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NUMERICAL ANALYSIS OF THE INFLUENCE OF NATURAL CONVECTION ON THE PROCESS OF CONDENSATION OF ATMOSPHERIC POLLUTANT COMPOUNDS ON THE SURFACE OF NEAR-GROUND PLANTS

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Numerical investigations of the process of condensation of deleterious atmospheric impurities on the surface of near-ground plants under the conditions of natural convective flows have been carried out. The influence of the latter near the surface of phytocenosis elements on the intensity of the process of condensation has been evaluated.

The problem of technogenic action on vegetation has been particularly aggravated in the last decade in connection with regional and global pollution of the atmosphere. Air pollutants substantially reduce the biological productivity of plants and lead to their degradation. To investigate the influence of anthropogenic emissions on near-ground plants one must primarily study the possible pathways by which atmospheric pollutant compounds arrive at the elements of phytocenosis. A great body of data on experimental study of the acid and dry deposition of pollutant compounds on plants is available in the literature; the concentrations of the pollutants in the atmosphere are usually higher than the maximum permissible levels [1–5].

It is common knowledge that the arrival of deleterious substances from aqueous solutions on the surface of leaves at the elements of the internal structure of near-ground plants occurs at night mainly through the covering tissues. It has been established that young leaves are affected most strongly [6]. If the surface of a leaf is moist, deleterious substances penetrate more intensely (necrotic spots are left on the surface of the phytocenosis elements once dew has dried out). Therefore, it is expedient to study the process of condensation as another way in which atmospheric pollutants arrive at the surface of plants.

This work seeks to numerically investigate the regularities of the process of condensation of atmospheric pollutant compounds on the surface of plants with decrease (caused by the solar diurnal cycle) in the air temperature and to evaluate the influence of natural convective flows appearing near the plants' surface on the condensation.

Systematic experimental investigations of the process of condensation of anthropogenic atmospheric impurities on the surface of plants are impossible because of the relatively low absolute values of the quantities (concentration, film, thickness) measured and the large errors in their determination [7, 8].

Since the condensation is accompanied by a considerable release of heat, it becomes necessary to numerically evaluate the influence of natural convection on the intensity of the process in question.

Physical Model. As a result of experimental study of the process of condensation (dewfall) of a steam from the atmosphere on the surface of phytocenosis elements [7, 8], it has been established that this process is realized at night during the warm season on condition that the air temperature decreases, the velocity of wind is no higher than 1–2 m/sec, and the sky is clear. Based on an analysis of the empirical information published [7–9], we have formulated a physicomathematical model of the process of condensation of atmospheric pollutants on the surface of phytocenosis elements with allowance for natural convection.

In the model proposed, a phytocenosis element is taken in the form of a rectangular plate. On the plate surface, the process of condensation is realized and accumulation of a condensate film occurs (the firm contains deleterious components and water) (see Fig. 1).

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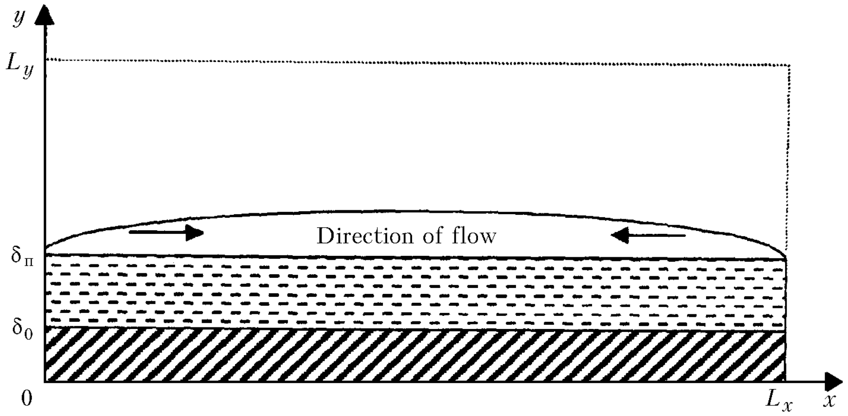

Fig. 1. Diagram of the process of condensation of anthropogenic atmospheric compounds on the surface of phytocenosis elements ($0 \le y \le \delta_0$, phytocenosis element; $\delta_0 \le y \le \delta_f$, condensate film; $\delta_f \le y \le L_y$, gas layer adjacent to the condensate surface).

