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A numerical model of bio-aerosols transformation in the atmosphere*

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Abstract. A non-stationary mathematical model of the bio-aerosols dynamics is considered. It is stated as the initial boundary value problem for integral-differential equation, describing the particle size spectrum dynamics with respect to coagulation, condensation and evaporation processes. The numerical scheme for solving the equation is presented. It is based on the splitting scheme and discrete analytical approximations with fundamental solutions of local adjoint problems.

Keywords: mathematical modeling, aerosol populations, pollutant transformation, coagulation, integral-differential equations, bio-aerosols.

1. Introduction

This paper is an extension of the research into discrete analytical schemes presented in [1–3]. We apply them to the aerosol dynamics problems. The currently used numerical methods for the aerosol dynamics modeling and a detailed literature review of the studies in this area are presented in [4]. By now, different versions of the Smoluchowski equation describe a variety of phenomena, such as bacterial growth [5], fish individual size schooling [6], astronomical phenomena [7, 8], evolution of aerosol compositions [9], and meteorological phenomena [10]. Presently, just several analytical solutions for certain cases are known. That is why many numerical methods of solving the Smoluchowski equation, such as the finite element method [11, 12], the finite difference methods based on special kernel presentations [13, 14], the finite volume methods [15, 16], successive approximations method [17], the moments method [18, 19], Monte Carlo methods [20, 21], and the grid less approach based on the radial functions [22] were developed. A detailed comparison of numerical methods is presented in [23]. In the current research we use discrete analytical schemes with applying the adjoint integrating factors [1, 2]. It has not been used for solving the Smoluchowski coagulation equation yet. The quasisteady-state Approximation (QSSA) method for solving problems of atmospheric chemistry [2] and exponential Runge-Kutta methods, are mainly used for solving parabolic equations [24].

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2. Problem statement

The model of aerosols transformation processes in the atmosphere depending on the particle sizes (including coagulation, evaporation or condensation and diffusion) is considered. It is presented as an initial-boundary value problem for an integral-differential equation according to [4, 25, 26]. The model time interval is $[0, T_{\max}]$, the particle sizes interval is $[r_{\min}, r_{\max}]$:

$$\begin{aligned}
&\frac{\partial c(r,t)}{\partial t} + [\alpha_D(r) + \alpha_S(r)]c(r,t) - \\
&\quad \frac{1}{2}\int_0^r K(q(r,r'),r')c(q(r,r'),t)c(r',t)w(r,r')\,dr' + \\
&\quad c(r,t)\int_0^{r_{\max}} K(r,r')c(r',t)\,dr' + \frac{\partial}{\partial r}(U(r)c(r,t)) - \\
&\quad \frac{\partial^2}{\partial r^2}(U_D(r)c(r,t)) = 0, \quad (r,t) \in (r_{\min}, r_{\max}) \times (0, T_{\max}), \qquad (1)\\
&\quad c(r_{\min},t) = c(r_{\max},t) = 0, \quad c(r,0) = c_0(r).
\end{aligned}$$

We study the dynamics of biologically active substances and, in this connection, designations and physical content of the main variables from (1) taken from [25, 27]: $c(r,t) \in Z(D_t)$ is concentration of suspended particles with radii in the range $[r, r+dr]$ in time moment t, $Z(D_t)$ is space of sufficiently smooth functions, $D_t = [r_{\min}, r_{\max}] \times [0, T_{\max}]$,

$$\begin{gathered}
q(r,r') = (r^3 - r'^3)^{1/3}, \quad w(r,r') = \frac{r^2}{q(r,r')^2},\\
K(r,r') = K_g(r,r') + K_B(r,r'),\\
K_g(r,r') = \pi\varepsilon(r+r')^2|U_S(r) - U_S(r')|,\\
K_B(r,r') = 4\pi kT(r+r')(B(r) + B(r')),\\
\alpha_D(r) = \frac{kTB(r)A_D}{\delta_D V}, \quad \alpha_S(r) = \frac{4}{3}\pi r^3\,\frac{\rho g B(r) A_H}{V}, \quad \varepsilon = \frac{r^2}{2(r+r')^2},
\end{gathered}$$

