

MATHEMATICAL MODELS AND SIMULATION IN ENVIRONMENT

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Contents

1. Introduction
 2. Mathematical model for regional transport and transformations of gaseous pollutants and aerosols
 - 2.1. Main Equations of Atmospheric Thermo-hydrodynamics
 - 2.2. Atmospheric Surface Layer Model and Heat-balance Equation
 - 2.3. Turbulent Exchange Coefficients
 - 2.4. Initial and Boundary Conditions
 - 2.5. Numerical Model of Transport and Transformations of Multicomponent Gaseous Pollutants and Aerosols.
 - 2.6. Gas and Aerosol Fluxes in the Atmospheric Surface Layer.
 - 2.7. Initial and Boundary Conditions
 - 2.8. Photochemical Model
 - 2.9. Nucleation and Condensation/Evaporation Model
 - 2.10. Coagulation Model
 3. Application of the combined model of atmospheric thermo-hydrodynamics and pollution transport to solving specific environmental problems.
 - 3.1. Secondary Photochemical Air Pollution
 - 3.2. Formation of Primary Aerosols in the Atmosphere due to Kinetic Processes of Nucleation, Condensation, and Coagulation
 4. Numerical model of global transport and transformations of multicomponent gaseous pollutants and aerosols
 - 4.1. Binary Homogeneous Nucleation
 - 4.2. Photochemical Transformations in the Upper Troposphere and Stratosphere
 - 4.3. Formation of Sulfuric Aerosol Contrails in the Atmosphere of the Northern Hemisphere.
- Acknowledgements
Glossary
Bibliography
Biographical Sketches

Summary

Human economic activities result in emission of a great number of gaseous and aerosol pollutants into the atmosphere. Then, these species pass through a series of transformations that lead to formation of more toxic species than the original emissions. All these mechanisms are connected with one another, forming part of the general environmental protection problem. Among the anthropogenic emissions, nitrogen and sulfur oxides, metallic dust etc. are of particular importance. For example, sulfuric oxide in the atmosphere can transform into the aerosol phase and give rise to acid rain, which is harmful to the biosphere. Also, they bring about smog-inherent toxic effects. To describe these processes in solving environmental protection problems, complex mathematical models are needed. These models include modules for regional atmospheric thermohydrodynamics, transport, diffusion, and transformation of gasses and aerosols, as well as kinetic processes of nucleation, condensation/evaporation, and coagulation.

In the photochemical transformation model, anthropogenic nitrogen-sulfur-carbon species emissions typical for large industrial areas are accounted for and spatio-temporal variability of secondary environmental pollutions is studied. The kinetic models of condensation and coagulation allow one to study the new-particle formation and their further growth, which leads to aerosol formation and development in the environment. The results of numerical experiments performed using these models are demonstrated for specific environmental applications in the regional and global scales.

1. Introduction

At present, aerosol particles are undoubtedly known to play a critical role in forming the physical and chemical state of the atmosphere. However, many atmospheric aerosol related processes have not yet been clearly understood. In particular, the micro-to-macro-scale transition path has not yet been fully studied. The impact of aerosol macrotransport on microprocesses, which control essentially the composition and size distribution of aerosols, is treated in a very simplified form. The macroscopic transport and atmospheric turbulence play an important role in setting boundary conditions far away from the particle surface. Particularly, the turbulence results in fluctuations of condensing particle concentrations as well as in spontaneous generation of particles, whose concentration fluctuations lead to formation of super-critical particles in the atmosphere. Currently, this mechanism of particle formation has not been clearly studied. So, some difficulties arise in constructing complex mathematical models (consisting of dynamical and turbulence factors, generation, transformation, and removal of gases and aerosols, gas- and aqueous-phase chemistry, and atmospheric circulation). Also, there is no reliable estimate for the influence of particle size distribution on the oxidation processes in liquid particles and for the role of turbulent fluctuations in condensation, coagulation, and photochemistry.