The process of condensation occurs with a fairly intense release of heat; therefore, transverse temperature gradients causing natural convective flows are formed near the surface of the condensate film in the gas phase. Since the phytocenosis element has a finite shape, symmetric convective flows converging at the center will appear at both ends of the surface. Figure 1 shows the directions of these flows.

In formulating the problem, we made the following assumptions:

(1) there is no chemical interaction between the deleterious component and moisture;

(2) the steam density is low as compared to the condensate density;

(3) consideration is given to film condensation;

(4) surface-tension forces on the free surface of the film exert no influence on the character of its flow;

(5) inertia forces arising in the condensate film are negligible as compared to viscous and gravity forces;

(6) motion of the steam along the condensate-film surface in the gas phase is described in the approximation of the "boundary-layer" model [10];

(7) change in the environmental temperature due to the solar diurnal cycle follows the cosine law [11].

Formulation of the Problem. A mathematical model of the process of condensation of anthropogenic atmospheric impurities on the surface of phytocenosis elements represents a system of nonlinear unsteady two-dimensional equations of mathematical physics that describe heat and mass transfer in the system gas phase–condensate film–phytocenosis element with corresponding boundary and initial conditions [9, 12]. The mathematical model allows for the space-time inhomogeneity of the parameters of heat and mass transfer, the presence of the moving boundaries of the solution domain and phase transitions, radiative-convective heat exchange with the ambient medium, and natural convective flows near the condensate film due to the release of heat in condensation.

It is suggested that flow and energy transfer giving rise to the flow are mainly confined to a thin air layer adjacent to the surface. Beyond this layer, the steam is immobile. A consequence of this suggestion is the assumption that the gradients along the condensation surface are much smaller than those along the normal to it [10].

The system of differential equations describing the process of heat and mass transfer in the problem in question has the form

$$\frac{c_f \rho_f}{\lambda_f} \frac{\partial T_f}{\partial t} = \frac{\partial^2 T_f}{\partial x^2} + \frac{\partial^2 T_f}{\partial y^2}, \quad \frac{c_c \rho_c}{\lambda_c} \frac{\partial T_c}{\partial t} = \frac{\partial^2 T_c}{\partial x^2} + \frac{\partial^2 T_c}{\partial y^2},$$

$$\frac{c_g \rho_g}{\lambda_g} \left[\frac{\partial T_g}{\partial t} + U \frac{\partial T_g}{\partial x} + V \frac{\partial T_g}{\partial y} \right] = \frac{\partial^2 T_g}{\partial y^2}, \quad U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} = -\frac{1}{\rho_g} \frac{\partial P}{\partial x} + \frac{\mu_g}{\rho_g} \frac{\partial^2 U}{\partial y^2},$$

$$\frac{\partial U}{\partial x}+\frac{\partial V}{\partial y}=0\,,\quad \frac{1}{D_i}\frac{\partial C_i}{\partial t}=\frac{\partial^2 C_i}{\partial x^2}+\frac{\partial^2 C_i}{\partial y^2}\,,\quad \frac{P_\Sigma M_\Sigma}{\rho_\Sigma}=RT$$

with the initial

$$t=0:\quad T_{\rm g}=T_{\rm g0}\,,\quad T_{\rm c}=T_{\rm c0}\,,\quad C_i=C_{i0}\,,\quad \delta_{\rm f}=\delta_0$$

and boundary conditions

$$0\le x\le L_x\,,\quad y=0:\quad -\lambda_{\rm c}\frac{\partial T_{\rm c}}{\partial y}=\alpha\,(T_{\rm g}-T_{\rm c})+\sigma\varepsilon_{\rm red}\,(T_{\rm g}^4-T_{\rm c}^4)\,;$$

$$0\le x\le L_x\,,\quad y=\delta_0:\quad \begin{cases}-\lambda_{\rm c}\dfrac{\partial T_{\rm c}}{\partial y}=-\lambda_{\rm f}\dfrac{\partial T_{\rm f}}{\partial y}\,,\\ T_{\rm f}\,(x)=T_{\rm c}\,(x)\,;\end{cases}$$

$$0\le x\le L_x\,,\quad y=\delta_{\rm f}:\quad \begin{cases}-\lambda_{\rm f}\dfrac{\partial T_{\rm f}}{\partial y}=-\lambda_{\rm g}\dfrac{\partial T_{\rm g}}{\partial y}+\sigma\varepsilon_{\rm red}\,(T_{\rm g}^4-T_{\rm f}^4)+W_\Sigma Q\,,\\ \rho_i D_i\dfrac{\partial C_i}{\partial y}=W_i\,(1-C_{\rm s})\,.\end{cases}$$

The adhesion condition $U = 0$ and $V = 0$ is formulated on the surface of the condensate film in the gas phase.

