Numerical Simulation of Cloud Dynamics and Microphysics

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Abstract. It is well known that convective clouds play an essential role in the evolution of the aerosol particles in the atmosphere by providing spatial redistribution and transformation of aerosol due to in cloud chemical reactions, dynamical and microphysical processes. The influence of the clouds upon the aerosol properties increase greatly in extreme conditions, such as volcano eruptions, explosions, large fires, when enormous number of aerosol particles of different size and chemical compound are injected in the atmosphere. In this paper the overview of the main results, obtained by the authors in the field of numerical modeling of the convective clouds, developing in natural and extreme conditions and the investigation of their role in the evolution of the atmospheric aerosol is presented.

1 Introduction

Computational fluid dynamics and meteorology in particular are among the major consumers of high performance computer technology. Effective numerical modeling of convective flows developing in natural and extreme conditions allows to calculate online transport and transformation of the atmospheric particles and effluents in real time thus making possible to use the model for the operational forecast of the local pollution propagation. A detailed analysis of the processes of such kind requires development of the effective algorithms of its numerical realization including high-performance algorithms for modern supercomputer calculations. The effective numerical algorithms will allow to incorporate the model into in the operational regional or global climate models for online forecasting of the pollutant propagation in the certain area and possible prevention of undesirable effects of catastrophic phenomenon frequently accompanied by the convective cloud development.

A role of clouds in evolution of atmospheric pollutant is quite significant. Cloud dynamics strongly modifies the distribution of pollutant through advection and more local eddy motions over the edges of the cloud. Cloud microphysics participates in pollutant evolution by means of condensation/evaporation and collection processes transferring them to the drops during precipitation formation and reinjecting back into the air by evaporation of droplets and raindrops. On the one hand, the processes in the clouds result in cleaning the atmosphere by wet removal of the pollution. On the other hand they are responsible for so called acid rains, damaging the material surfaces of aquatic and forest ecosystems. In addition, clouds participate actively in trace

chemical redistribution, affect the global radiation budget and thus influence global background atmosphere.

Though clouds of all types contribute significantly to atmospheric processes, the case of so called deep convection, when the upper boundary of the cloud can reach the tropopause level, is the most interesting one from the view point of pollutant delivering to the upper levels of troposphere. Besides, deep convection plays an exclusively important role as pollutant converter and transport mean in various extreme situations when enormous amount of chemically active aerosol particles are being injected into the atmosphere.

Convective clouds are very complex natural objects, with a wide spectrum of interacting processes of different time/space scales (convective transport, microphysical interactions, chemical reactions, etc.). A brief review of the recent cloud models where the most complete set of the in-cloud processes are considered [1]-[6] shows, that in each model only a few features of cloud processes interaction are being considered rigorously while the rest ones are treated approximately, with the use of strong simplifying assumptions and crude parameterizations. Thus, an urgent need does exist in a numerical model capable of representing properly all the essential interactions between dynamical, microphysical, chemical and aerosol processes. This model implementation will apparently demand supercomputer facilities and the effective numerical algorithms including special techniques for supercomputer applications.

This paper is dedicated to the description of the numerical algorithms used for simulation dynamical, turbulent, microphysical and chemical processes in convective clouds developing in natural and extreme conditions. Algorithms were realized in the frame of one and two-dimensional numerical models. The first one is intended for natural clouds investigation, the second – primarily for investigation of the clouds developing in extreme conditions. The second model was also used for describing the polluted cloud formation that occurs during buoyant thermal rising.

2 Algorithms Used in the One-Dimensional Model

A time-dependent, one-dimensional model is used for an isolated warm cumulus cloud life cycle simulation. In this model the cloud is assumed to have a cylindrical form with constant radius R in an environment at rest. All equations expressed in cylindrical coordinates and all cloud variables are represented with mean values averaged over the horizontal cross section of the cloud [7]. The system of equations combines the equations of vertical motion, the equation of continuity, the first law of the thermodynamics, and the equations of water vapor and liquid hydrometeors transport. The dynamic interaction between the cloud and its environment is modeled by two entrainment terms: turbulent entrainment representing lateral mixing at the side boundaries of the cloud and dynamic entrainment, representing the systematic inflow or outflow of air required to satisfy mass continuity. Time splitting method is used for numerical solution of the equations. The formation and growth of drops by nucleation, condensation and stochastic collection are modeled in detail with the help of stochastic collection equation. For calculation of the terms describing processes of condensation/evaporation the Lagrangian scheme was chosen [8], which guarantee

the conservation of cloud drops number. For the calculation of coalescence process the modification of the well-known Kovetz and Olund method [9] is used, which allows to obtain good solution of stochastic collection equation at the relatively low number of drop size intervals and provides precise fulfillment of the mass conservation law.