$K(r,r')$ is operator describing the process of particle coagulation, $K_g(r,r')$ is gravitational coagulation, $K_B(r,r')$ is the Brownian coagulation, k is the Boltzmann constant, T is temperature, A_D and A_S are vertical and horizontal deposition surfaces of the particles, α_D and α_S are particles removal rates, V is volume of aerosols localization, ρ is particle density, g is acceleration of gravity, δ_D is thickness of the boundary layer, η is gas viscosity, ε is effectiveness of particle collisions,

$$B(r) = \frac{\mathrm{Cn}(r)}{6\pi\eta r}, \quad \mathrm{Cn}(r) = 1 + 1.246\,\mathrm{Kn}(r) + 0.42\,\mathrm{Kn}(r)\exp\Big(-\frac{0.87}{\mathrm{Kn}(r)}\Big),$$

$$U(r) = 4\pi\Big(\frac{3}{4\pi\rho}\Big)^{1/3} D_g r C_\nu (S - \exp(\mathrm{Ke}(r)))\Big(1 + \frac{1.333\,\mathrm{Kn}(r) + 0.71}{1 + \mathrm{Kn}(r)^{-1}}\Big)^{-1},$$

$$U_S(r) = \frac{2\rho_{\mathrm{eff}} g}{9\eta} r^2\,\mathrm{Cn}(r), \quad \mathrm{Kn}(r) = \frac{l}{r}, \quad \mathrm{Ke}(r) = \frac{4\sigma\gamma}{2rkT},$$

$B(r)$ is mobility of the particles of radius r, $\mathrm{Cn}(r)$ is the Cunningham empirical correction factor, $U(r)$ is condensation growth rate, $U_S(r)$ is particles gravitational settling rate (Stokes' law), $U_D(r)$ is diffusion rate from kinetic theory, $\mathrm{Kn}(r)$ is the Knudsen number, $\mathrm{Ke}(r)$ is the Kelvin number, l is the mean free path of gas molecules, ρ_{eff} is effective density of spherical particles, $D_g = \frac{1}{3}vl$ is vapor diffusion coefficient, v is the mean molecular velocity, $S = \frac{C_*}{C_\nu}$ is super-saturation ratio, C_ν is vapor mass concentration in terms of the bulk liquid vapor pressure at system temperature T, C_* vapor mass concentration, σ is surface tension, and γ is molecular volume of particles.

The task of this study is to develop and to test an efficient numerical scheme keeping solution positiveness, and to apply the developed scheme to the simulation of the aerosol population dynamics.

3. Numerical scheme

We will consider problem (1) over the time interval $t_j \le t \le t_{j+1}$; $(r,t) \in (r_{\min}, r_{\max}) \times (t_j, t_{j+1})$. Let us introduce a grid domain on $[0,T]$ and split (1) with respect to physical processes [28]:

$$\frac{\partial c_1(r,t)}{\partial t} + A(c_1(r,t),r,t)c_1(r,t) = f(r,t), \tag{2}$$

$$c_1(r,t_j) = c(r,t_j), \;\; c_1(r_{\min},t_j) = c_1(r_{\max},t_j) = 0, \;\; c_1(r,0) = c_0(r), \tag{3}$$

$$\frac{\partial c_2(r,t)}{\partial t} + (\alpha_D(r) + \alpha_S(r))c_2(r,t) + \frac{\partial}{\partial r}(U(r)c_2(r,t)) - \frac{\partial^2}{\partial r^2}(U_D(r)c_2(r,t)) = 0, \tag{4}$$

$$c_2(r,t_j) = c_1(r,t_{j+1}), \;\; c_2(r_{\min},t_j) = c_2(r_{\max},t_j) = 0, \;\; c(r,t_{j+1}) = c_2(r,t_{j+1}). \tag{5}$$

At the first splitting stage we solve the equation that describes the coagulation process, the result is treated as the initial value for the second stage (as concentration from the previous step). Then we solve the second equation, obtaining the result that is treated as the solution at the end of the interval $[t_j, t_{j+1}]$. Repeat this cycle till the end of sub-intervals.

In the following sections, numerical algorithms by which we solve problems (2)–(5) are presented.