At the external boundary of the boundary layer, the velocity is equal to zero in the case of natural convective flow [9]:

$$0\le x\le L_x\,,\quad y=L_y:\quad T_{\rm g}=T_{\rm env}(t)\,,\quad C_i=C_{i0}\,;$$

$$0\le y\le\delta_0\,,\quad x=0:\quad -\lambda_{\rm c}\frac{\partial T_{\rm c}}{\partial x}=\alpha\,(T_{\rm g}-T_{\rm c})+\sigma\varepsilon_{\rm red}\,(T_{\rm g}^4-T_{\rm c}^4)\,;$$

$$0\le y\le\delta_0\,,\quad x=L_x:\quad -\lambda_{\rm c}\frac{\partial T_{\rm c}}{\partial x}=\alpha\,(T_{\rm g}-T_{\rm c})+\sigma\varepsilon_{\rm red}\,(T_{\rm g}^4-T_{\rm c}^4)\,;$$

$$\delta_0\le y\le\delta_{\rm f}\,,\quad x=0:\quad -\lambda_{\rm f}\frac{\partial T_{\rm f}}{\partial x}=\alpha\,(T_{\rm g}-T_{\rm f})+\sigma\varepsilon_{\rm red}\,(T_{\rm g}^4-T_{\rm f}^4)\,;$$

$$\delta_0\le y\le\delta_{\rm f}\,,\quad x=L_x:\quad -\lambda_{\rm f}\frac{\partial T_{\rm f}}{\partial x}=\alpha\,(T_{\rm g}-T_{\rm f})+\sigma\varepsilon_{\rm red}\,(T_{\rm g}^4-T_{\rm f}^4)\,;$$

$$\delta_{\rm f}\le y\le L_y\,,\quad x=0:\quad -\lambda_{\rm g}\frac{\partial T_{\rm g}}{\partial x}=0\,,\quad -\rho_i D_i\frac{\partial C_i}{\partial x}=0\,;$$

$$\delta_{\rm f}\le y\le L_y\,,\quad x=L_x:\quad -\lambda_{\rm g}\frac{\partial T_{\rm g}}{\partial x}=0\,,\quad -\rho_i D_i\frac{\partial C_i}{\partial x}=0\,.$$

The mass rate of condensation was calculated from the formula [11]

$$W_i=A\,(P_i^{\rm sat}-P_i)/\sqrt{2\pi RT/M_i}\,.$$

The coordinate of the external boundary of the film was determined from the condensation rate

$$\delta_f(t) = \delta_0 + \int_0^t W_i/\rho_f dt .$$

The accommodation coefficient A as a function of the saturation pressure was determined, according to [13], from the formula

$$A = \frac{35}{(P_i^{\text{sat}})^{0.56}} .$$

On the condition that the environmental temperature decreased from 20 to 10°C in the evening, we found its value at a specific instant of time t from the cosine law

$$T_{\text{env}} = 288 + 5\cos\left(\frac{\pi t}{t_{\text{fin}}}\right).$$

Method of Solution. The problem was solved in a two-dimensional formulation with allowance for the conductive and radiative modes of transfer of heat, the condensation of deleterious components on the surface of phytocenosis elements, the diffusion of deleterious components to the condensation surface, and the unsteadiness of the processes of heat and mass transfer. Condensation began at temperatures lower than the corresponding critical temperature. Account was taken of the release of the heat of phase transition and of natural convective flows appearing near the surface.

We used the finite-difference method [14]. Difference analogs of the differential equations were solved by the splitting method with the use of the iteration method and the implicit four-point difference scheme for solution of one-dimensional equations [10].

In calculating concentration fields, we used a grid with an irregular step that was determined from the arithmetic-progression formula.

