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## ATMOSPHERIC RADIATION, OPTICAL WEATHER, AND CLIMATE

# Numerical Model of Bioaerosol Transformation in the Atmosphere

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**Abstract**—A nonstationary mathematical model of bioaerosol dynamics is considered. It is based on nonlinear integral-differential equations that describe coagulation, condensation, and evaporation processes versus particle sizes. A definitely positive numerical scheme for solution of the problem of aerosol transformation in the atmosphere is presented. The model is numerically compared with the models that describe individual processes in the composition of the former. The relative contribution of each process in the overall dynamics of aerosol populations is studied in numerical experiments.

*Keywords:* mathematical modeling, aerosol populations, impurity transformation, coagulation, integral-differential equations

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## INTRODUCTION

This work continues the series of works devoted to the development of numerical models for the solution of environmental protection problems. Mathematical models are among the most important instruments in modern natural science, since they allow the observed and unobservable parameters to be connected. This makes it possible to formulate inverse problems, where it is necessary to find such model parameters with which the simulation results correspond to the measurements. The algorithms for solution of the inverse problems often require multiple solutions of direct problems, and the algorithms for data assimilation require multiple solutions of the inverse problems. Hence, the question of the computational efficiency becomes important. In this work, we study numerical models of aerosol dynamics, where discrete-analytical schemes suggested in [1–3] are applied. They have some advantages in the description of multiscale processes. The numerical methods currently used for the simulation of atmospheric aerosol dynamics and the detailed review of the related literature are presented in [4]. Coagulation, convection–diffusion, and condensation and evaporation are among the main processes taken into account in the aerosol dynamics models.

Coagulation is simulated with the help of different versions of the Smoluchowski equation, which is applied in the description of variabilities of different natures, e.g., evolution of aerosol composition [5], cloud and precipitation microphysics [6], growth of bacteria [7], changes in the sizes of schooling fishes [8], etc. Theoretical questions of the existence and stability and the analysis of the properties of their solutions are described in [9]. At present, only several analytical solutions of this equation are known, and only for certain cases. Therefore, different numerical methods for the solution of the Smoluchowski equation were developed, such as the method of finite elements [10]; finite difference methods based on special representations of the coagulation kernels [11, 12]; the method of finite volumes [13, 14]; the method of successive approximations [15]; the method of moments [16, 17]; Monte Carlo methods [18–20]; the meshless approach on the basis of radial functions [21], etc. Numerical methods are compared in detail in [22].

In this work, we use original discrete-analytical schemes constructed using the concept of conjugated Eulerian multipliers [1, 2]. The main advantages of these schemes are computational efficiency and unconditional monotonicity for models of aerosol populations in particle-size spaces. Let us emphasize that the state functions of objects under study are to be kept nonnegative at all computation steps. In fact, we develop a complex of algorithms for the study of the internal dynamics of aerosol transformation. These algorithms are intended for use in parallel computations according to the structure of a system of finite volumes in 4D models of the convection–diffusion–

reaction type of multicomponent gas-aerosol atmospheric substances.

## PROBLEM STATEMENT

Let us consider the problem of atmospheric aerosol admixture transformation versus the particle size accounting for the coagulation, evaporation (condensation), and diffusion processes. The particle mass, volume, or radius of a sphere of the same volume is used as a quantitative characteristic of the size of an arbitrary configured particle. The structure of the basic integral-differential operator of the model is to be defined following [4, 23–25] in the spatiotemporal domain $D_t = D \times [0; T_{\max}]$, where $D = [r_{\min}, r_{\max}]$ is the particle size range and $T_{\max}$ is the time interval length. The model is specified by the initial-boundary value problem

$$\begin{gathered}\frac{\partial c(r,t)}{\partial t} + (\alpha_D(r) + \alpha_S(r))\, c(r,t) \\ - \frac{1}{2}\int_0^r K(q(r,r'),r')c(q(r,r'),t)c(r',t)w(r,r')dr' \\ + c(r,t)\int_0^{r_{\max}} K(r,r')c(r',t)dr' + \frac{\partial}{\partial r}(U(r)c(r,t)) \\ - \frac{\partial^2}{\partial r^2}(U_D(r)c(r,t)) = 0, \quad (r,t) \in D_t, \end{gathered} \tag{1}$$

