

HEAT AND MASS TRANSFER IN CONDENSATION OF HARMFUL AIR-POLLUTING SUBSTANCES ON THE PHYTOCENOSIS SURFACE

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A mathematical model for the condensation of harmful air-polluting substances on the phytocenosis surface is formulated. Results of a numerical study of the problem of heat and mass transfer are presented. The temperature and concentration fields, the time dependence of the condensation rate, and the distribution of the condensate film over the phytocenosis surface are obtained.

Every year hundreds of millions of tons of sulfur and nitric oxides, halogen derivatives, and other compounds get into the atmosphere. The pollution sources are power plants (they use oil, coal, and slates), enterprises of ferrous and nonferrous metallurgy and the chemical and petrochemical industry, and aircraft and automobiles [1]. These compounds readily enter into chemical reactions with atmospheric components, forming secondary polluting substances. From the standpoint of the action on vegetation, secondary polluting substances are more dangerous than primary atmospheric pollutants. The accumulation of a significant quantity of toxic substances in a plant or on its surface leads to damage to leaves, formation of necroses, and destruction of plants [2].

Many works that deal with the fallout of harmful atmospheric pollutants on the phytocenosis surface are known in the literature. Most of them are concerned with experimental study of the processes of acid and dry sedimentation [1]. However, polluting substances can also get to the phytocenosis surface in condensation. Such processes have not been studied previously.

This work seeks to model physically and mathematically the condensation of harmful atmospheric pollutants on the phytocenosis surface with a decrease in the air temperature due to the diurnal cycle of the position of the sun.

Physical Model. In the evening and at night the air temperature falls and the phytocenosis surface cools down. The vapor of condensable substances residing in the air (in the atmospheric boundary layers) approaches the saturation state. If the temperature of the phytocenosis surface reaches the "dew point," condensation begins. The process continues until dawn, when the air temperature rises and the condensation on the phytocenosis surface is replaced by transpiration. A simplified scheme of the condensation is presented in Fig. 1. In the model proposed, the gas phase can include air, water vapor, and the vapor of acid components. As an example, consideration is given to the case with a single acid component. Its initial concentration was taken to be equal to the daily mean maximum permissible concentration [3]. The thermophysical properties of the phytocenosis were assumed to be known [4].

Since the phytocenosis has a curvilinear surface with a small angle of curvature, this problem can be considered in a rectangular coordinate system. However, it should be taken into account that the angle of curvature of the surface is sufficient for the condensate film to spread.

The phytocenosis was taken to be in the form of a rectangular plate measuring $\delta_0 \times L_x$ (Fig. 1). The origin of coordinates coincided with the phytocenosis boundary at which no condensation occurs.

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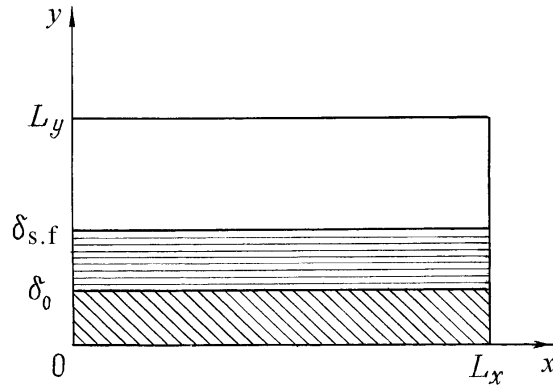


Fig. 1. Scheme of the condensation of harmful air-polluting substances on the phytocenosis surface ($0 \leq y \leq \delta_0$, phytocenosis; $\delta_0 \leq y \leq \delta_{c.f}$, condensate film; $\delta_{c.f} \leq y \leq L_y$, gas layer adjacent to the condensation surface).

The external pressure was assumed to be constant and equal to 10^5 Pa. The problem was solved in a two-dimensional formulation with allowance for the conductive and radiative mechanisms of heat transfer, the condensation of acid components on the phytocenosis surface, the diffusion of acid components to the condensation surface, and the unsteadiness of the heat and mass transfer. The condensation of the components on the phytocenosis surface began at temperatures below the corresponding critical temperature. The liberation of the heat of phase transition in the condensation was taken into account.

