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THEORETICAL AND MATHEMATICAL PHYSICS

Simulation of the Temperature Distribution at the Water–Air Interface Using the Theory of Contrast Structures

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Abstract—A mathematical model for describing the temperature distribution in the near-surface layer at the water–air interface is proposed. The model is composed based on the theory of contrast structures. Using numerical calculations, the temperature distribution in a 10-cm wide near-boundary layer has been obtained. The calculation results coincide well with the experimental data.

Keywords: water–air interface, contrast structures, transition layer, heat-exchange coefficient.

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INTRODUCTION

A layer with a thickness on the order of several centimeters near a boundary plays a special part in studying the temperature distribution at the water–air interface. Figure 1 presents the plot of the temperature variation in the near-surface layer on the order of 10 cm at the water–air interface according to measurements in laboratory conditions [1]. In the plot one can clearly see the presence of several intervals in which the temperature varies in different ways. According to the performed measurements, monotonic variation in the temperature from lower to larger values, generally speaking, does not occur; on the contrary, near the surface, regions with an inverse temperature distribution are observed. The clear distinction between intervals with different behaviors of the temperature plot indicates the presence of stratification according to the time of carrying out the experiment both in the water medium and air. The aim of this work is to develop a mathematical model that allows one to describe the nonmonotonic temperature variation in the transition layer at the water–air interface.

The model is based on experimentally verified data about the stepwise change in the heat-exchange coefficient, both at the water–air interface and at boundaries of layers caused by the stratification of each of the media. To describe sharp changes in the temperature at the layer boundaries, we used the theory of contrast structures. A contrast structure is a function whose domain contains an interval with a sharp change in values of this function. This region is called the internal transition layer. The theory of contrast structures is often used for simulating phase transitions, in particu-

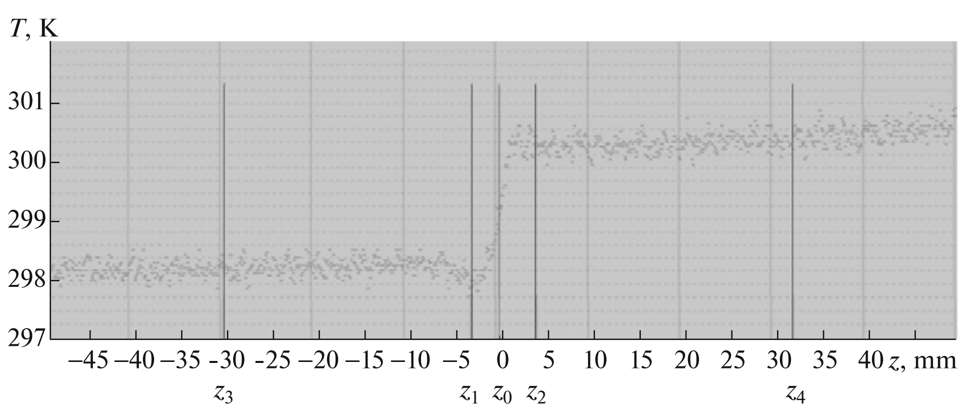

Fig. 1. An experimental plot of the temperature variation in the near-surface water–air layer.

lar, processes of combustion and other autowave processes [2].

1. THEORETICAL MODEL

To describe the temperature distribution over a segment of a straight line that is perpendicular to the interface, we pose the following initial boundary value problem for the heat-conductivity equation:

$$\frac{\partial}{\partial \tilde z}\left(K(\tilde z)\frac{\partial T}{\partial \tilde z}\right) - c\rho\frac{\partial T}{\partial \tilde t} = \tilde f(T,\tilde z,\tilde t),$$
$$\tilde z \in (-\tilde a,\tilde a), \quad \tilde t \in (0;\tilde t_0); \qquad (1)$$
$$\left.\frac{\partial T}{\partial \tilde z}\right|_{\tilde z=-\tilde a} = 0; \quad \left.\frac{\partial T}{\partial \tilde z}\right|_{\tilde z=\tilde a} = 0; \quad T(\tilde z,0) = T_0(\tilde z).$$

Here, T is temperature in K, $\tilde z$ is the coordinate along the straight line that is perpendicular to the water–air boundary (in meters), $\tilde t$ is time in seconds (the dimensional spatial and temporal variables are marked with a tilde), c is the specific heat capacity of the medium in J/(kg K) (for a gas, at a constant pressure), and ρ is the medium density in kg/m^3. The heat-exchange coefficient in Ω/(m K) is denoted by $K(\tilde z)$. As is seen from the experimental plots (see Fig. 1), zones of the inverse temperature distribution are located at a distance on the order of several centimeters from this boundary; for this reason, problem (1) is solved on the segment $\tilde z \in [-\tilde a, \tilde a]$ at $\tilde a = 0.05$ m during $\tilde t_0$ seconds. The function $T_0(\tilde z)$ specifies the initial temperature distribution that is necessary for numerical calculations by the method of establishing a steady state. The Neumann boundary conditions mean that the total heat flow through the boundaries of the region is zero.