The atmosphere is a complex dynamical system with a number of different physical and chemical processes whose intensity depends on the features of a specific region and latitude-longitude-altitude localization. The gas-phase chemical reactions take place with some intensity in the bulk of the atmosphere, while the heterogeneous reactions

occur only on the surfaces of liquid and solid particles in the troposphere and stratosphere. It should be noted that the natural aerosols play a significant role in the chemistry of the lower stratosphere: stratospheric sulfate aerosols (SSA), triple supercooled solution particles, and polar stratospheric clouds as cooled solution (PSC-1) and as crystalline (PSC-2). At midlatitude temperatures ($205^{\circ} < T < 220^{\circ}$ K), the SSA exist as binary supercooled solutions of $\text{H}_2\text{SO}_4/\text{H}_2\text{O}$. The formation and removal of aerosol particles are due to a number of processes: nucleation, condensation / evaporation, coagulation, gas- and aqueous-phase chemical transformations, thermo-hydrodynamical processes, interphase exchange, dry and wet deposition, etc. The chemical composition of particles mainly depends on size distribution, which is of great significance for aerosols physics and atmospheric chemistry. In the atmosphere, sulfate aerosols are of particular importance; they can have climate effects both directly and indirectly. These particles are formed in different parts of the atmosphere: free troposphere, marine boundary layer, Arctic region, etc. Numerical experiments indicate that new sulfate particles can nucleate both in the stratosphere and urban polluted air; they are formed through homogenous nucleation, for example, of water and sulfuric acid. Aerosol particle size distribution is known to be affected by coagulation and gas-to-particle conversion. Gas-to-particle conversion rate can be determined from the rate of diffusion of vapor molecules to the surface of particle and the rate of reaction between a molecule of the adsorbed vapor and a species of the particle surface.

Most three-dimensional aerosol dynamics models assume an instantaneous equilibrium in the gas-aerosol system. However, under some conditions, this equilibrium is established rather slowly relative to the timescales of other processes. Thus, it is necessary to use a non-equilibrium distribution function in the numerical models, which are required to meet the laws of particle mass-number conservation.

In modeling the aerosol formation processes, the species resulting in photochemical transformations are of prime importance. Saturation of these species' vapors leads to formation of primary clusters and aerosols. Then, they can interact with the nuclei of the background atmosphere uniting with some water drops and later coagulating. The regional and global-scale mathematical models that describe these processes account for the photochemical transformations and kinetic processes of nucleation, condensation/evaporation, and coagulation. Aerosol size distribution is given for 25 bins starting from 10^{-5} μm with doubling the subsequent sizes. The model includes SO_2 - H_2SO_4 oxidation through a series of photochemical reactions. At certain levels, this brings about supersaturation of SO_2 - H_2SO_4 and later deposition onto the surfaces of condensation nuclei. Depending on the location and physical medium, the drops can either grow in size or evaporate; in the latter case, their interiors turn to be solid nuclei. Now let us consider numerical models for the gas-aerosol interaction in the regional and global scales.

2. Mathematical Model for Regional Transport and Transformations of Gaseous Pollutants and Aerosols.

Since the atmospheric pollutants generally have multiple dispersion character; their dynamics can be mathematically simulated using the following two mechanisms: (1) pollution transport and diffusion, (2) change of concentrations of gaseous species

through photochemical transformations and variation of aerosol size distribution and concentration through kinetic processes of nucleation, condensation, coagulation, etc. As these processes take place in the turbulent atmosphere and the earth's surface is generally inhomogeneous (orographically and thermally), the gas-aerosol dynamics model should be combined with thermohydrodynamical models. This approach allows a more comprehensive reproduction of the spatial and temporal variations of the meteorological variables, turbulent characteristics and aerosol features.

2.1. Main Equations of Atmospheric Thermo-hydrodynamics

The model is based on the thermo-hydrodynamic equations for the regional-scale atmospheric processes. To take into account the orography here we turn from the Cartesian system of coordinates (x, y, z) to the generalized system $(\bar{x}, \bar{y}, \sigma)$ with the help of the following formulas:

$$x = \bar{x}, \quad y = \bar{y}, \quad \sigma = \frac{z - \tilde{\zeta}(x, y)}{H - \zeta(x, y)} \hat{H}, \quad (1)$$

where H and \hat{H} - are heights of the upper boundary in the z - and σ - system of coordinates, respectively; $\tilde{\zeta}(x, y)$ - is a function describing the relief.