3.1. Numerical schemes for the coagulation equation. In order to obtain numerical schemes for (1), we use the variation principle described in [2]. We compose an integral identity for (2) with the function $c^* \in Z(D_t)$:

$$\int_{t_j}^{t_{j+1}} \Big(\frac{\partial c(r,t)}{\partial t} + A(c,r,t)c(r,t) - F(c,r,t) \Big) c^*(r,t)\, dt = 0, \tag{6}$$

where

$$A(c,r,t) = \int_{r_{\min}}^{r_{\max}} K(r,r')c(r',t)\, dr',$$

$$F(c,r,t) = \int_{r_{\min}}^{r} K((r^3 - r'^3)^{1/3}, r')c((r^3 - r'^3)^{1/3}, t)c(r,t) \frac{r^2}{(r^3 - r'^3)^{2/3}}\, dr'.$$

Let us introduce grids on the intervals $[0, T_{\max}]$, $[r_{\min}, r_{\max}]$:

$$\omega_t^h = \big\{ t_j = t_{j-1} + \Delta t_j,\ t_0 = 0,\ t_{J_0} = T_{\max},\ j = \overline{1, J_0} \big\},$$
$$\omega_r^h = \{ r_k = r_{k-1} + \Delta r_k,\ r_0 = r_{\min},\ r_{N_0} = r_{\max},\ k = \overline{1, N_0} \},$$

where N_0 is the number of particles ranges.

Integrating identity (6) by parts, we obtain

$$c(r_k,t)c^*(r_k,t)\big|_{t_j}^{t_{j+1}} + \int_{t_j}^{t_{j+1}} \Big(-\frac{\partial c^*(r_k,t)}{\partial t} c(r_k,t) + A(c,r_k,t)c(r_k,t)c^*(r_k,t) \Big) dt = \int_{t_j}^{t_{j+1}} F(c,r_k,t)c^*(r_k,t)\, dt. \tag{7}$$

To simplify expression (7), we choose c^* from the solution of the local adjoint problems [3]:

$$\frac{\partial c^*(r_k,t)}{\partial t} - A(c,r_k,t)c^*(r_k,t) = 0, \quad c^*(r_k,t_{j+1}) = 1,$$

which can be approximated as

$$c^*(r_k,t) \simeq e^{A(c,r_k,t_j)(t-t_{j+1})}. \tag{8}$$

After this we obtain a discrete analytical expression for the concentration at the step $j+1$:

$$c(r_k, t_{j+1}) = c(r_k, t_j)c^*(r_k, t_j) + \int\limits_{t_j}^{t_{j+1}} F(c, r_k, t)c^*(r_k, t)\, dt.$$

Replacing $c^*(r_k, t)$ with its approximation from (8), we arrive at

$$c(r_k, t_{j+1}) = c(r_k, t_j)e^{A(c,r_k,t_j)(t_j - t_{j+1})} + \int\limits_{t_j}^{t_{j+1}} F(c, r_k, t)e^{A(c,r_k,t_j)(t-t_{j+1})}\, dt. \quad (9)$$

Now we replace integrals in the operators A and F with their discrete analogues (obtained with the method of trapezoids [29]):

$$A(c, r_k, t) = \int\limits_{r_{\min}}^{r_{\max}} K(r_k, r')c(r', t)dr' \simeq$$

$$\bar{A}(c, r_k, t) = \sum_{i=1}^{N_0} \frac{K(r_k, r_i)c(r_i, t) + K(r_k, r_{i+1})c(r_{i+1}, t)}{2}\Delta r_k,$$

$$F(c, r_k, t) = \frac{1}{2}\int\limits_{r_{\min}}^{r_k} K(q(r_k, r'), r')c(q(r_k, r'), t)c(r', t)w(r_k, r')\, dr' \simeq$$

$$\bar{F}(c, r_k, t) = \frac{1}{4}\sum_{i=1}^{k-1}\Big\{K(\bar{q}(r_k, r_i), r_i)c(\bar{q}(r_k, r_i), t)c(r_i, t)w(r_k, r_i) +$$

$$K(\bar{q}(r_{k+1}, r_{i+1}), r_{i+1})c(\bar{q}(r_{k+1}, r_{i+1}), t)c(r_{i+1}, t)w(r_{k+1}, r_{i+1})\Big\}\Delta r_k,$$

where

$$q(r_k, r') = (r_k^3 - r'^3)^{1/3}, \quad w(r_k, r') = \frac{r_k^2}{(r_k^3 - r'^3)^{2/3}},$$
$$\bar{q}(r_k, r_i) = \arg\min_{r \in \omega_r^h} |q(r_k, r_i) - r|.$$