In such kind of problems the major part of computation time is consumed during the solution of stochastic coalescence equation especially when the real collection kernel is calculated directly in calculation process. To reduce the run time the collection kernel of such equation, being once calculated must be stored in computer memory. This demands the array of the size $n^2 m$, where n is the number of droplet size classes and m is the number of space grid points. It is evidently needs great amount of computer memory, but allows reducing run time essentially.

To investigate the role of convection in aerosol pollutant redistribution a very effective numerical algorithms are needed which could be incorporated into the dynamical block of the model without a significant growth of the computational expenses. Development and implementation of such algorithms will allow assessing more accurately the effect of the aerosol particles size distribution on the pollutant concentrations.

For the problem solution the model was modified in nucleation block description. Nucleus vertical transport and reinjecting back into the air by evaporation of cloud drops were taken into account. The particle was assumed to be activated when achieving critical supersaturation for given size. The results of numerical investigation of the cloud effect upon aerosol pollution redistribution in the atmosphere revealed strong feedback between cloud and aerosol parameters. Vertical distribution of the aerosol particles in different outer atmospheric conditions with unstable temperature distribution (case 1) and the other (case 2) with the small layer of the temperature inversion on the 50 min of cloud development is represented in Fig.1.

Fig. 1. Vertical profiles of aerosol particles obtained on the 50min of cloud development, where 1- initial aerosol distribution, 2 - hydrophobic particles (case 1), 3 - cloud condensation nucleus (case 1), 4 - hydrophobic particles (case 2), 5 - cloud condensation nucleus (case 2).

For the analyses of the calculation results a special viewer was elaborated, which allowed looking through the output data which structure was not prescribed in advance. This was obtained by special output procedure, which created data base with all necessary information about the structure of the output data fields and its content. The viewer utilizes this data to form the user's menu system and provide all features necessary for visualization.

Calculations with the model gave the results, which were in good agreement with observations of the dynamical and microphysical properties of warm cumulus cloud (Fig.2). The development of the droplet spectrum during cloud evolution up to the precipitation formation was particularly well simulated.

Fig. 2. Numerical and experimental data comparison. (drop size distribution) Dark columns - numerical data, light columns - numerical data.

One-dimensional model was used for investigation of the effect of the convective cloud droplets on the chemical composition of the troposphere. For this purpose effective and computationally cheap numerical scheme of chemical species redistribution along the droplet spectrum due to the processes of condensation and evaporation was elaborated [8]. In general, numerical simulation of cloud droplet – chemical species interaction is very complicated problem, demanding solution of the kinetic equation for multicomponent composition distribution function [10]. Proposed approach is based upon the following simple assumptions: if the droplet spectrum is divided into several size classes, fraction of the chemical species redistributed due to the microphysical processes is proportional to the ratio of the droplet mass flux between classes to the total droplet mass class contains. Nevertheless it allows obtaining satisfactory results using relatively small computer resources.

Calculation showed that the main effect of the convective cloud on the chemical composition of the air is the depletion of the well-dissolved species concentrations and their removal by precipitation. The transformation of aqueous species in different size droplets due to their coagulation is very important for the cloud and precipitation

chemistry. The vertical transport in the convective cloud may affect essentially the vertical distribution of chemical species of the troposphere, especially if there is a surface pollution source.

Test calculations showed that the method application for simulation intensive collection at high aerosol particle concentrations required essential reduction of the time step for obtaining positive solution. For overcoming this constraint the following modification of the initial scheme was proposed. A solution is obtaining in two stages as the time step is splitting. On the first stage the following equation is solved (see [9]):

$$\frac{M_j^{n+1/2} - M_j^n}{\Delta t} = -S_j^-, \quad (1)$$

where M_j – aerosol particle mass in the interval $m_{j-1/2}, m_{j+1/2}$, m_j , $j=0,1,\dots,N$ – coordinates of the grid points in the mass space.

$$S_j^- = \sum_{l=1}^{N-1} S_{jl}^- \quad (2)$$

$$S_{jl}^- = K(m_j, m_l) \frac{M_j^{n+1/2} M_l^n}{m_l} \quad (3)$$

$K(m_j, m_l)$ – is collection kernel.

Solution of the equation (1) is as follows:

$$M_j^{n+1/2} = \frac{M_j^n}{1 + \Delta t \sum_{l=1}^{N-1} K(m_j, m_l) M_l^n / m_l} \quad (4)$$

The further calculations are conducted according to the formulas:

$$\frac{M_j^{n+1} - M_j^n}{\Delta t} = S_j^+ - S_j^- \quad (5)$$

$$S_j^+ = \sum_{k=1}^{N-1} \sum_{l=1}^{N-1} S_{jkl}^+ \quad (6)$$

$$S_{gil}^+ = \alpha_{gil} S_{jl}^- \quad (7)$$

$$\alpha_{gil} = \begin{cases} \frac{m_{g+1} - m_j - m_l}{m_{g+1} - m_g} & \text{at } m_g < m_j + m_l \leq m_{g+1} \\ \frac{m_j + m_l - m_{g-1}}{m_g - m_{g-1}} & \text{at } m_{g-1} < m_j + m_l \leq m_g \\ 0 & \text{in the other cases} \end{cases} \quad (8)$$