The time interval during which the measurements are performed is long enough to establish a steady-state temperature distribution and, at the same time, short enough to treat the change in the environment as insignificant and not capable of having an effect on this distribution. Taking this condition of the experiment into account, we considered the function $\tilde f(T, \tilde z, \tilde t)$ in the right-hand side of Eq. (1) in the process of constructing the model as time-independent.

The heat exchange in different layers of a stratified medium is affected by different factors. At a distance of several millimeters from the water-air boundary, the exchange is molecular; with an increase in the distance from the boundary, it becomes turbulent. The heat-exchange coefficient that is due to molecular interactions is lower by two orders of magnitude than that via the turbulent interactions. As well, the turbulent exchange in the air occurs more intensely than in the water; therefore, the heat-exchange coefficient in the air is larger by an order of magnitude than in the water. It is also known from experimental data that inside the transition layer a plane exists along which the heat-exchange coefficient varies discontinuously by several times. This plane is accepted to be the water–air interface. Therefore, four regions in which the heat-exchange coefficient takes different values exist:

$$K(z) = \begin{cases} 100\cdot D, & \tilde z \le \tilde z_1; \\ D, & \tilde z_1 < \tilde z \le \tilde z_0; \\ m\cdot D, & \tilde z_0 < \tilde z \le \tilde z_2; \\ 1000\cdot D, & \tilde z > \tilde z_2. \end{cases} \qquad (2)$$

Here, $1 < m < 10$, $\tilde z_1$ and $\tilde z_2$ are boundaries of the transition layer, and $\tilde z_0$ is a point at the interface. The lines $\tilde z = \tilde z_i$, $i = 0, 1, 2$, are marked in Fig. 1.

Let us reduce problem (1) to the dimensionless form. For the scales of measuring the length, temperature, and time, we take the corresponding quantities that were mentioned in [3]. For the unit of length, we use the length of capillary waves $h_\sigma = \sqrt{\frac{\sigma}{\rho_w g}} \approx 2.77 \times 10^{-3}$ m, where σ and ρ_w are the surface tension and density of water, respectively, and g is the acceleration of gravity. For the characteristic time, we select $t_* = \frac{h_\sigma}{v_\sigma} \approx 0.017$ s, where $v_\sigma = \sqrt{h_\sigma g}$ is the phase velocity of capillary waves. The scale of the temperature variation is chosen for reasons of convenience in the numerical calculations. We take $T_* = 0.5$ K. We denote $u = \frac{T}{T_*}$; $u_0 = \frac{T_0}{T_*}$; $z = \frac{\tilde z}{h_\sigma}$; $a = \frac{\tilde a}{h_\sigma}$; $t = \frac{\tilde t}{t_*}$; and $t_0 = \frac{\tilde t_0}{t_*}$.

Problem (1) written in dimensionless quantities has the form

$$\frac{\partial}{\partial z}\left(k(z)\frac{\partial u}{\partial z}\right) - \frac{\partial u}{\partial t} = f(u,z),$$
$$z \in (-a,a), \quad t \in (0;t_0); \qquad (3)$$
$$\left.\frac{\partial u}{\partial z}\right|_{z=-a} = 0; \quad \left.\frac{\partial u}{\partial z}\right|_{z=a} = 0; \quad u(z,0) = u_0(z).$$

Here, $k(z) = K(\tilde z)\frac{t_*}{h_\sigma^2}\frac{1}{c\rho}$ is the dimensionless coefficient of the heat conductivity.

According to data in [4], the quantity D in expression (2) for the heat-exchange coefficient should take the value of 0.6 W/(m K); then, for the dimensionless coefficient of heat conductivity in the region of molecular heat exchange from water, we obtain $k(z_0 - 0) \times 3.1 \times 10^{-4}$.