At the external boundary, a temperature is specified that is time-varying in connection with the diurnal cycle of the sun [4].

It was supposed that the condensate film is accumulated on the phytocenosis surface over the entire condensation process. Since the phytocenosis surface is concave, the film produced runs off to the surface edges due to gravity. Since the film thickness and the rate are small quantities, the flow is laminar.

The problem was solved under the following assumptions:

- 1) there is no chemical interaction between the harmful component and moisture;
- 2) the vapor density is low in comparison with the condensate density;
- 3) film condensation is considered;
- 4) convective mass and heat transfer is disregarded;
- 5) the surface-tension forces on the free surface of the film have no effect on its flow;
- 6) the inertial forces arising in the condensate film are negligible in comparison with the viscous and gravity forces.

The investigations were carried out in two stages: 1) the problem of heat and mass transfer was solved in a rectangular coordinate system and the phytocenosis was taken to be in the form of a rectangular plate and 2) the spread of the condensate film was calculated with allowance for the curvilinear condensation surface.

Mathematical Model. The system of differential equations with appropriate initial and boundary conditions that describes the heat and mass transfer in the condensation of anthropogenic atmospheric pollutants on the phytocenosis surface, by analogy with [4, 5], is of the form

$$\frac{c_g \rho_g}{\lambda_g} \frac{\partial T_g}{\partial t} = \frac{\partial^2 T_g}{\partial x^2} + \frac{\partial^2 T_g}{\partial y^2}, \quad \frac{c_c \rho_c}{\lambda_c} \frac{\partial T_c}{\partial t} = \frac{\partial^2 T_c}{\partial x^2} + \frac{\partial^2 T_c}{\partial y^2},$$

$$\frac{c_{c.f} \rho_{c.f}}{\lambda_{c.f}} \frac{\partial T_{c.f}}{\partial t} = \frac{\partial^2 T_{c.f}}{\partial x^2} + \frac{\partial^2 T_{c.f}}{\partial y^2}, \quad \frac{1}{D_i} \frac{\partial C_i}{\partial t} = \frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2}; \quad \frac{P_\Sigma M_\Sigma}{\rho_\Sigma} = RT$$

with the following initial and boundary conditions:

$$\begin{aligned}
t=0: & \quad T_g = T_{g0}, \quad T_c = T_{c0}, \quad C_i = C_{i0}, \quad \delta_{c.f} = \delta_0; \\
y=0: & \quad -\lambda_c \frac{\partial T_c}{\partial y} = \alpha (T_g - T_c) + \sigma \varepsilon_r (T_g^A - T_c^A); \\
y=\delta_0: & \quad -\lambda_c \frac{\partial T_c}{\partial y} = -\lambda_{c.f} \frac{\partial T_{c.f}}{\partial y}, \quad T_{c.f}(x) = T_c(x); \\
y=\delta_{c.f}: & \quad -\lambda_{c.f} \frac{\partial T_{c.f}}{\partial y} = -\lambda_g \frac{\partial T_g}{\partial y} + \sigma \varepsilon_r (T_g^A - T_{c.f}^A) + W_\Sigma Q; \\
& \quad \rho_i D_i \frac{\partial C_i}{\partial y} = W_i (1 - C_w); \\
y=L_y: & \quad T = T(x), \quad C_i = C_{i0}; \\
& \quad 0 \leq y \leq \delta_{c.f}; \\
x=0: & \quad -\lambda_c \frac{\partial T_c}{\partial x} = \alpha (T_g - T_c) + \sigma \varepsilon_r (T_g^A - T_c^A); \\
x=L_x: & \quad -\lambda_c \frac{\partial T_c}{\partial x} = \alpha (T_g - T_c) + \sigma \varepsilon_r (T_g^A - T_c^A); \\
& \quad \delta_{c.f} \leq y \leq L_y; \\
x=0: & \quad -\lambda_g \frac{\partial T_g}{\partial x} = 0, \quad -\rho_i D_i \frac{\partial C_i}{\partial x} = 0; \\
x=L_x: & \quad -\lambda_g \frac{\partial T_g}{\partial x} = 0, \quad -\rho_i D_i \frac{\partial C_i}{\partial x} = 0.
\end{aligned}$$