For approximation of equation (9), we use the single-stage numerical scheme presented in [1, 2, 30]:

$$c(r_k, t_{j+1}) = c(r_k, t_j)e^{-\bar{A}(c,r_k,t_j)\Delta t} + \frac{1 - e^{-\bar{A}(c,r_k,t_j)\Delta t}}{\bar{A}(c, r_k, t_j)\Delta t}\bar{F}(c, r_k, t_j)\Delta t, \quad (10)$$

$k = \overline{1, N_0}$. We choose Δt from the condition of expression $e^{-\bar{A}(c,r_k,t_j)\Delta t}$ significance:

$$|\bar{A}(c, r_k, t_j)\Delta t| \le 1.$$

3.2. The process of vaporization (condensation). The full convection-diffusion model is the following:

$$\frac{\partial c(r,t)}{\partial t} + (\alpha_D(r) + \alpha_S(r))c(r,t) + \frac{\partial}{\partial r}(U(r)c(r,t)) - \frac{\partial^2}{\partial r^2}(U_D(r)c(r,t)) = 0.$$

According to [25], the diffusion term can be neglected because of its non-significant contribution. Then we will consider the model

$$\frac{\partial c(r,t)}{\partial t} + (\alpha_D(r) + \alpha_S(r))c(r,t) + \frac{\partial}{\partial r}(U(r)c(r,t)) = 0.$$

For the difference scheme we use the Godunov upwind scheme, described in [31]. We obtain the difference scheme of the first order of accuracy:

$$\frac{c(r_k,t_{j+1}) - c(r_k,t_j)}{\Delta t} + (\alpha_D(r_k) + \alpha_S(r_k))c(r_k,t_{j+1}) +$$
$$U^+\frac{c(r_k,t_{j+1}) - c(r_{k-1},t_{j+1})}{\Delta r} + U^-\frac{c(r_k,t_{j+1}) - c(r_{k+1},t_{j+1})}{\Delta r} = 0, \quad (11)$$
$$U^+ = \frac{|U(r_k)| + U(r_k)}{2}, \quad U^- = \frac{|U(r_k)| - U(r_k)}{2}, \quad k = \overline{1, N_0}.$$

As a result, we obtain the concentration value $c(r, t_{j+1})$. The equations system is solved by the three-point sweep method [32].

4. Algorithm validation on analytical solutions of the Smoluchowski equation

In order to check algorithms, we will apply the numerical scheme obtained to the problem having an analytical solution. Equation (2) is written down in radii variables:

$$\frac{\partial c(r,t)}{\partial t} + c(r,t)\int_0^{r_{\max}} K(r,r')c(r',t)\,dr'$$
$$= \frac{1}{2}\int_0^r K((r^3 - r'^3)^{1/3}, r')c((r^3 - r'^3)^{1/3}, t)c(r',t)\frac{r^2}{(r^3 - r'^3)^{2/3}}\,dr'. \quad (12)$$

Usually, it is studied in volume variables and is known as the Smoluchowski equation. Let us show the equivalence of the equations in radii and volume variables according to [25]. Denote

$$I_1 = \int_0^r K((r^3 - r'^3)^{1/3}, r')c((r^3 - r'^3)^{1/3}, t)c(r',t)\frac{r^2}{(r^3 - r'^3)^{2/3}}\,dr',$$

$$I_2 = \int_0^{r_{\max}} K(r, r')c(r', t)\, dr'.$$

In order to reduce (12) to the equation in volume variables, we make use of the relation between radii and volume:

$$V = \frac{4}{3}\pi r^3, \quad V' = \frac{4}{3}\pi r'^3, \quad dV' = d\Big(\frac{4}{3}\pi r'^3\Big) = 4\pi r'^2 dr'.$$

In addition, according to [25] there are the following relations between concentrations in volume variables and concentrations in radii variables:

$$c(r, t) = 4\pi r^2 c_v(V, t), \quad c(r', t) = 4\pi r'^2 c_v(V', t),$$
$$c((r^3 - r'^3)^{1/3}, t) = 4\pi(r^3 - r'^3)^{2/3} c_v(V - V', t), \quad K(r, r') = \bar{K}(V, V').$$

