)
WUT	Warsaw University of Technology (Poland)

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Received: November 13, 2008; accepted: July 13, 2009.

NOWE WYZWANIA W MODELOWANIU JAKOŚCI POWIETRZA I KLIMATU

W obecnej chwili, gdy alarmująco wysokie stężenia pyłów w atmosferze powodują przedwczesną śmiertelność tysięcy mieszkańców Europy, a zmiany klimatu są największym wyzwaniem ochrony środowiska naszej planety, matematyczne modelowanie jakości powietrza i klimatu staje się niezbędnym narzędziem badawczym, jak również niezwykle potrzebnym narzędziem wspomagania polityki ochrony środowiska. W ostatnich latach osiągnięto wielki postęp w omawianej dziedzinie. W pracy przedstawiono zadania i cele modelowania jakości powietrza oraz podstawy modelowania deterministycznego. Ukazano rozwój modeli regulatoryjnych oraz numerycznych modeli Eulerowskich, które aktualnie przyjmują postać tzw. systemów modelowania (modeli trzeciej generacji), pracujących zarówno w trybie *off-line* jak i *on-line*. Zaprezentowano najnowsze rozwiązania stosowane w modelowaniu meteorologicznym, w modelowaniu przemian chemicznych oraz w regionalnych modelach klimatycznych, wskazując na rozwój modelowania na świecie, w Europie i w Polsce. Omówiono także kwestę implementacji modeli oraz ich weryfikacji. Pracę podsumowują wnioski i rekomendacje związane z koniecznością rozwoju i integracji modelowania jakości powietrza i klimatu w Polsce.