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AEROSOL DYNAMICS AND TRANSPORT IN AIR-QUALITY MODELS AT THE URBAN AND REGIONAL LEVELS

An attempt is made to present the aerosol dynamics and transport in air-quality models used for short-term simulations of pollutant fields at urban and regional levels. Two groups of aerosol dynamics models built into air quality models are distinguished and characterised, i.e., sectional and modal models. Methods of solving aerosol dynamic and transport equation are described. A critical analysis of aerosol modelling is given.

1. INTRODUCTION

Gas-phase species and aerosols interact with each other in the atmosphere. In order to be able to assess the effect of these interactions on the air quality, gas-phase species and aerosol particles have to be modelled together. As a result, the air-quality models for the mixture of gases and aerosols are developed. In these models, the concentrations of gas-phase species and size distributions and composition of aerosol particles are calculated simultaneously.

The physical and chemical principles that govern the pollutant behaviour are complex. In the simulation of the evolution of the fields of the gas-phase and aerosol phase pollutants in the atmosphere, the following processes need to be included: the emission, transport and diffusion, chemical transformations, removal from the atmosphere by wet and dry deposition, nucleation, condensation, evaporation, sublimation, coagulation and gravitational setting.

Air-quality models have usually a modular structure. Aerosol processes are usually described in an independent module called an aerosol dynamics model.

In this article, aerosol dynamics models are reviewed. A classification of the aerosol dynamics models is presented and the types of these models are distinguished and

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characterised. The methods of the numerical description of the aerosol dynamics and transport equation are presented. Some research topics for further considerations and the improvements necessary for modelling the atmosphere with the focus on the aerosol modelling are listed. The review concerns the models applied in short-term air-quality simulations at urban and regional levels in which the Eulerian type of a framework is used.

2. AIR-QUALITY MODELS SIMULATING THE EVOLUTION OF GAS-PHASE SPECIES AND AEROSOL PARTICLES

The models used in air-quality assessments can be classified using different criteria such as: the temporal scale, spatial scale, modelling approach or mathematical assumptions [24], [26], [51]. Recently, in a modelists' community, it has been quite popular to distinguish, depending on the period of the model development, three types of the following air-quality models: the first-generation, the second-generation and the third-generation models [8], [32]. In the models which belong to the second-generation (some models) and third-generation we deal with the aerosol modelling, while in the first-generation models, the aerosol modelling is not indispensable in each case.

The second-generation air-quality models used in short-term simulations of gas-phase species and aerosol particle distributions on the urban and regional scale were developed in conjunction with the gas-phase models developed in the 1980's or even the 1970's. The late 1990's was just the beginning of the third-generation models. As one can expect the time of their development has a great influence on general model characteristics. The advances concern the description of specific physical and chemical processes, the machine used as well as numerical, uncertainty and sensitivity analyses [8], [32], [37], [39].

In the case of the tools of the newest generation, the term *modelling system* instead of a *model* is used and the gas–aerosol air quality models can be run on-line or off-line with the meteorological models. In these systems, a mathematical description of real phenomena is based on the newest theory, computational experiments and measurements. Here the most powerful computers are used. The numerical algorithms addressing massive parallel architecture of machine are introduced. They all are capable of carrying out sensitive and uncertainty analyses. The development of more friendly interfaces allows us to apply the air-quality modelling systems to scientific and control strategy calculations that can be used by much broader spectrum of users including the so-called average staff.

The examples of the gas–aerosol air quality models (systems) applied in short-term urban and regional scale simulations are presented in table.

Table

The examples of the Eulerian air quality models/systems currently applied in short-term simulations of gas-phase and aerosol-phases species' distributions on urban and regional scale [26]

Air quality model/system	Gas-phase model	Aerosol dynamics model	Some other features	Application
CIT-AERO	CIT [27, 28]	Aerosol model of PILINIS and SEINFELD [34]	Second generation model Off-line modelling	south coast basin of California
UAM-AERO [50]	UAM IV	IMADE (internally mixed aerosol dynamic equation based model)	Second generation model Off-line modelling	south coast basin of California [23], [45], [46]
GATOR/MTDM [19]	GATOR	Sectional aerosol model of JACOBSON [19]	Second generation modelling system with some features of the third generation system On-line modelling	south coast basin of California
EURAD-AERO [1]	EURAD (European air dispersion model) [17], [22]	MADE (modal aerosol dynamics model for Europe) [3]	Second generation modelling system Off-line modelling	Central Europe [1], North-Reine-Westfalia [26]
Models-3 /CMAQ (community multi-scale air quality model) [5]		RPM (regional particulate model) [2], [3]	Third generation modelling system On-line modelling	North America

3. A CLASSIFICATION OF THE AEROSOL DYNAMICS MODELS

The aerosol dynamics models can be divided into classes using different criteria. Based on the behaviour of a probability density function of the aerosol particle-size distribution during model simulation two classes of models can be distinguished: *moments' models* (*modal models*) and *sectional models* [6], [15], [16], [26], [35]. In the first class of the aerosol dynamics models, the type of this function does not change during the whole model simulation. In the second class, it may change.