Then integrals I_1 and I_2 take the form:

$$I_1 = r^2 \int_0^V \bar{K}(V - V', V') \frac{4\pi(r^3 - r'^3)^{2/3} c_v(V - V', t)}{(r^3 - r'^3)^{2/3}} 4\pi r'^2 c_v(V', t) \frac{dV'}{4\pi r'^2},$$
$$I_2 = \int_0^{V_{\max}} \bar{K}(V, V') 4\pi r'^2 c_v(V', t) \frac{dV'}{4\pi r'^2}.$$

Equation (12) takes the form

$$4\pi r^2 \frac{\partial c_v(V, t)}{\partial t} = \frac{1}{2} I_1 - 4\pi r^2 c_v(V, t) I_2.$$

Finally, we will obtain

$$\frac{\partial c_v(V, t)}{\partial t} = \frac{1}{2} \int_0^V \bar{K}(V - V', V') c_v(V - V', t) c_v(V', t)\, dV' -$$
$$c_v(V, t) \int_0^{V_{\max}} \bar{K}(V, V') c_v(V', t)\, dV'. \tag{13}$$

When $V_{\max}(r_{\max})$ tends to ∞, equation (13) takes the form of the Smoluchowski equation. Analytical solutions of the Smoluchowski equation for some $\bar{c}_v(x, 0)$ and $\bar{K}(x, y)$ are provided in [33]. Let us present them here:

4.1. The case $\bar{K}(x, y) = 1$. If $\bar{c}_v(x, 0) = \exp(-x)$, then

$$\bar{c}_v(x, t) = N^2(t) \exp(-N(t)x), \quad N(t) = \frac{2}{2 + t}.$$

4.2. The case $\bar{K}(x,y) = xy$. If $\bar{c}_v(x,0) = \exp(-x)/x$, then

$$\bar{c}_v(x,t) = \exp(-T(t)x)\frac{I_1(2xt^{1/2})}{x^2t^{1/2}},$$

where

$$T(t) = \begin{cases} 1+t, & t \le 1, \\ 2t^{1/2}, & t > 1, \end{cases} \quad I_1(x) = \frac{1}{\pi}\int\limits_0^\pi \exp(x\cos\theta)\cos\theta\, d\theta.$$

4.3. The case $\bar{K}(x,y) = x + y$. If $\bar{c}_v(x,0) = \frac{1}{2\pi x^{3/2}}\exp(-x/2)$, then

$$\bar{c}_v(x,t) = \frac{\exp(-t)}{2\pi x^{3/2}}\exp(-\exp(-2t)x/2).$$

We verify the effectiveness of the proposed method using the exact solutions presented in Cases 4.1–4.3. The above-described method of calculation has been implemented in C++. The results are shown in the table. The order of a relative error $\|\bar{c}_v(r,t) - c_v(r,t_{j+1})\|/\|\bar{c}_v(r,t)\|$ is presented depending on the time step Δt, where the norm of the space L_2 is used. The number of radii ranges is 5000.

Accuracy of the Smoluchowski equation solution obtained by the discrete analytical method from 3.1

Case	Δt							
	10^{-8}	10^{-7}	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}
4.1	10^{-10}	10^{-9}	10^{-8}	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}
4.2	10^{-12}	10^{-11}	10^{-10}	10^{-9}	10^{-6}	10^{-5}	10^{-4}	10^{-3}
4.3	10^{-8}	10^{-7}	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}