The boundary-layer thickness $\delta_{\text{b.layer}}$ was estimated by the value of the Grashof number Gr and from the condition that the value of $\delta_{\text{b.layer}}$ is low as compared to the characteristic dimension (length of the phytocenosis element) [15]:

$$\text{Gr} = \frac{g\beta L_x^3 (T_s - T_{\text{env}})}{\nu^2} , \quad \delta_{\text{b.layer}} = O\left(\frac{L_x}{\sqrt[4]{\text{Gr}}}\right).$$

In addition to the main grid, we introduced an auxiliary "half-integral" grid to approximate the equation of motion. The transverse velocity component on the half-integral layer was found from the continuity equation. We determined the value of the longitudinal velocity component on the integral layer by solution of the equation of motion and found the value of U on the half-integral layer by interpolation [10]:

$$U_{k+1/2,j} = (U_{k,j} + U_{k+1,j})/2 .$$

Selection of the initial profile was the main difficulty in calculating the velocities of natural convection. The maximum possible velocity in a fixed (nonzero) cross section x_1 was determined as a first approximation according to [15]:

$$U(x_1) = \sqrt{g\beta x_1 (T_s - T_{\text{env}})} .$$

Thereafter, by successive iterations, we calculated the value of the velocity in the cross section x_1. The resulting profile was taken as the initial one.

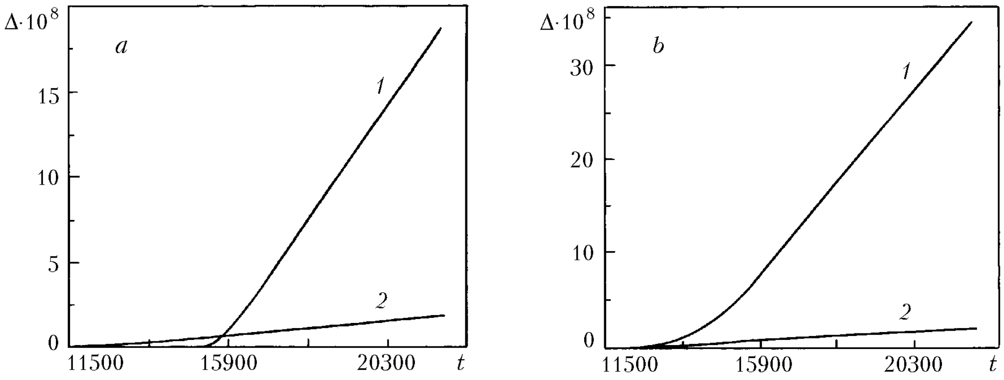

Fig. 2. Condensate-film thickness Δ vs. time t in the presence of deleterious components (a) 1) tridecane vapor; 2) sulfuric-acid vapor; b) 1) pentadecane vapor; 2) sulfuric-acid vapor) in the gas phase. Δ, m; t, sec.

Calculation of the velocity profiles with variation in the coordinate x was organized as follows. As a first approximation we took the functions sought on the kth layer as the velocity values on the $(k + 1)$th layer. The second iteration and all the iterations that followed began with obtaining running coefficients in whose computation we used the values of the velocities obtained in the previous iteration. The process of computation was completed when the required accuracy was attained.

Analysis of Results and Discussion. Numerical investigations of the process of condensation of anthropogenic atmospheric impurities on the surface of phytocenosis elements were carried out for the following environmental parameters:

(1) the pressure was assumed to be constant and equal to 10^5 Pa;

(2) the air temperature decreased from 20 to 10°C for 6 h;

(3) the value of the relative humidity was taken to be 58, 60, and 62%;

(4) the atmospheric air contained two deleterious components, one of which was sulfuric acid (the strongest phytotoxicant [1]);

(5) the concentrations of atmospheric pollutants (C_{pol}) varied within $\text{MPC}_{\text{d.m}} < C_{\text{pol}} < \text{MPC}_{\text{w.z}}$) ($\text{MPC}_{\text{d.m}}$ is the daily-mean maximum permissible concentration and $\text{MPC}_{\text{w.z}}$ is the maximum permissible concentration of the working zone);

(6) compounds belonging to the class of hydrocarbons, alcohols, and acids were considered as the atmospheric pollutants.

In the course of the numerical experiments, it was established that such compounds as sulfuric acid, ethylene glycol, propylene glycol, trimethylene glycol, dipropylene glycol, butane-1,3-diol, and saturated hydrocarbons from $C_{12}H_{26}$ to $C_{15}H_{34}$ and unsaturated ethylene hydrocarbons from $C_{12}H_{24}$ to $C_{15}H_{30}$ for certain values of their concentrations lower than $\text{MPC}_{\text{d.m}}$ in the atmosphere are capable of condensing on the surface of the phytocenosis element.