3.1. MOMENTS' (MODAL) AEROSOL MODELS

In the moments' aerosol models, the continuous distribution is used to describe the variability of aerosol particle sizes. The range of particle diameters is divided into a series of overlapping intervals, called the *modes*. Each mode is represented by a single-density function of the aerosol size distribution, whose type is fixed. The type of this function is arbitrary but usually a lognormal distribution is assumed. Integral parameters, called *moments of the distribution*, are used to characterise the particles belonging to a specific mode. The moment of order k (M_k) is defined by the relation [1]:

$$M_k = \int_{-\infty}^{\infty} D_p^k n_n^e (\ln D_p) d(\ln D_p), \quad (1)$$

where:

D_p – the aerosol particle diameter,

$n_n^e(\ln D_p)$ – the normalised probability density function of the particle-size distribution.

The size distribution of the whole population of the atmospheric aerosol is represented by a sum of the overlapping lognormal distributions. Usually the number of these distributions does not exceed 4. This resembles the nature of the size distributions measured in the atmosphere [30].

The aerosol dynamics and transport within each mode are described by tracing the change of moments. Assuming the lognormal distribution within each mode, relation (1) takes the form:

$$M_k = N \overline{D}_{pg,N}^k \exp\left[\frac{k^2}{2} \ln^2 \sigma_{g,N}\right], \quad (2)$$

where:

N – the total particle number concentration of the mode,

$\overline{D}_{pg,N}$ – the median diameter,

$\sigma_{g,N}$ – the standard deviation of the distribution.

In order to fully characterise the size distribution of aerosol particles, three independent variables are needed. Most often as these prognostic variables the following moments of the size distribution are used: M_0, M_2, and M_3. The first variable is the total particle number concentration of the mode. The second variable is proportional to the particle surface area, and the third one is proportional to the particle volume area. Computational costs are considered to be the reasons for using these moments as the prognostic variables [3]. The conservation equation used to predict the aerosol size distribution formulated in terms of the integral moments for the mode j is the following [1]:

$$\frac{\partial M_{k,j}}{\partial t} + \frac{\partial (u M_{k,j})}{\partial x} + \frac{\partial (v M_{k,j})}{\partial y} + \frac{\partial (w M_{k,j})}{\partial z} = \left(\frac{\partial M_{k,j}}{\partial t}\right)_{df} + S_{k,j} \quad (3)$$

for $k = 0, 2, 3$ and $j = 1, 2, 3, ..., L_j$,

where:

$M_{k,j}$ – the moment of the order k for the particles of the mode j,

$\left(\frac{\partial M_{k,j}}{\partial t}\right)_{df}$ – the change of the moment due to diffusion,

$S_{k,j}$ –the source and sink terms of the moment $M_{k,j}$,

L_j – the number of modes.

This is one of the forms of the equations describing the pollution transport in the atmosphere. The source and sink terms represent the following processes: chemical reactions, dry deposition, wet deposition, nucleation, evaporation, sublimation, coagulation, gravitational setting. It can be noticed that the interactions between gas phase and aerosol phases are included implicitly in the term $S_{k,j}$. The concentrations of gas-phase species concentrations are calculated based on the host model.

Among the moments' aerosol models the most popular are the MADE model and the RPM model incorporated respectively in the EURAD-AERO system [1] and in the Model-3/CAQM system [5].

3.2. SECTIONAL MODELS

In the sectional models, the discrete distribution describes the variability of aerosol particle sizes. The range of particle-size diameters is discretised into separate sections. In these models, different treatment of the particle-size bin structure is realised. A full-stationary size structure, the full-moving size structure, or mixed schemes can be applied [26], [35].

In the *full-stationary size structure* (fixed-size bins, stationary-size bins) [34], the values determining the boundaries of each size section are fixed during simulation. It is assumed that aerosol particles belonging to a specific section are represented by a fixed size diameter and have the same composition. When particles grow their diameters do not change, but if the particles become large enough they belong to another section. Similarly, coagulation of particles is taken into account. This approach is convenient as far as the description of the transport, coagulation, nucleation and emission of aerosol particles is concerned. There are problems with the description of condensation. In order to reduce the numerical diffusion, which changes the shape of the aerosol-size distribution, one can increase the number of size sections or use more sophisticated numerical techniques [18].

In the *full-moving size structure* [12], [34], the boundaries of each section are extended independently of the boundaries of the neighbouring sections. Therefore the boundaries between two neighbouring or even further ranges can overlap. The full-moving size structure is not used in the Eulerian-type aerosol models. It is used in the

Lagrangian-type models. This approach allows elimination of errors related to the numerical diffusion, but the description of coagulation, nucleation, emission and transport of aerosol particles still poses some problems.