2. CHOOSING THE INHOMOGENEITY IN THE RIGHT-HAND SIDE PROCEEDING FROM THE THEORY OF CONTRAST STRUCTURES

This model was developed to describing laboratory experiments that are carried out during a time interval that is sufficiently short to make the effects of such factors as solar radiation, intense evaporation, intermixing, or waviness of the water surface on a considered object negligible. The model is based on the assumption that the entire water–air transition layer is an active medium, i.e., a medium that is far from the state of thermodynamic equilibrium [2]. The main property of an active medium is the ability to remain in one of the possible states that is determined by specified external factors for a long period of time and to switch from one such state to another state under the influence of an intense external action. The medium temperature in the boundary water–air layer can have two states under given external physical conditions: the temperature in the water, u_w, and the temperature in the air, u_a. The role of the external action that switches the medium state from the temperature u_w to the temperature u_a is played by the interface between the two media. In Eq. (3), according to the calculations that were presented in the previous section, there is a small parameter at the highest derivative with respect to the coordinate, i.e., the equation is singularly perturbed. To construct a model that describes the stationary transition layer, we draw on the investigations that were performed in a cycle of works that were devoted to studying singularly perturbed boundary problems that admit solutions in the form of contrasting structures [5–9]. When modeling the temperature distribution at the water–air boundary, the solution with an internal transition layer whose localization area does not vary during the considered time interval is of interest, i.e., in fact, this is the solution of the stationary problem for a second-order differential equation according to (3). In [9], the existence of a solution in this form was shown for the boundary problem for an ordinary differential equation of the second order in the case where the inhomogeneity in its right-hand side is a piecewise-continuous function. Relying on the results of this work, we chose the function $f(u, z)$ in the right-hand side of Eq. (3) in the form

$$f(u,z) = \begin{cases} u - (u_w + \delta W), & z < z_0; \\ u - (u_a + \delta A), & z \geq z_0. \end{cases}$$

Here, u_a and u_w are the known values of the temperature in the air and water, respectively. In laboratory conditions, these quantities are on the order of 300 K. Small-magnitude (on the order of several Kelvin) summands δA and δW are different from zero only on intervals of nonmonotonic variation in temperature; the intervals are clearly seen in the experimental plots. In particular, the quantity δA is different from zero at $z_2 < z < z_4$ (see Fig. 1); the quantity δW in the layer $z_3 < z < z_1$. The piecewise-continuous summand in the right-hand side of the heat-conductivity equation can be interpreted as a heat source that provides the existence of a transition layer whose position does not vary in time.

3. NUMERICAL CALCULATION

Problem (3) was solved numerically on the segment $z \in \left[-\frac{\tilde{a}}{h_\sigma}; \frac{\tilde{a}}{h_\sigma}\right]$, where $\tilde{a} = 0.05$ m and $h_\sigma = 2.7 \times 10^{-3}$ m. On this segment, a uniform grid of $N = 10\,000$ steps was introduced. The solution involved a six-point implicit scheme that is also called "the scheme with a half-sum" [10]. The temporal iterations were executed

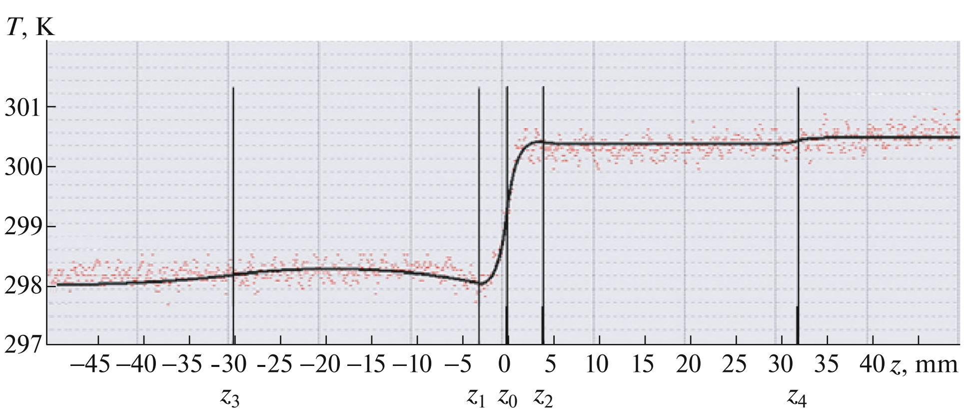

Fig. 2. A plot of the temperature distribution in a 10-cm wide near-boundary layer at the water–air interface in the case where the temperature of the water is lower than the temperature of air. The dots are the experimental measurements; the solid line is the result of the numerical calculation according to the proposed model.