The mass rate of condensation was calculated from the formula

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

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

$$\delta_{c.f}(t) = \delta_0 + \int_0^t W_i / \rho_{c.f} dt.$$

Method of Solution. The problem was solved by the finite-difference method [6]. Difference analogs of the initial differential equations were solved by the splitting method using an iteration method and an implicit four-point difference scheme for solving one-dimensional equations. Concentration fields were calculated using a grid with an irregular step. Diffusion coefficients were calculated using the method of Fuller,

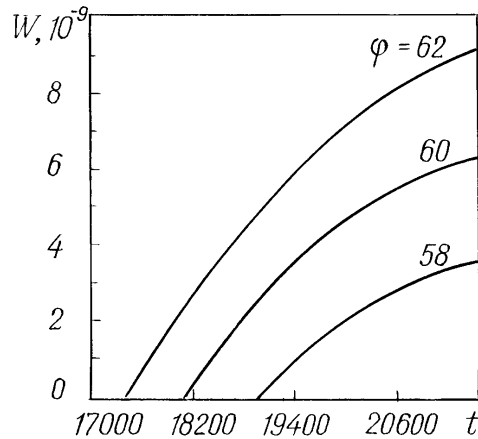


Fig. 2. Mass rate of condensation of the acid component W as a function of the time t for different relative humidities.

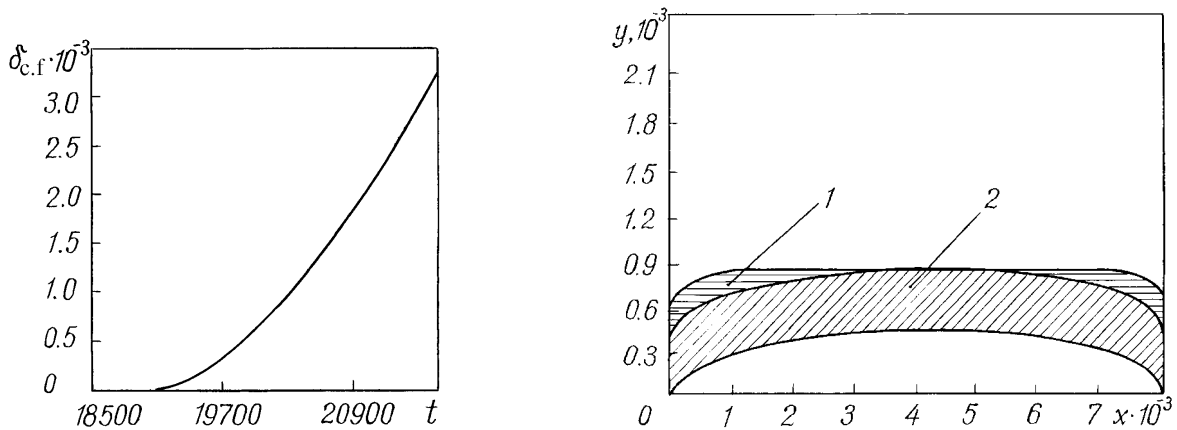


Fig. 3. Thickness of the condensate film Δ as a function of the time t .

Fig. 4. Distribution of the condensate film over the phytocenosis surface: 1) condensate film; 2) phytocenosis.

Shettler, and Giddings [7]. The thermal conductivity of the gas mixture was calculated by the method of Mason and Saxena [7].

The spreading of the condensate film over the phytocenosis surface was determined using the approach of Isachenko [8], who considered condensation on a horizontal tube. Using the solution of [8] with allowance for the geometric features of the adopted model, the film distribution over the surface was determined as

$$\Delta(x) = \sqrt[3]{\frac{3\mu_{\text{liq}} W_i x}{\rho_{\text{liq}}^2 g}} f^{-1/3}(x);$$

the function $f(x) = \sin(\pi x)$ specifies the shape of the condensation surface and the orientation relative to the normal to the surface of the earth.