$$q(r,r') = (r^3 - r'^3)^{\frac{1}{3}}, \quad w(r,r') = r^2 / q(r,r')^2,$$

$$c(r_{\min},t) = 0, \quad c(r_{\max},t) = 0, \quad c(r,0) = c_0(r).$$

For particularization, let us consider the dynamics of biologically active substances. Let us take the designations and physical sense of the main objects in problem (1) from [23–25]: $c(r,t) \in Z(D_t)$ is the concentration of airborne particles with sizes in the range $[r, r + dr]$, $Z(D_t)$ is the space of quite smooth functions where the problem solution is searched for, and $K(r_i, r_k)$ is the kernel that describes the particle coagulation, defined for any $r_i, r_k \in D$:

$$K(r_i,r_k) = K_{\mathrm{g}}(r_i,r_k) + K_{\mathrm{B}}(r_i,r_k),$$

$$K_{\mathrm{g}}(r_i,r_k) = \pi\varepsilon(r_i + r_k)^2 \left|U_S(r_i) - U_S(r_k)\right|,$$
$$K_{\mathrm{B}}(r_i,r_k) = 4\pi kT(r_i + r_k)(B(r_i) + B(r_k)).$$

Here $K_{\mathrm{g}}(r_i,r_k)$ is the gravity coagulation, $K_{\mathrm{B}}(r_i,r_k)$ is the Brownian coagulation, $k$ is the Boltzmann constant, and $T$ is the temperature;

$$\alpha_D(r) = kTB(r)A_D/(\delta_D V),$$

$$\alpha_S(r) = [(4/3)\pi\rho r^3 gB(r)A_H]/V,$$

$A_D$ and $A_H$ are the parameters that consider the vertical and horizontal precipitation of particles on surfaces, $\alpha_D$ and $\alpha_S$ are the wash-out rates of particles, $V$ is the volume of aerosol localization, $\rho$ is the particle density, $g$ is the gravitational acceleration, $\delta_D$ is the boundary layer depth, $B(r) = Cn(r)/(6\pi\eta r)$ is the mobility of particles of radius $r$, $\eta$ is the gas viscosity;

$$Cn(r) = 1 + 1.246K_n(r) + 0.42K_n(r)\exp(-0.87/K_n(r))$$

is the empirical Cunningham correction factor, $K_n(r) = l/r$ is the Knudsen number, $l$ is the mean free path of the molecules;

$$\varepsilon = 0.5\left(r_i/(r_i + r_k)\right)^2$$

is the efficiency of particle collisions;

$$U_S(r) = 2\rho_{\mathrm{eff}}gr^2Cn(r)/(9\eta)$$

is the rate of gravitational sedimentation of particles (the Stokes law), $\rho_{\mathrm{eff}}$ is the effective density of a spherical particle;

$$U(r) = \frac{4D_iM_i}{2RTr\rho_{\mathrm{eff}}}(P_i - P_{\mathrm{eq},i})Cn(r)$$

is the condensation growth rate of particles,

$$P_i - P_{\mathrm{eq},i} = \Delta P$$

is the parameter that determines the physical sense of the process: the condensation occurs at $\Delta P > 0$, and evaporation, at $\Delta P < 0$; $D_i$ is the diffusion coefficient; $M_i$ is the molar weight; $R$ is the gas constant; $U_D(r) = |U(r)|\Delta r/2$ is the diffusion rate.

## NUMERICAL SCHEMES

Let us consider initial problem (1) in the time interval $t_j \le t \le t_{j+1}$. The splitting method [26] is used at each step. As a result, we obtain two interrelated subproblems:

$$\begin{gathered}\frac{\partial c_1(r,t)}{\partial t} + A(c_1,r,t)c_1(r,t) = F(c_1,r,t), \\ A(c_1,r,t) = (\alpha_D(r) + \alpha_S(r))c_1(r,t) \\ + \int_{r_{\min}}^{r_{\max}} K(r,r')c_1(r',t)dr', \\ F(c_1,r,t) = \frac{1}{2}\int_{r_{\min}}^{r} K((r^3 - r'^3)^{\frac{1}{3}},r') \\ \times c_1((r^3 - r'^3)^{\frac{1}{3}},t)c_1(r,t)\frac{r^2}{(r^3 - r'^3)^{\frac{2}{3}}}dr', \end{gathered} \tag{2}$$