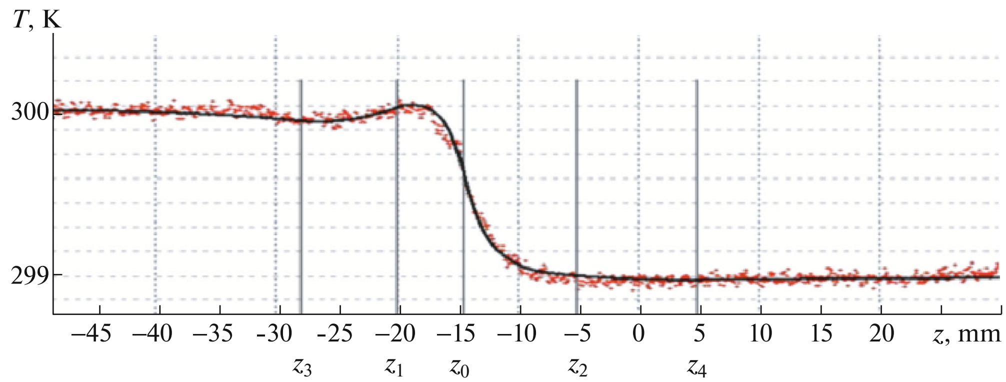

Fig. 3. The plot of the temperature distribution in a 10 cm wide near-boundary layer at the water–air interface in the case where the temperature of the water is higher than the temperature of air. The dots are the experimental measurements; the solid line is the result of the numerical calculation according to the proposed model.

with a step of $\tau = 0.001$ up to completion. The initial distribution was chosen in the form

$$u_0(z) = \begin{cases} u_w + 0.5(u_a - u_w)\exp(10(z - z_0)), & z < z_0; \\ u_a - 0.5(u_a - u_w)\exp(-10(z - z_0)), & z > z_0. \end{cases}$$

4. THE RESULTS OF THE NUMERICAL EXPERIMENTS

Figure 2 presents two plots of the temperature distribution in a 10-cm wide transition layer near the interface in the case where the air temperature is higher than the temperature of the water. The dots denote the results of experimental measurements [1]; the solid line denotes the result of the numerical solution of problem (3). The dimensionless heat-exchange coefficient was chosen as a piecewise-continuous function of the following form:

$$k(z) = \begin{cases} 2\cdot 10^{-2}, & z \le z_1; \\ 10^{-4}, & z_1 < z \le z_0; \\ 1.5\cdot 10^{-4}, & z_0 < z \le z_2; \\ 10^{-1}, & z > z_2. \end{cases}$$

Here, the designations $z_i = \dfrac{\tilde{z}_i}{h_\sigma}$, $i = 0, 1, 2$, are introduced. The parameters of the model are presented in Table 1.

Figure 3 presents plots of the temperature distribution in the transition layer in the case where the air temperature is lower than the temperature of the water. Here, the following expression for the dimensionless heat-exchange coefficient is used:

$$k(z) = \begin{cases} 3.1\cdot 10^{-2}, & z \le z_1; \\ 2\cdot 10^{-4}, & z_1 < z \le z_0; \\ 4\cdot 10^{-4}, & z_0 < z \le z_2; \\ 10^{-1}, & z > z_2. \end{cases}$$

The parameters of the model are presented in Table 2.

As is seen from the plots, the numerical calculations that were obtained based on the proposed model coincide well with the experimental data.

CONCLUSIONS

In this work, a mathematical model that describes the temperature distribution in the near-boundary layer at the water–air interface was proposed. The model was constructed using the theory of contrast

Table 1. The parameters of the model in the case where the temperature of the water is lower than the temperature of the ai

$u_a(K)$	$\delta A(K)$	$u_w(K)$	$\delta W(K)$	$\tilde{z}_0(m)$	$\tilde{z}_1(m)$	$\tilde{z}_2(m)$	$\tilde{z}_3(m)$	$\tilde{z}_4(m)$
300.4	–0.2	297.9	1.4	0	–0.003	0.004	–0.03	0.032

Table 2. The parameters of the model in the case where the temperature of the water is higher than the temperature of the air

$u_a(K)$	$\delta A(K)$	$u_w(K)$	$\delta W(K)$	$\tilde{z}_0(m)$	$\tilde{z}_1(m)$	$\tilde{z}_2(m)$	$\tilde{z}_3(m)$	$\tilde{z}_4(m)$
299	–1.5	300.1	–3	–0.0145	–0.02	–0.005	–0.028	0.005

structures. Based on this theory, the model boundary problem is formulated such that its solution has an internal transition layer whose position does not vary in time. Using this model makes it possible to determine the relationships between heat-exchange coefficients in different layers of a stratified medium, as well as the width of each of the layers and the quantity of heat that is released or absorbed in regions with an inverse temperature distribution. One should also note that this model can be modified. In particular, using this model one can describe temperature distributions that vary in time, e.g., daily or seasonal oscillations in near-surface layers of basins.

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