In the *mixed technique*, the aerosol dynamics is analysed using either the combination of the moving section size grid and the stationary section size grid [12], [23] or the moving centre size structure [20]. In the first scheme, the moving section technique is used in the aerosol module internally, but after the completion of the time step the solutions obtained are converted into a stationary size grid. In the second scheme, the structure size bin edges are fixed but a mean diameter of particles within the size bin is allowed to vary. The description of the coagulation, nucleation, emission and transport is almost identical to that in the stationary-size structure, but the description of the condensation is modified. This allows reduction of a numerical diffusion.

The full-stationary size structure is used, for example, in the aerosol dynamic model of Pilinis and Seinfeld built in the gas-phase CIT model developed by MCRAE [27], [28] and in the IMADE model applied in the UAM-AERO model [49], [50]. The description of aerosol dynamics and transport is realised by tracing the change in the mass concentration of the species i in the aerosol particles of the diameter size j:

$$\frac{\partial C_{m,i,j}}{\partial t}+\frac{\partial (uC_{m,i,j})}{\partial x}+\frac{\partial (vC_{m,i,j})}{\partial y}+\frac{\partial (wC_{m,i,j})}{\partial x}=\left(\frac{\partial C_{m,i,j}}{\partial t}\right)_{df}+S_{i,j} \tag{4}$$

$$\text{for } i = 1, 2, 3, ..., L_i, j = 1, 2, 3, ..., L_j,$$

where:

$C_{m,i,j}$ – the mass concentration of the species i in the aerosol particles of the diameter size j,

u, v, w –the components of the wind velocity,

$\left(\frac{\partial C_{m,i,j}}{\partial t}\right)_{df}$ – the change in the mass concentration due to diffusion,

$S_{i,j}$ –the source and sink terms,

L_i – the number of species,

L_j – the number of diameter sizes.

The **moving centre size structure** is used, for example, in the GATOR system [19], [20]. Here the aerosol dynamics and transport are described by tracing the change in the number concentration of particles of the diameter j and the change in the volume concentration of the particle component i in the particles of the diameter j:

$$\frac{\partial C_{n,j}}{\partial t}+\frac{\partial(uC_{n,j})}{\partial x}+\frac{\partial(vC_{n,j})}{\partial y}+\frac{\partial(wC_{n,j})}{\partial z}=\left(\frac{\partial C_{n,j}}{\partial t}\right)_{df}+S_j\,, \tag{5}$$

$$\frac{\partial C_{\upsilon,i,j}}{\partial t}+\frac{\partial(uC_{\upsilon,i,j})}{\partial x}+\frac{\partial(vC_{\upsilon,i,j})}{\partial y}+\frac{\partial(wC_{\upsilon,i,j})}{\partial z}=\left(\frac{\partial C_{\upsilon,i,j}}{\partial t}\right)_{df}+S_{i,j} \tag{6}$$

for $i = 1, 2, 3, ..., L_i$, $j = 1, 2, 3, ..., L_j$,

where:

$C_{n,j}$ – the number concentration of aerosol particles of diameter j,

$C_{\upsilon,i,j}$ – the volume concentration of the substance i in the aerosol particles of the diameter j,

$\left(\frac{\partial C_{n,j}}{\partial t}\right)_{df}$, $\left(\frac{\partial C_{\upsilon,i,j}}{\partial t}\right)_{df}$ – represent the change in the number concentration and the volume concentration due to diffusion, respectively,

S_j, $S_{i,j}$ – are the sink and source terms related to the number and the volume concentration, respectively.

In the sectional models, the interactions between the gas-phase and aerosol-phase species are also included implicitly, and the gas-phase pollutant concentrations should be calculated in the host model.

4. SOLUTION METHOD OF THE AEROSOL DYNAMIC AND TRANSPORT EQUATIONS

The equations describing the dynamic and transport of gas-phase substances and aerosol particles are complex. In most of air quality models, they are solved using an operator splitting technique introduced by MARCHUK [25]. It is assumed that within a short period Δt the processes influencing the behaviour of the species in the atmosphere are independent of each other. Specific terms in the equations describing single processes are integrated separately using the most efficient and accurate numerical algorithms. The final solution is obtained in a sequence. This allows us to shorten the solution time and in general to improve numerical accuracy [31].

To integrate partial differential equations the differential schemes, finite element method, spectral methods or pseudospectral methods are used [33], [36], [41], [43], [52]. In order to solve the ordinary differential equations, which describe the processes hidden in the source term, the general purpose methods [4], [11], [14], [21], [44], [48] or specific methods developed to solve the specific air pollution processes are used [9], [10], [19], [20], [47].