It is easy to show that

$$M_j^{n+1} = M_j^n + \Delta t (S_j^+ - S_j^-) = M_j^n - \Delta t S_j^- + \Delta t S_j^+ = M_j^{n+1/2} + \Delta t S_j^+, \quad (9)$$

Test calculations showed that at relatively small time step the solution obtained by explicit and implicit schemes practically coincided. At large time step implicit scheme produces a certain error. Nevertheless it provides positive solution at any time step (as it is clear from [8]) and guarantees mass conservation similar to the original scheme.

3 Algorithms Used in the Two-Dimensional Model

The numerical study of the convective flows developing in extreme conditions was based upon the system of equations of the turbulent convection, described in detail in [11] and [12]. In case of deep convection, especially associated with the extreme conditions, the problem is strengthened by the presence of crucial variations of the system thermodynamic parameters. At such conditions the conventional Boussinesq approximation becomes unjustified and one has to use the full compressible Navier - Stokes equations. However at low Mach numbers typical for clouds convection, these equations becomes acoustically "stiff" and their solution presents an extremely complicated computational problem [13]. Besides, one of the most difficult physical issues associated with the cloud dynamics modeling is an appropriate treatment of turbulent transport. A turbulence model used for this purpose should be capable of providing an adequate description of the strong stream-line curvature, flow rotation, and buoyancy effects being crucial in deep clouds convection.

Two-dimensional model is the model based upon the solution of equations, describing the axisymmetric turbulent flow of compressible two-phase two-component medium considering condensation of water vapour and precipitation formation. The model is appropriate for the description of the flows with arbitrary vertical scales and temperature variations. The description of the processes of turbulent mixing is provided with the help of k - ϵ model modified by taking into account the influence of the streamline curvature and buoyancy forces. It was shown in [11], that for the correct description of the stratified flows one of the constants in the k - ϵ turbulence model should have different values in the stable and unstable conditions. The alternative directions scheme is used for the numerical solution of the system of equations. The suppression of the nonphysical oscillations is provided by means of the specially elaborated monotonization procedures [14] Calculation of the processes of turbulent energy generation and dissipation is separated in the additional step of the

splitting procedure, where fully explicit scheme is used. As the dimensions of the disturbed region of calculation vary greatly, the simulations were performed in the domain with movable external boundaries where movable grid with fixed number of points was inserted. The model is intended for the investigations of the flows developing at the presence of high-energy sources on the ground surface or in the air. As a matter of fact this problem is converged to the simulation of the buoyant thermal rising in the stratified medium.

The numerical simulation provided with this model allowed to obtain the description of all stages of the thermal evolution, including the stage of its transformation to the buoyant vortex ring, which is characterized by the fully coincidence of the regions of maximum temperature and maximum vorticity. Such structure is preserved till the end of the thermal rising when its speed begins to decrease due to the generation of the secondary vortex system in the stable stratified atmosphere.

For taking into account the phase transitions of the water vapor the main model equations are written for the general case of two-phase two-component flow movement. In this case the processes of cloud droplets evaporation-condensation were described in the equilibrium approach, for the description of precipitation formation the Kessler parameterization scheme was used. Moist convection numerical experiments results showed, that while thermal ascending the condensed water once appeared in the updraft region near the axis of symmetry propagates then to the whole cloud volume. The further cloud evolution depends essentially upon the environmental conditions. When the relative humidity of the air is more than 50% in the lower 5km atmospheric layer release of the latent heat of condensation resulted in the development of the convective flow similar to that in the natural convective clouds. In the regions of high water content the formation of the precipitation particles capable to reach the ground takes place.

This model appended with the equations describing the aerosol-droplet interaction [15] was used for the investigations of the vertical transport of the aerosol particle injected in the atmosphere as a result of the powerful explosion. The results of numerical experiments showed that the process of so called «nucleation coalescence» [16] is responsible for the rate of the capture of the large aerosol particles by the cloud drops. Regions with low concentration of dry aerosol particles locate near cloud lower boundary and under the vortex core, where the ambient air is involved into the cloud.

4 Conclusions

Several numerical algorithms intended for simulation of dynamical, microphysical and chemical processes in convective clouds are presented. The algorithms provide development and operation of adequate cloud models and effective codes of their numerical realization. Special technique elaborated for supercomputer applications allows conducting a wide set of numerical experiments with reasonable/affordable computation resources. Wide set of numerical experiments was conducted aimed to investigate the processes of pollutant source formation transport and transformation.

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