5. Numerical modeling of bio-aerosols dynamics

Algorithm based on proposed discrete analytical scheme (10), (11) was developed in C++ language. The functions $K(r_i, r_k)$, $\alpha_D(r)$, $\alpha_S(r)$, $U(r,t)$, and $U_D(r,t)$ are set according to the definitions of Section 2. The following values were used in the numerical experiments:

$$\begin{gathered} \eta = 1.82\cdot 10^{-8}\ \text{Pa}\cdot\text{s}, \quad \rho_{\text{eff}} = 10^3\ \text{kg/m}^3, \quad \rho = 1\ \text{kg/m}^3, \\ A_D = 200\ \text{m}^2, \quad A_S = 600\ \text{m}^2, \quad U_S = 0.00002\ \text{m/s}, \\ l = 6.53\cdot 10^{-8}\ \text{m}, \quad T = 298\ \text{K}, \quad V = 2000\ \text{m}^3, \\ \sigma = 3.5\cdot 10^{-4}\ \text{N/m}, \quad S = 1.0379, \quad N_0 = 300, \\ C_\nu = 1.5496\cdot 10^{-11}\ \text{kg/m}^3, \quad C_* = 1.6083\cdot 10^{-11}\ \text{kg/m}^3. \end{gathered} \tag{14}$$

In [34], aerosols of the biological origin are under consideration. According to this classification, various bio-aerosols categories can be specified by characteristic parameters — concentration in the air, mass concentration, aerosol particles radii sizes. The proposed numerical algorithm for solving (1) was tested on two species of bio-aerosols — pollen and bacteria.

For the numerical modeling of pollen species, the following input values are used according to [34]:

$$\begin{aligned} &r_{\min} = 10^{-6} \text{ m}, \quad r_{\max} = 40 \cdot 10^{-6} \text{ m}, \quad T_{\max} = 3 \cdot 10^{7} \text{ s}, \\ &\Delta t = 5 \cdot 10^{4} \text{ s}, \quad \min c(r_k, t) = 10 \text{ m}^{-3}, \quad \max c(r_k, t) = 10^{3} \text{ m}^{-3}. \end{aligned} \tag{15}$$

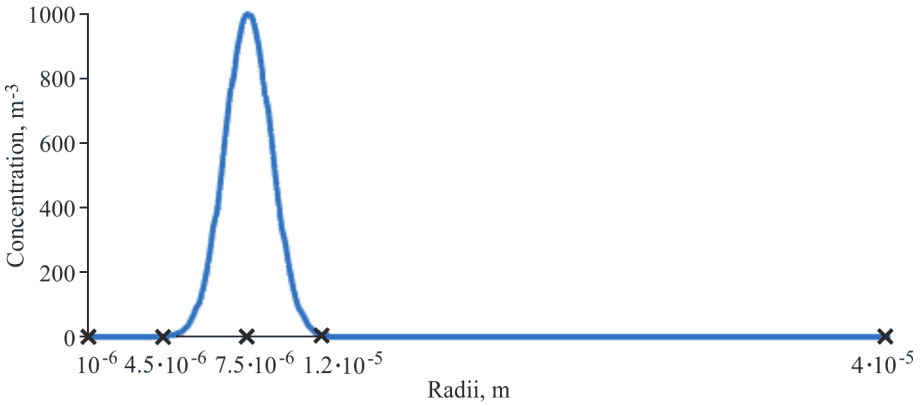

Figure 1. Initial distribution of pollen

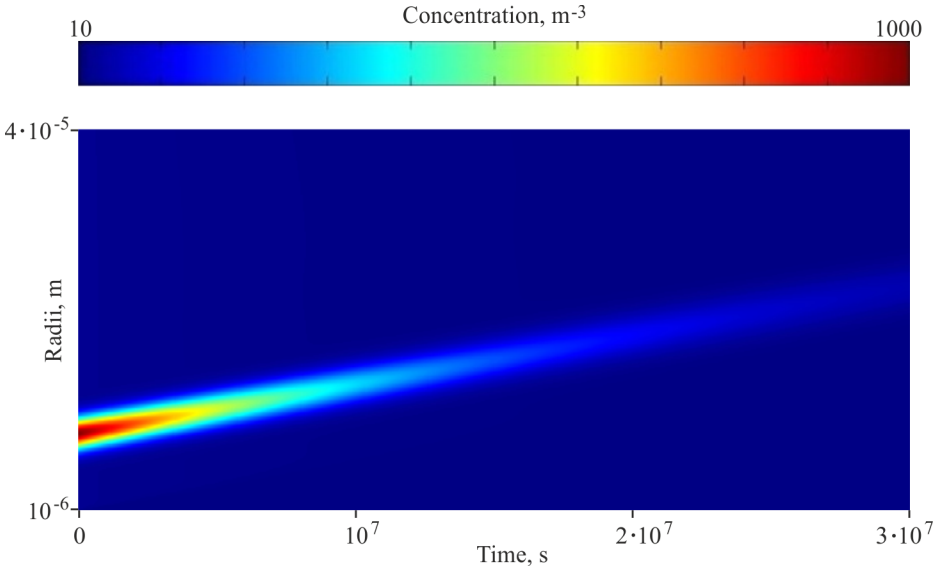

Figure 2. Solution of (1) with the parameters (14), (15)