The equations in the new system of coordinates take the form

$$\frac{\partial \hat{u}}{\partial t} + \text{div} \bar{u} \hat{u} = - \frac{\partial p}{\partial x} + a_1 \frac{\partial p}{\partial \sigma} + 1 \hat{v} + F_u \quad (2)$$

$$\frac{\partial \hat{v}}{\partial t} + \text{div} \bar{u} \hat{v} = - \frac{\partial p}{\partial y} + a_2 \frac{\partial p}{\partial \sigma} + 1 \hat{u} + F_v \quad (3)$$

$$\frac{\partial \hat{w}}{\partial t} + \text{div} \bar{u} \hat{w} = - a_3 \frac{\partial p}{\partial \sigma} + \lambda \vartheta (1 + 0.61q) + F_w \quad (4)$$

$$\frac{\partial \hat{\vartheta}}{\partial t} + \text{div} \bar{u} \hat{\vartheta} + \frac{S}{a_3} (\hat{w} + \tilde{\zeta}_x \hat{u} + \tilde{\zeta}_y \hat{v}) = \frac{L_w \Phi \bar{\rho}}{C_p} + F_\vartheta \quad (5)$$

$$\frac{\partial \hat{q}}{\partial t} + \text{div} \bar{u} \hat{q} = - a_3 \hat{w} \frac{\partial Q}{\partial \sigma} - \Phi \bar{\rho} + F_q \quad (6)$$

$$\frac{\partial \hat{u}}{\partial x} + \frac{\partial \hat{v}}{\partial y} + \frac{\partial \hat{w}}{\partial \sigma} = 0 \quad (7)$$

Here the following notation is used:

$$\operatorname{div} \bar{u} \hat{\varphi} = \frac{\partial u \hat{\varphi}}{\partial x} + \frac{\partial v \hat{\varphi}}{\partial y} + \frac{\partial w \hat{\varphi}}{\partial \sigma}, \hat{\varphi} = \rho \varphi, \varphi = (u, v, w, \vartheta, q), \tilde{\zeta}_x = \frac{\partial \tilde{\zeta}}{\partial x}, \tilde{\zeta}_y = \frac{\partial \tilde{\zeta}}{\partial y} \quad (8)$$

F_u, F_v, F_w are the turbulent fluxes for wind components:

$$F_u = \frac{\partial \tau_{11}}{\partial x} + \frac{\partial \tau_{12}}{\partial y} + \frac{\partial}{\partial \sigma} (a_1 \tau_{11} + a_2 \tau_{12}) + a_3^2 \frac{\partial}{\partial \sigma} \rho v_u \frac{\partial}{\partial \sigma} \left(\frac{\hat{u}}{\bar{\rho}} \right) \quad (9)$$

$$F_v = \frac{\partial \tau_{21}}{\partial x} + \frac{\partial \tau_{22}}{\partial y} + \frac{\partial}{\partial \sigma} (a_1 \tau_{21} + a_2 \tau_{22}) + a_3^2 \frac{\partial}{\partial \sigma} \rho v_u \frac{\partial}{\partial \sigma} \left(\frac{\hat{v}}{\bar{\rho}} \right) \quad (10)$$

$$F_w = \frac{\partial \tau_{31}}{\partial x} + \frac{\partial \tau_{32}}{\partial y} + \frac{\partial}{\partial \sigma} (a_1 \tau_{31} + a_2 \tau_{32}) + a_3^2 \frac{\partial}{\partial \sigma} \rho v_u \frac{\partial}{\partial \sigma} \left(\frac{\hat{w}}{\bar{\rho}} \right) \quad (11)$$

F_q and F_ϑ are the turbulent fluxes for heat and moisture respectively :

$$F_\vartheta = \frac{\partial H_1}{\partial x} + \frac{\partial H_2}{\partial y} + \frac{\partial}{\partial \sigma} (a_1 H_1 + a_2 H_2) + a_3^2 \frac{\partial}{\partial \sigma} \rho v_\vartheta \frac{\partial}{\partial \sigma} \left(\frac{\hat{\vartheta}}{\bar{\rho}} \right) \quad (12)$$

$$F_q = \frac{\partial Q_1}{\partial x} + \frac{\partial Q_2}{\partial y} + \frac{\partial}{\partial \sigma} (a_1 Q_1 + a_2 Q_2) + a_3^2 \frac{\partial}{\partial \sigma} \rho v_q \frac{\partial}{\partial \sigma} \left(\frac{\hat{q}}{\bar{\rho}} \right) \quad (13)$$

$$a_1 = \tilde{\zeta}_x \frac{\sigma - \hat{H}}{H - \tilde{\zeta}(x, y)}, \quad a_2 = \tilde{\zeta}_y \frac{\sigma - \hat{H}}{H - \tilde{\zeta}(x, y)}, \quad a_3 = \frac{\hat{H}}{H - \tilde{\zeta}(x, y)} \quad (14)$$