5. CRITICAL ANALYSIS OF AIR QUALITY MODELLING WITH THE FOCUS ON AEROSOL MODELLING

Although much progress has been achieved in the field of air quality modelling over the last decade, a number of topics warrant further consideration. RUSSEL and DENNIS [37] have suggested the following needs:

- better understanding and the parameterisation of the vertical mixing,
- an improvement in the cloud formation modelling,
- a more detailed treatment of radiative transfer and heterogeneous chemical processes,
- an application of interrogation techniques (including the uncertainty analysis) in the model evaluation,
- further development of databases and monitoring programs.

As far as the aerosol modelling is concerned the following postulates are formulated:

- the treatment of secondary inorganic aerosols occurring simultaneously with fog and clouds as well as the treatment of secondary organic aerosols in general have to be improved [40],
- the aerosol particle scavenging during cloud formation, capture of aerosol particles by cloud drops, their resuspension by evaporation of cloud drops and their impact on photolysis rate have to be accurately assessed [32],
- the more reliable emission inventories including the more detailed data of aerosol emission have to be developed [37].

It seems that wide application of the air-quality models is basically limited by the lack of input databases. Input data necessary for system of the air-quality modelling covers: meteorological data, emission rates, physiographic data, and concentrations of species. Typically, inputs are specified at hourly intervals for each computational cell. Most researchers are of the opinion that emissions are one, if not the most, uncertain inputs into air quality models. Effort should be made to obtain the accurate and reliable input data, in particular emission estimates. Typically, in order to assess the transport and dynamics of gas/aerosol, the hourly, spatially grided estimates of the emissions of CO, NO, NO_2, SO_2 VOCs as well as emissions of SO_3, NH_3, PM2,5, PM10 are needed.

6. SUMMARY

The air quality models/systems simulating the gas and aerosol behaviour in the atmosphere can be classified using different criteria. Recently, in the air-quality models their three generations have been separated, depending on the time of their development. The time of the model development greatly influences the description of specific processes and numerical techniques applied. The tools of the newest generation are most advanced. The aerosol modelling is included in the air quality models belonging to the second and the third generations. Depending on the behaviour of the probability density function of the aerosol particle-size distribution, two types of the aerosol dynamics models are distinguished, i.e., moments' models and sectional models. The moments' models are based on the continuous distribution, and the type of the probability density function of this distribution does not change during the simulation. The sectional models are based on the discrete distribution and the function may change.

Despite a considerable progress in modelling the distributions of gas-phase and aerosol-phase species on the urban and regional scale the further development of this procedure is needed. It seems that widespread application of the gas–aerosol air-quality models is basically limited by the lack of input databases, in particular emission inventories including aerosol data. It is worth adding that the difficulties in collecting the emission data are thought of to be the main source of the model uncertainty.

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DYNAMIKA I TRANSPORT AEROZOLI W MODELACH JAKOŚCI POWIETRZA W SKALI MIASTA I REGIONU

Opisano transport i dynamikę aerozoli w modelach jakości powietrza stosowanych w obliczeniach krótkoterminowych w skali miasta i regionu. Dynamikę aerozoli pokazują modele jakości powietrza należące do drugiej i trzeciej generacji. Opis procesów oddziałujących na rozprzestrzenianie się zanieczyszczeń i numeryczne metody rozwiązywania równań matematycznych zależą od czasu powstania modelu. W modelach najnowszych stosuje się nowoczesne rozwiązania. Transport i dynamikę aerozoli w modelach jakości powietrza opisuje się, korzystając z modeli dynamiki aerozoli. Wyróżniono dwie grupy modeli, tzn. modele sektorowe i modele modalne. Aby opisać zmienność cząstek aerozoli pod względem wielkości, w modelach modalnych przyjmuje się ciągły rozkład. Typ funkcji gęstości prawdopodobieństwa tego rozkładu założony na początku symulacji nie zmienia się. W modelach sektorowych

zmienność cząstek aerozoli opisuje pod względem wielkości rozkład dyskretny i typ funkcji gęstości tego rozkładu może się zmieniać. Pomimo że w ostatnim dziesięcioleciu odnotowano istotny postęp w modelowaniu rozprzestrzeniania się zanieczyszczeń gazowych i cząstek aerozoli, należy nadal pracować nad rozbudową modeli jakości powietrza. Powinny być również podjęte prace zmierzające do opracowania baz danych odpowiedniej jakości, w tym szczegółowych baz danych o emisji. Dostępność takich baz umożliwi szersze zastosowanie modeli jakości powietrza opisujących rozprzestrzenianie się zanieczyszczeń gazowych i aerozoli w atmosferze. Uważa się, że jakość danych wejściowych do modeli, w tym jakość danych o emisji wpływa istotnie na niepewność modelowania i dane te powinny być określane bardzo starannie.