In the process of solution, we obtained the dependences of the rates of condensation of atmospheric pollutant compounds on time, the temperature and concentration distributions, and the dependences of the condensate-film thickness on time.

Two deleterious compounds (sulfuric acid and hydrocarbon) are present in the film formed in addition to water.

Figure 2 shows, as an example, the characteristic dependences of the thickness of the film of the deleterious-component condensate on time. It is seen in the figure that hydrocarbons are condensed more intensely than sulfuric acid.

Figure 3 shows the U distribution along a) the transverse coordinate and b) the longitudinal coordinate in natural convection in the boundary layer on the condensate-film surface. In Fig. 3a, it is seen that the velocity has a parabolic profile and the maximum value is attained at the center of the boundary layer, whereas in Fig. 3b it is seen that flow develops toward the center of the surface. A symmetric pattern will be realized for convective flow from the opposite edge of the condensate-film surface.

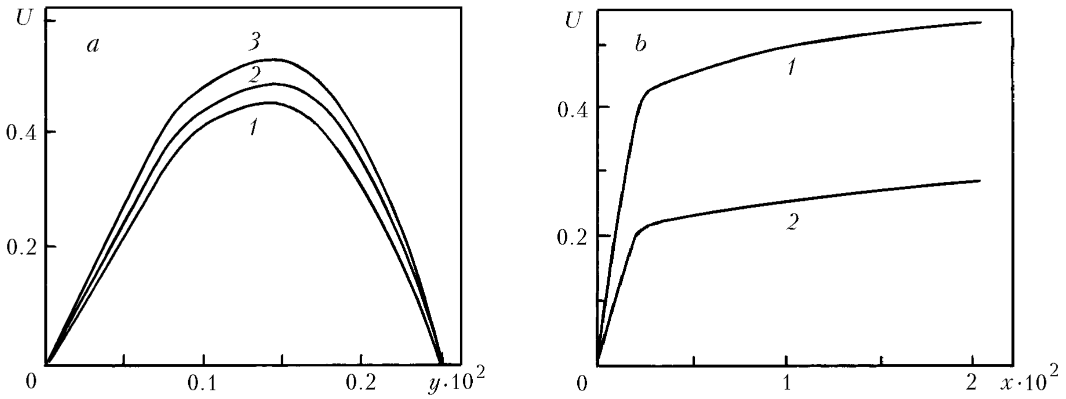

Fig. 3. Distribution of the longitudinal velocity component: a) along the transverse coordinate of the boundary layer in different cross sections in x (1) $x = 0.5 \cdot 10^{-2}$; 2) $1.2 \cdot 10^{-2}$; 3) $1.8 \cdot 10^{-2}$ m); b) along the longitudinal coordinate of the boundary layer in different cross sections in y (1) $y = 1.7 \cdot 10^{-3}$; 2) $2.5 \cdot 10^{-3}$ m). U, m/sec; x, y, m.

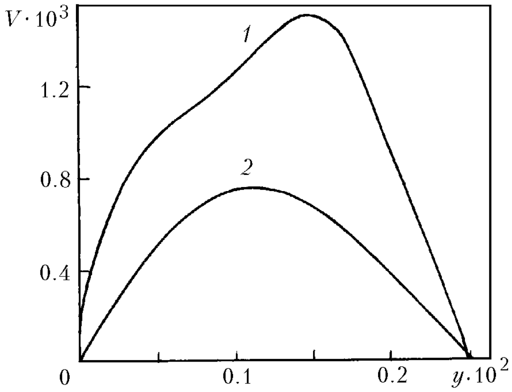

Fig. 4. Distribution of the transverse velocity component along the transverse coordinate of the boundary layer in different cross sections in x: 1) $x = 0.5 \cdot 10^{-2}$; 2) $1.2 \cdot 10^{-2}$ m. V, m/sec; y, m.

Figure 4 gives the distribution of the transverse velocity component V along the transverse coordinate of the boundary layer. It is seen in the figure that the quantity V is much lower than the value of U.

The model proposed was verified from the data [7] on condensation of a steam. In [7] Kobysheva described measurements of the fallen moisture by Yaroshevskii's drosometer. A comparison of the results of numerical modeling of the process of condensation of the steam on the surface of plants to the experimental data of [7] yields satisfactory agreement with a discordance no higher than 40%.