The following commonly – employed notation is used in the equations above: t is the time; u, v, w are wind velocity vector components along x, y, σ ; $\bar{u} = (u, v, w)$; ϑ is the potential temperature; ρ is the density; l the Coriolis parameter; q is the specific humidity; L_w is the latent heat of condensation; Φ is the water condensation rate; S is the stratification parameter; $\lambda = g/T$ is the buoyancy parameter; $\gamma = 0.61$; $\bar{\rho}(z)$ is the background density; τ_{ij}, h_i, Q_i ($i=1,2,3; j=1,2$) are the Reynolds viscous stress tensor and turbulent flows of heat and moisture; v_u, v_ϑ, v_q are the vertical turbulent coefficients for the moments of momentum, heat, and moisture.

2.2. Atmospheric Surface Layer Model and Heat-balance Equation

The structure of the lower atmospheric layer is described within the Monin-Obukhov similarity theory and the Businger empirical functions. The surface layer model can be written as:

$$\varkappa z \frac{\partial |\vec{u}|}{\partial z} = u_* \varphi_u(\zeta), \quad \varkappa \frac{\partial \vartheta}{\partial z} = \vartheta_* \varphi_\vartheta(\zeta), \quad \varkappa \frac{\partial q}{\partial z} = q_* \varphi_q(\zeta) \quad (15)$$

$$\begin{aligned} \varkappa |\vec{u}| &= u_* f_u(\zeta, \zeta_u), \quad \vartheta - \vartheta_0 \\ &= \vartheta_* f_\vartheta(\zeta, \zeta_\vartheta), \quad q - q_0 = q_* f_q(\zeta, \zeta_q), \quad \zeta = \frac{z}{L}, \quad \zeta_h = \frac{h}{L} \end{aligned} \quad (16)$$

$$v_i = \frac{u_* \varkappa z}{u_i(\zeta)}, \quad (v_i)_h = \frac{u_* \varkappa h}{\psi_i(\zeta_h)}, \quad a_i = \frac{\psi_i(\zeta)}{f_i(\zeta_h, \zeta_i)}, \quad L = -\frac{u_*^2}{\varkappa^2 \lambda \varphi_*}, \quad (17)$$

$$f_u(\zeta, \zeta_0) = \int_{\zeta_0}^{\zeta} \frac{\varphi_u(\zeta)}{\zeta} d\zeta, \quad f_\vartheta(\zeta, \zeta_0) = \int_{\zeta_0}^{\zeta} \frac{\varphi_\vartheta(\zeta)}{\zeta} d\zeta \quad (18)$$

where $|\vec{u}| = (u^2 + v^2)^{1/2}$ is ; u_* is the friction velocity; ϑ_*, q_* are the scales of the potential temperature and specific humidity; h is the surface layer height; L is the Monin-Obukhov length scale; z_u, z_ϑ are the roughness parameters for wind and temperature, respectively; $\zeta = \frac{z}{L}$ is a dimensionless height representing the hydrostatic stability parameter; φ_i, f_i are continuous universal functions.

The temperature over the water surface is assumed to be given and the relative humidity is computed by the Magnus formula. The earth's surface temperature is determined from the combined solution of the turbulence energy balance equation and the equation of heat conduction in soil. The heat balance on the boundary of atmosphere-soil separation is modeled by the equation.

$$G_S - \rho c_p \left(v_\vartheta \frac{\partial \vartheta}{\partial z} \right)_0 - \rho L_w \left(v_\vartheta \frac{\partial q}{\partial z} \right)_0 = I_0 (1 - A_S) - F, \quad (19)$$

where $G_s = \lambda_s \left(\frac{\partial T}{\partial z} \right)_s$ is the heat transfer through the soil surface (s denotes the values for $z = 0$, $\lambda_s = c_s \rho_s K_s$, ρ_s , c_s , K_s , T are density, specific heat capacity, coefficient of temperature conduction, and absolute temperature of soil, respectively; ρ is air density; I_0 is the shortwave radiation; A_s the surface albedo; and F is the effective longwave radiation.