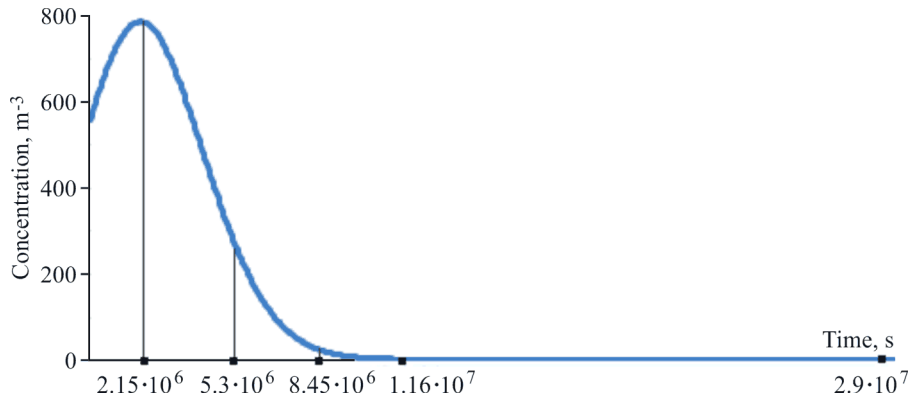

Figure 3. Cross-section of 10 micrometer radii particles for the solution of (1) with the parameters (14), (15)

The initial distribution and the solution are shown in Figures 1–3.

For the numerical modeling of bacteria species, the following parameters are chosen according to [34]:

$$r_{\min} = 0.1 \cdot 10^{-6} \text{ m}, \quad r_{\max} = 10 \cdot 10^{-6} \text{ m}, \quad T_{\max} = 6 \cdot 10^{6} \text{ s},$$
$$\Delta t = 10^{4} \text{ s}, \quad \min c(r_k, t) = 10^{2} \text{ m}^{-3}, \quad \max c(r_k, t) = 10^{4} \text{ m}^{-3}. \tag{16}$$

The initial distribution and the solution are shown in Figures 4–6.

In Figures 3 and 6, the upper boundaries for health-related particles ranges less than 10 and 2.5 micrometer are presented. In the carried out experiments, the respirable suspended particles concentration increases in the beginning of the experiment and then decays. As we can see from