Results and Discussion. Figure 2 gives the time dependence of the mass rate of condensation of the acid component for various relative air humidities. The condensation rate increases smoothly during the process. This is evidently caused by the decrease in the ambient temperature. With increase in the relative air humidity the condensation rate increases and, correspondingly, the thickness of the condensate film increases.

Figure 3 shows an increase in the thickness of the condensate film with time. In the beginning of the condensation the film grows slowly, which is explained by the fact that the condensation rate is a small quantity, and then it increases and the film thickness increases more rapidly.

Figure 4 presents the distribution of the condensate film over the phytocenosis surface. The concentration of the acid component is higher at the edges. This result accounts, for example, for the fact that damage to leaves and formation of necroses begin at the edges of the phytocenosis surface [2].

It follows from the results of numerical investigations that, under certain conditions, a condensate film that contains an acid component is formed on the phytocenosis surface. A comparison of the concentration of the acid component on the phytocenosis surface with the daily mean maximum permissible concentration indicated that the content of the harmful component in the condensate film is above normal.

Conclusion. From the results obtained it is possible to draw the conclusion that, under certain conditions, on the phytocenosis surface a condensate film can be formed with a content of the acid component much in excess of the maximum permissible concentrations (MPCs) with the MPC of the gas phase kept within the limits of the normal range. This model permits prediction of the effect of air-polluting substances on phytocenosis elements.

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NOTATION

T , temperature, K; t , time, sec; x , longitudinal coordinate, m; y , lateral coordinate, m; λ , thermal conductivity, W/(m·K); δ_0 , coordinate of the phytocenosis surface, m; Δ , thickness of the condensate film, m; $\Delta(x)$, distribution function of the thickness of the condensate film over the phytocenosis surface; $\delta_{c,f}$, coordinate of the surface of the condensate film; D , diffusion coefficient, m²/sec; C , mass concentration of the substance; C_w , mass concentration of the condensing substance at the phytocenosis surface; ρ , density, kg/m³; c_c , specific heat of the phytocenosis, J/(kg·K); c_g , specific heat of the gas, J/(kg·K); $c_{c,f}$, specific heat of the condensate film, J/(kg·K); g , acceleration due to gravity, m/sec²; Q , heat of the phase transition, J/kg; W , condensation rate, kg/(m²·sec); M , molecular weight, kg/mole; ϕ , relative humidity, %; μ , dynamic viscosity, kg/(m·sec); α , heat-transfer coefficient, W/(m²·K); P , pressure, Pa; R , gas constant, J/(mole·K); σ , Stefan–Boltzmann constant, J/K; A , accommodation coefficient; ϵ_r , reduced emissivity factor. Subscripts and superscripts: 0, initial value; g, gas phase; c, condensed phase; c.f, condensate film; i , number of the component; liq, liquid; Σ , overall values; s, saturated vapor.

REFERENCES

1. L. Horvat, *Acid Rain* [Russian translation], Moscow (1990).
2. M. Threshaw, *Air Pollution and Life of Plants* [Russian translation], Leningrad (1988).
3. G. P. Bepamyatnov, *Maximum Permissible Concentrations of Harmful Substances in Air and Water* [in Russian], Leningrad (1975).
4. A. M. Grishin, *Mathematical Models of Wood Fires* [in Russian], Tomsk (1981).
5. N. V. Pavlyukevich, G. E. Gorelik, V. V. Levdanskii, V. G. Leitsina, and G. I. Rudin, *Physical Kinetics and Transfer Processes in Phase Transitions* [in Russian], Minsk (1980).
6. A. A. Samarskii, *Theory of Difference Schemes* [in Russian], Moscow (1977).
7. R. Reed, J. Prausnitz, and T. Sherwood, *Properties of Gases and Liquids* [Russian translation], Leningrad (1982).
8. V. P. Isachenko, *Heat Transfer in Condensation* [in Russian], Moscow (1977).