$$\begin{gathered} c_1(r,t_j) = c(r,t_j), \quad c_1(r_{\min},t) = 0, \quad c_1(r_{\max},t) = 0, \\ c_1(r,0) = c_0(r), \quad (r,t) \in (r_{\min},r_{\max}) \\ \times (t_j,t_{j+1}) \equiv D_t^j \in D_t; \end{gathered}$$

$$\frac{\partial c_2(r,t)}{\partial t}+\frac{\partial}{\partial r}(U(r)c_2(r,t))-\frac{\partial^2}{\partial r^2}(U_D(r)c_2(r,t))=0,$$
$$c_2(r,t_j)=c_1(r,t_{j+1}),\quad c(r,t_{j+1})=c_2(r,t_{j+1}),\qquad (3)$$
$$c_2(r_{\min},t)=0,\quad c_2(r_{\max},t)=0,\quad (r,t)\in D_t^j.$$

Equations (2) are the Cauchy–Smoluchowski problems for the description of aerosol coagulation process in the subdomains $D_t^j \in D_t$. Equations (3) define the initial-boundary value problems for the aerosol substance condensation/evaporation, diffusion, and sedimentation, respectively.

To construct numerical schemes for the aerosol coagulation processes, let us use the variational approach suggested in [1, 2]. Its application allows derivation of the discrete-analytical scheme

$$\begin{gathered}
c_1(r_k,t_{j+1})=c_1(r_k,t_j)\mathrm{e}^{-\bar{A}(c_1,r_k,t_j)\Delta t}\\
+\frac{1-\mathrm{e}^{-\bar{A}(c_1,r_k,t_j)\Delta t}}{\bar{A}(c_1,r_k,t_j)\Delta t}\bar{F}(c_1,r_k,t_j)\Delta t,\quad k=\overline{1,N_0},\\
\bar{A}(c,r_k,t)=(\alpha_D(r_k)+\alpha_S(r_k))c(r_k,t)\\
+\sum_{i=0}^{N_0-1}\frac{K(r_k,r_i)c(r_i,t)+K(r_k,r_{i+1})c(r_{i+1},t)}{2}\Delta r_{i+0.5},\\
\bar{F}(c,r_k,t)=\frac{1}{4}\sum_{i=0}^{k-1}\{K(\bar{q}(r_k,r_i),r_i)\\
\times c(\bar{q}(r_k,r_i),t)c(r_i,t)w(r_k,r_i)\\
+K(\bar{q}(r_k,r_{i+1}),r_{i+1})c(\bar{q}(r_k,r_{i+1}),t)\\
\times c(r_{i+1},t)w(r_k,r_{i+1})\}\Delta r_{i+0.5},\\
\bar{q}(r_k,r_i)=\operatorname{Argmin}_{r\in\omega_r^h}|q(r_k,r_i)-r|,\\
\Delta r_{i+0.5}=r_{i+1}-r_i.
\end{gathered}\qquad (4)$$

The step $\Delta t$ is chosen from the condition $|\bar{A}(c_1,r_k,t_j)\Delta t|\le 10$.

To derive the difference scheme for convection–diffusion processes (3), let us use the directional difference approximations

$$\begin{gathered}
\frac{c_2(r_k,t_{j+1})-c_2(r_k,t_j)}{\Delta t}\\
+\frac{U^+(r_k)c_2(r_k,t_{j+1})-U^+(r_{k-1})c_2(r_{k-1},t_{j+1})}{\Delta r_{k-0.5}}\\
+\frac{U^-(r_k)c_2(r_k,t_{j+1})-U^-(r_{k+1})c_2(r_{k+1},t_{j+1})}{\Delta r_{k+0.5}}\\
-\frac{1}{\delta r_k}\left(\frac{U_D(r_{k+1})c_2(r_{k+1},t_{j+1})-U_D(r_k)c_2(r_k,t_{j+1})}{\Delta r_{k+0.5}}\right.\\
\left.-\frac{U_D(r_k)c_2(r_k,t_{j+1})-U_D(r_{k-1})c_2(r_{k-1},t_{j+1})}{\Delta r_{k-0.5}}\right)=0,\\
U^+(r)=(|U(r)|+U(r))/2,\\
U^-(r)=(|U(r)|-U(r))/2,\quad \delta r_k=\frac{1}{2}(\Delta r_{i+0.5}+\Delta r_{i-0.5}).
\end{gathered}\qquad (5)$$