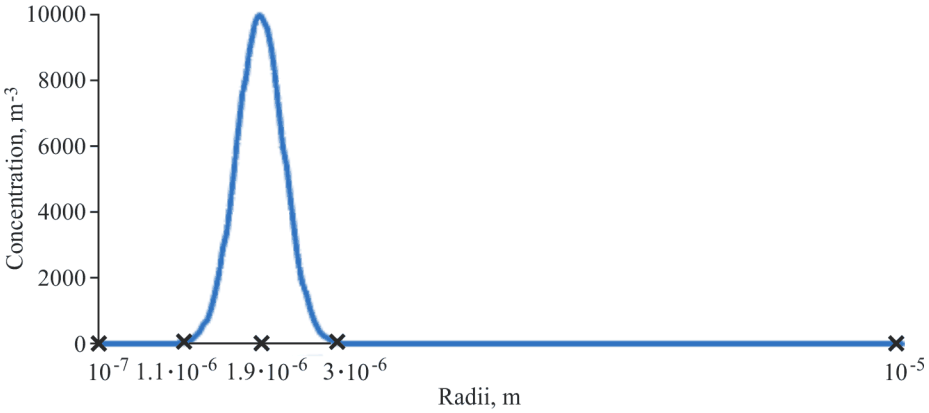

Figure 4. Initial distribution of bacteria

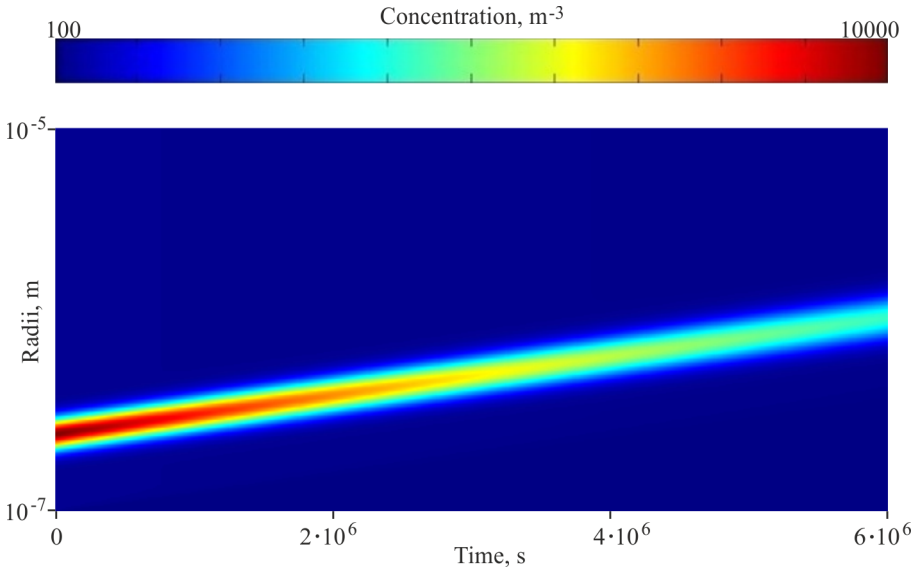

Figure 5. Solution of (1) with the parameters (14), (16)

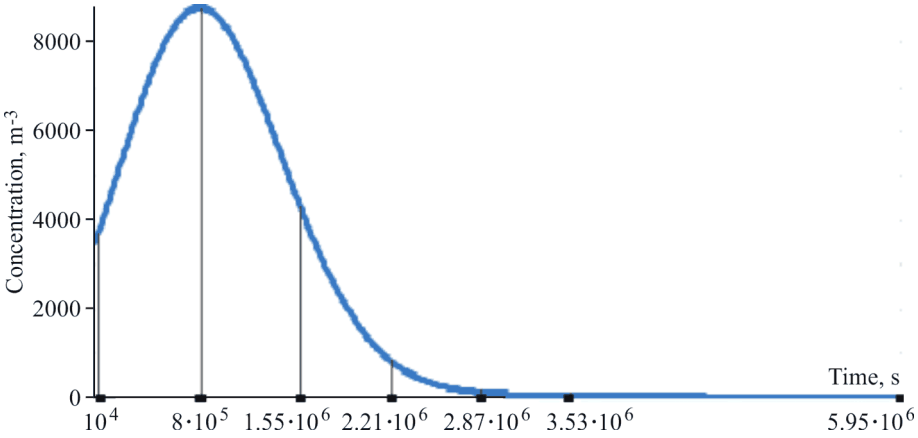

Figure 6. Cross-section of 2.5 micrometer radii particles for the solution of (1) with the parameters (14), (16)

Figures 3 and 6, the time scale of pollen and bacteria reaction duration are measured in months, and in [27] it is measured in hours. This difference is explained by different orders of initial concentrations: in our bio-aerosols experiment maximal concentration has 10^4 order, in [27] — 10^8. Note that the duration of the reaction with a bigger amount of particles is lesser. The time scale revealed in the experiments can correspond to the long-range (global) bio-aerosols atmospheric transport processes.

6. Conclusion

The discrete-analytical scheme approach has been applied to the aerosol populations dynamic model. The splitting technique was used to split the model to physical processes: coagulation and evaporation. The splitting scheme allows building efficient algorithms for complex problems. For the splitting step, corresponding to coagulation processes, the explicit discrete-analytical scheme has been built. The time step restriction for this scheme is weaker than it is for standard explicit schemes. Moreover, the scheme provides non-negative solutions for non-negative initial data. The algorithms check has been done for the Cauchy–Smoluchowski problem with three versions of the coagulation kernel, whose exact analytical solutions are known. The comparison of calculations results has shown algorithm efficiency. The results of calculation with realistic parameters values for the bio-aerosols dynamics model are presented.

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