The earth's surface temperature and humidity are determined from the equations of heat balance, heat- and moisture-exchange in soil.

2.3. Turbulent Exchange Coefficients

Since $Re \gg 10^3$ (Re is the Reynolds number) in the majority of problems in aerophysics, we should write the subgrid turbulent motions in a parameterized form thus separating motions with scales less than the dimension of the calculated cell. It follows

from the dimension considerations that the energy spectrum contains a wavenumber region where the viscous dissipation effect can be neglected as compared to inertia-induced energy transport. So, the characteristic timescale of the processes in a reference grid cell is within the inertial range. Then, on averaging by volume in the cell, new terms describing the subgrid scale Reynolds stress appear in the thermo-hydrodynamic equations. Thus, the turbulent exchange operators are approximated by the viscous stress tensor, $\tau_{i,j}$, as a function depending on the mean-motion deformation tensor D_{ij} as follows

$$\tau_{ij} = \bar{\rho} K_M D_{ij} \quad (20)$$

where K_M is the coefficient of kinematic viscosity; D_{ij} , ($i = 1, 2, 3$; $j = 1, 2, 3$) are the components of deformation tensor:

$$D_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \quad (21)$$

2.4. Initial and Boundary Conditions

The problem (2)-(21) is solved in the region $D_t = D \times [0, \bar{t}]$, $D = \{(x, y, \sigma) : x \in [-X, X], y \in [-Y, Y], \sigma \in [\zeta, \hat{H}]\}$ under the following initial and boundary conditions

$$u = u^0, v = v^0, w = w^0, \vartheta = \vartheta^0, q = q^0, \text{ for } t = 0 \quad (22)$$

$$\frac{\partial \hat{u}}{\partial x} = \frac{\partial \hat{v}}{\partial x} = \frac{\partial \hat{w}}{\partial x} = 0, \quad \frac{\partial \hat{\vartheta}}{\partial x} = 0, \quad \frac{\partial \hat{q}}{\partial x} = 0 \text{ for } x = \pm X \quad (23)$$

$$\frac{\partial \hat{u}}{\partial y} = \frac{\partial \hat{v}}{\partial y} = \frac{\partial \hat{w}}{\partial y} = 0, \quad \frac{\partial \hat{\vartheta}}{\partial y} = 0, \quad \frac{\partial \hat{q}}{\partial y} = 0 \text{ for } y = \pm Y \quad (24)$$

At the upper boundary of the atmosphere we have

$$u = u^0, v = v^0, w = w^0, \vartheta = \vartheta^0, q = q^0, \text{ for } \sigma = \hat{H} \quad (25)$$

Here the zero indices stand for the background values.

$$a_3 h \frac{\partial \hat{u}}{\partial \sigma} = a_u \hat{u}, \quad a_3 h \frac{\partial \hat{v}}{\partial \sigma} = a_u \hat{v}, \quad a_3 h \frac{\partial \hat{\vartheta}}{\partial \sigma} = a_\vartheta (\hat{\vartheta} - \hat{\vartheta}_0), \text{ for } \sigma = h \quad (26)$$

$$a_3 h \frac{\partial \hat{q}}{\partial \sigma} = a_{\vartheta} (\hat{q} - \hat{q}_0), \quad \frac{\hat{w}}{h} = - \left(\frac{\partial \hat{u}}{\partial x} + \frac{\partial \hat{v}}{\partial y} \right), \quad \text{for } \sigma = \frac{\hat{H}}{\hat{H} - \hat{\zeta}(x, y)} \quad (27)$$

$$\hat{w} = 0 \quad \text{for } \sigma = \zeta(x, y) \quad (28)$$

The system of equations under these initial and boundary conditions describes the temperature and humidity changes that initiate perturbations in the atmospheric flow dynamics.