Solving them, we find the value of concentration $c(r,t_{j+1})$ at the $(j+1)$th step. The resulting set of equations is solved by the three-point run method. Let us note that the above versions of numerical schemes (4) and (5) are simplified; they are effectively implemented and have properties of approximation, stability, and unconditional monotonicity. More precise discrete-analytical schemes are given in [1, 2].

## NUMERICAL SIMULATION OF BIOAEROSOL DYNAMICS

An algorithm based on discrete-analytical schemes (4) and (5) was written in C++ [27]. Let us study how the dynamics of solution by the model from [24], which is defined by Eqs. (2) during the corresponding splitting phase, changes when adding the condensation processes (according to [23]), which compose the phase of splitting of Eq. (3). For this, let us compare the solutions by model (2) with the results of the model that consider only condensation processes (3) and with the results of the general numerical model (1). The following parameters of the model of processes [24] and grid domains are used in the numerical experiments:

$$\begin{gathered}
\eta=1.82\times10^{-8}\ \text{Pa s},\quad \rho_{\text{eff}}=10^3\ \text{kg/m}^3,\\
A_D=200\,\text{m}^2,\quad \delta_D=0.0001\ \text{m},\quad A_H=600\ \text{m}^2,\\
U_S=0.00002\ \text{m/s},\quad l=6.53\times10^{-8}\,\text{m},\\
T=298\ \text{K},\quad V=2000\,\text{m}^3,\\
D_i=10^{-5}\ \text{m}^2/\text{s},\quad M_i=0.1\ \text{kg/mole},\\
P_i-P_{\text{eq},i}=10^{-4}\,\text{Pa},\quad R=8.31\ \text{J/(mole K)},\\
N_0=200,\quad r_{\min}=0,\quad r_{\max}=10\times10^{-6}\,\text{m},\\
\Delta t=300\ \text{s},\quad T_{\max}=50\times3600\ \text{s}.
\end{gathered}$$

The initial distribution of the concentration is shown in Fig. 1. This is a Gaussian curve centered at $0.59\times10^{-6}$ m, with a standard deviation of $0.25\times10^{-6}$ m and the factor that ensures the $c(r,0)dr$ distribution maximum of $8\times10^6$ particle/m$^3$.

The solutions by models (2), (3), and (1) are compared in Fig. 2. It can be seen that the concentration maxima calculated by models (1) and (3) are in the inner points of the spatiotemporal region, which agree with the results from [23] in the properties of condensation processes.

In addition, the concentration in the coagulation–sedimentation–condensation model (Fig. 2c) decreases more rapidly than in the coagulation–sedimentation model (Fig. 2a).

The combined consideration of the coagulation and condensation/evaporation processes modifies the dynamics of particle distribution in the space of their radii. A gradual displacement of the initial mode in the

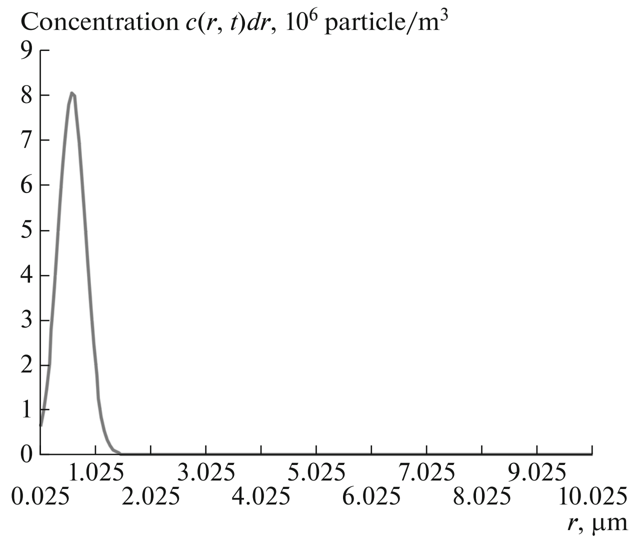


**Fig. 1.** Initial particle distribution over the radius.

particle spectrum toward large radii can be noted in the numerical experiments performed, while the initial mode remains in place in the coagulation–sedimentation model. In addition, it was found in the numerical experiments that the concentration decreases more rapidly in the presence of condensation/evaporation processes, which is important in the study of bioaerosol pollution processes.