Numerical investigations have shown that the influence of natural convective flows on the process of condensation of deleterious atmospheric impurities on the surface of phytocenosis elements is insignificant. Table 1 shows the temperature distribution along the coordinate y with allowance for the process of natural convective flow and without allowance for it. It is seen in the table that the temperatures differ in the fifth decimal place. Consequently, the amount of pollutant fallen out onto the surface of the phytocenosis element is independent of the convective flows appearing.

It has been established that a condensate film is formed on the surface of phytocenosis elements over a period of 6 to 8 h (average period of time over which the process of condensation is realized). Of course, not the entire pollutant fallen out from the atmosphere penetrates into the plant, but in the case of a periodic action we have the accumulation of deleterious compounds even when the penetration is slight, which influences the life activity of plants.

Based on an analysis and generalization of the results of the investigations carried out, we can draw the basic conclusions.

TABLE 1. Temperature Distribution along the Transverse Coordinate *y* of the Boundary Layer

No. of the node of the difference grid along the coordinate *y*	T_g, K	
	with allowance for natural convection	without allowance for natural convection
0	291.7725585955	291.7725585955
1	291.7703811200	291.7703790469
2	291.7681965422	291.7681944891
3	291.7660067924	291.7660049190
4	291.7638121126	291.7638103323
5	291.7616124767	291.7616107249
6	291.7594078839	291.7594060930
7	291.7571983840	291.7571964329
8	291.7549835401	291.7549817408

1. A physicomathematical model of the process of condensation of anthropogenic atmospheric impurities on the surface of phytocenosis elements with allowance for conductive and radiative modes of transfer of heat, the condensation of deleterious components on the phytocenosis surface, the diffusion of deleterious components to the condensation surface, and the unsteadiness of the processes of heat and mass transfer has been formulated. Account has been taken of the release of heat of phase transition in condensation and of natural convective flows.

2. The influence of natural convection on the process of condensation is insignificant. As the numerical investigations have shown, with allowance for natural convective flows (that appear in heat release in the process of condensation), the temperature near the surface increases only slightly, which does not result in a significant growth in the condensation rate. Accordingly the amount of atmospheric pollutant fallen out onto the surface of the phytocenosis element does not depend, in practice, on the convective flows appearing.

3. The investigations carried out demonstrate the possibility of realizing the process of condensation of atmospheric pollutant compounds on the surface of phytocenosis elements, which enables one to consider this process as another way in which pollutants can arrive at near-ground plants.

NOTATION

A, accommodation coefficient; C, mass concentration of the atmospheric pollutant component; c_c, specific heat of the condensed phase (phytocenosis element), J/(kg·K); c_g, specific heat of the gas, J/(kg·K); c_f, specific heat of the condensate film, J/(kg·K); D, diffusion coefficient, m^2/sec; g, free fall acceleration, m/sec^2; Gr, Grashof number; L_x, length of the phytocenosis-element surface, m; M, molecular weight, kg/mole; P, pressure, Pa; P^{sat}, saturation pressure, Pa; Q, heat of phase transition, J/kg; R, universal gas constant, J/(mole·K); T, temperature, K; T_{env}, environmental temperature, K; t, time, sec; t_{fin}, final time of the process, sec; U and V, longitudinal and transverse velocity components, m/sec; W, condensation rate, kg/(m^2·sec); x and y, longitudinal and transverse coordinates, m; α, heat-exchange coefficient, W/(m^2·K); β, coefficient of thermal volumetric expansion, 1/K; ν, kinematic viscosity, m^2/sec; $\delta_{b.layer}$, boundary-layer thickness, m; δ_f, coordinate of the condensate-film surface, m; δ_0, coordinate of the phytocenosis-element surface, m; Δ, condensate-film thickness; ε_{red}, reduced emissivity factor; λ, thermal conductivity, W/(m·K); μ, coefficient of dynamic viscosity, kg/(m^2·sec); ρ, density, kg/m^3; σ, Stefan–Boltzmann constant, W/(m^2·K^4). Subscripts and superscripts: 0, initial value; g, gas phase; c, condensed phase; f, condensate film; i, No. of the component; Σ, total value; sat, saturated steam; s, condensation surface; k and j, No. of the node of the sought function; b.layer, boundary layer; env, environment; fin, final time of the process; d.m, daily-mean; pol, pollutant; w.z, working zone; red, reduced.

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