2.5. Numerical Model of Transport and Transformations of Multicomponent Gaseous Pollutants and Aerosols.

The governing equations for the change rate of gas-aerosol concentrations in the general case have the following form:

$$\frac{\partial C_i}{\partial t} + \nabla(u_i C_i) = F_{\text{gas}} - P_{\text{nucl}} - P_{\text{cond}} + P_{\text{phot}} + \nabla(k \nabla C_i) \quad (29)$$

$$\frac{\partial \varphi_k}{\partial t} + \nabla(u_i \varphi_i) = F_{\text{aer}} + P_{\text{cond}} + P_{\text{coag}} + P_{\text{nucl}} + \nabla(k \nabla \varphi_i) \quad (30)$$

Here C_i , ($i=1, N_g$), φ_k , ($k=1, N_a$) are the concentrations of gases and aerosols; N_g and N_a are the numbers of gaseous species and aerosol fractions, respectively; $u_i = (u, v, w - w_g)$ are wind velocity components along x, y, z , respectively; w_g is the gravitational settling velocity; k , turbulent exchange coefficients in the horizontal and vertical directions, respectively; F_{gas} and F_{aer} are sources of gas and aerosol emissions; and $P_{\text{nucl}}, P_{\text{cond}}, P_{\text{coag}}$ and P_{phot} are the nucleation, condensation, coagulation and photochemistry operators, respectively.

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Biographical Sketches

Guri Marchuk is a scientific counselor of the Presidium of the Russian Academy of Sciences. Between 1962 and 1980 he worked in the Siberian Branch of the USSR Academy of Sciences, first as a director of the Computer Center and then as the Chairman of the Siberian Branch and Vice- President of the USSR Academy of Sciences. Between 1980 and 1986 he was a Deputy Prime Minister of USSR and the Chairman of the State Committee of Science and Technology. From 1986 to 1991 he was the President of the USSR Academy of Sciences. Guri Marchuk is an outstanding scholar in the field of numerical and applied mathematics. He has received many honors, including the Fridman, Keldysh, and Karpinski prizes; he is a member of the Academies of Sciences of Bulgaria, Czechoslovakia, Europe, Finland, France, Germany, India, Poland, and Rumania, and an Honorary Professor of Calcutta, Houston, Karlov, Tel-Aviv, Toulouse, and Oregon Universities, and Budapest and Dresden Polytechnic Universities. He is also a member of the editorial boards of many international and several Russian journals, and the Editor-in-Chief of the Russian Journal of Numerical Analysis and Mathematical Modelling, published by the Institute of Numerical Mathematics, RAS, in the Netherlands. Guri Marchuk is the author of a series of monographs on numerical mathematics, numerical simulation of nuclear reactors, numerical methods for the problems in the atmosphere and ocean dynamics, immunology, medicine, and environmental protection. For notable progress in scientific and organizational activities, Guri Marchuk has been awarded with prestigious state honors.

Kiril Kondratyev is a member of the Russian Academy of Sciences, Department of Oceanology, Atmospheric Physics and Geography. He is the Editor in chief of the journal *Issledovanie Zemli iz Kosmosa (Remote Sensing)*.

Academician Kondratyev is the cochairman of the National Oceanographic Committee, a member of the Governmental Oceanographic Committee, the chief of the Navigation and Oceanography Headquarters of the Russian Defence Ministry. Between 1964 and 1970, he was the rector of the Leningrad University. Academician Kondratyev is an outstanding scientist in the field of atmospheric radiation, greenhouse effect, numerical simulation of the ecological problems. He is the author of a number of monographs, including *Longwave Radiation Transfer in the Atmosphere, Nuclear Winter, Multivariate Global Changes, Climate Effects of Aerosols and Clouds*.

Artash Aloyan is an highly qualified specialist in the field of numerical modeling of atmospheric dynamics and environmental protection problems. He is engaged in development of mathematical models for transport of gaseous and aerosol pollutants in the atmosphere accounting for their transformation (photochemistry, condensation, coagulation, nucleation). From 1969 to 1987, he was a senior researcher at the Computer Center of the Siberian Branch of the USSR Academy of Sciences (Novosibirsk). Artash Aloyan earned his Ph.D. degree in 1975 in the field of numerical modeling of mesometeorological problems. In 1985, he earned his Dr. Sci. degree in mathematical modeling of the atmosphere dynamics and environmental protection problems. From 1987 on, he is a leading research scientist at the Institute of Numerical Mathematics of the Russian Academy of Sciences in Moscow, Russia. During his past research years, Aloyan has published two monographs and more than 100 papers in different scientific journals.