## CONCLUSIONS

The new versions of the numerical models of aerosol dynamics are presented. The splitting method by physical processes of the coagulation and evaporation (condensation)–diffusion in the space of radii was used for the problem solution. This allowed consideration of all processes separately and estimation of the role of every process in the general problem. The explicit discrete-analytical scheme was constructed for the split step that corresponds to the coagulation processes. The possibility of effective parallelization is an advantage of the explicit schemes, which is also important for effective computations. Due to the exponential character, the scheme provides for the nonnegative and stable solution with nonnegative initial data and does not require time step fragmentation for this, in contrast to classical explicit Euler schemes.

The model is numerically compared with the models that take into account only coagulation or only evaporation (condensation)–diffusion processes. A higher speed of concentration decrease was obtained in the numerical experiments with participation of condensation/evaporation processes, which is important in the study of air pollution processes with bioaerosols and, especially, of air quality in closed rooms.

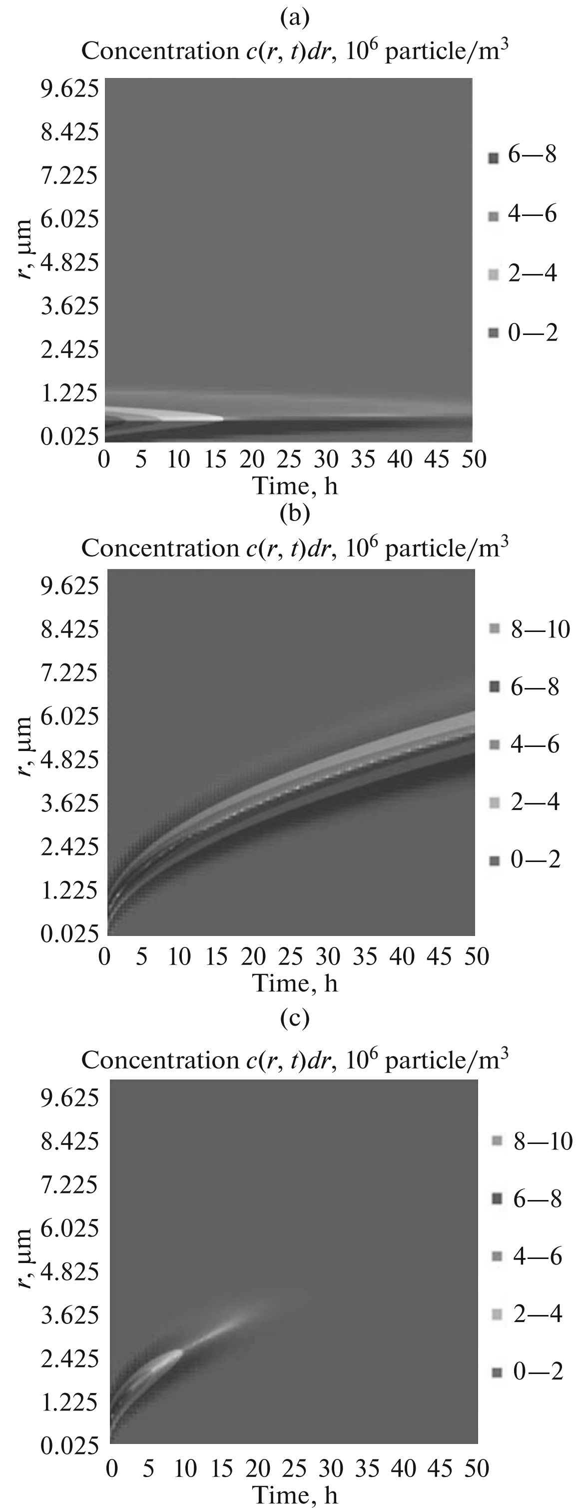


**Fig. 2.** Solution by (a) model (2), (b) model (3), and (c) model (1).

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