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Boundary Value Problem of Mass and Heat Transfer of an Evaporating Spherical Droplet

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Abstract—Approximate solutions of stationary diffusion and thermal conductivity equations are obtained for the power-law dependence of the molecular transfer coefficients (thermal conductivity, diffusion) and the density of a binary viscous non-isothermal gas medium on temperature.

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1. PROBLEM STATEMENT

Transfer phenomena are nonequilibrium processes that occur in a thermodynamically nonequilibrium system—the spatial transfer of energy, matter, momentum or some other physical quantity. The reason for this transfer is disturbances that violate the state of thermodynamic equilibrium. For example, the presence of spatial inhomogeneities of temperature, composition, or average velocity of the particles of the system. The transfer of a physical quantity occurs in the direction opposite to its gradient, as a result of which the thermodynamic system isolated from external influences approaches the state of thermodynamic equilibrium. Transfer phenomena occur stationary if external influences are maintained constant.

The significance of heat and mass exchange processes in production, nature, etc. is determined by the fact that the properties of bodies depend most significantly on their thermal state, which, in turn, is itself determined by the conditions of heat and mass exchange. These conditions have a significant impact on the processes of changing the state of matter, mechanical, thermal, magnetic and other properties of bodies. This explains the intensive development of the theory of heat and mass transfer and the extremely important importance that they are given in industry, medicine, energy, agriculture and nature.

As a rule, the transfer of heat (matter) in solids, liquids and gases is subject to conditionally accepted linear dependencies. For example, heat transfer—Fourier's law: the density of the heat flux (specific heat flux) is proportional to the temperature gradient; molecular transfer of matter—Fick's diffusion law: the density of the flow of matter is proportional to the concentration gradient (the difference in diffusion chemical potentials). Based on these linearized laws, the corresponding differential equations are derived.

When describing the behavior of particles suspended in thermodynamically nonequilibrium in temperature and concentration of viscous gaseous media, a dimensionless parameter Θ is introduced, characterizing the relative temperature difference between the average surface temperature of the particle (T_S) and the temperature of the gaseous medium away from it (T_∞) to the latter, i.e. $\Theta = (T_S - T_\infty)/T_\infty$. The relative temperature difference is considered small if the inequality $\Theta \ll 1$ is satisfied and significant if $\Theta \sim (1)$. When the first condition is met, the coefficients of molecular transport (viscosity, thermal

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conductivity, diffusion) and density of a viscous gaseous medium can be considered constant values, and the medium itself isothermal. This condition significantly simplifies the mathematical procedure for finding expressions for the fields of temperatures, concentrations, pressures, etc. in a thermodynamic system (see, for example, (see, for example, [4–6]). If $\Theta \sim (1)$, the particle is called heated (heating of the particle surface can be caused, for example, by the course of a volumetric chemical reaction, the process of radioactive decay of the particle substance, absorption of electromagnetic radiation by the particle, etc.), and the viscous medium is non-isothermal. In this case, it is already necessary to take into account the dependence of the molecular transfer coefficient and the density of the gaseous medium on temperature, and the system of gas-dynamic equations describing such a medium becomes essentially nonlinear. There are few works in the scientific literature devoted to the study of this case, for example (see, for example, [7, 8]).

2. STATEMENT OF THE PROBLEM: BASIC EQUATIONS AND BOUNDARY CONDITIONS

The steady-state diffusion process is considered between an evaporating spherical drop of radius R with density ρ_i, thermal conductivity λ_i, viscosity μ_i and a viscous non-isothermal binary gas mixture with density ρ_e, thermal conductivity λ_e, diffusion D_{12} and viscosity μ_e during its flow a plane-parallel flow directed along the Oz axis with a velocity of $\mathbf{U}_\infty$. Heat sources with a density of q_i operate inside the particle. This leads to the fact that the average surface temperature of the particle differs significantly from the temperature away from it, i.e. $\Theta \sim (1)$. The gas medium consists of two components C_1 and C_2. The component C_2 is considered the main (carrier), and the boundary surface is impervious to it. The substance of which the drop consists experiences a phase transition at the spherical interface of the drop-binary gas mixture. We will assume that this is a component of C_1, i.e. in its physicochemical composition it coincides with the substance of a liquid drop and the boundary surface for it is continuous. Here $C_1 = n_1/n_e$, $C_2 = n_2/n_e$ are the relative concentrations of the first and second components, $n_e = n_1 + n_2$, $\rho_e = \rho_1 + \rho_2$, $\rho_1 = m_1 n_1$, $\rho_2 = m_2 n_2$, m_1, n_1 and m_2, n_2 mass and numerical concentration of molecules of the first and second components of the mixture. From the definition of relative concentrations, it follows that $C_1 + C_2 = 1$ and the first component satisfies the condition $C_1 \ll C_2$. This inequality means that the evaporation of the droplet proceeds in a diffusion mode, i.e. when the main influence on the process of heat and mass transfer in the vicinity of a drop is determined by molecular diffusion, described by the equation (1) [4, 5].

$$\operatorname{div}\left(\frac{n_e^2 m_1 m_2}{\rho_e} D_{12} \nabla C_1\right) = 0. \tag{1}$$

The steady-state diffusion process is considered in a spherical coordinate system $(y = r/R, \theta, \varphi)$ associated with the center of mass of the particle. With the specified choice of the origin of the coordinate system, the distributions of velocities, pressures, concentrations and temperatures outside and inside the evaporating droplet have axial symmetry with respect to the Oz axis, i.e. they are functions of two variables y, θ. The indices "e" and "i" hereafter refer to the binary gas mixture and the evaporating droplet, and the index "∞" are physical quantities characterizing the gas medium in an undisturbed flow.

A TASK. A viscous non-isothermal binary gas mixture occupies an unlimited region $\Omega \subset R^3$. You want to find the distribution the relative concentration of C_1 in the binary mixture that satisfies the diffusion equation (1), and distribution outside temperature (T_e) and in (T_i) of the evaporating liquid droplets are described by the heat conduction equations (2) [5]

$$\operatorname{div}\left(\lambda_e \nabla T_e\right) = 0, \quad \operatorname{div}\left(\lambda_i \nabla T_i\right) = -q_i, \tag{2}$$

with boundary conditions

$$\lim_{y\to\infty} T_e = T_\infty, \quad \lim_{y\to\infty} C_1 = C_{1\infty}, \qquad \lim_{y\to 0} T_i \neq \infty. \tag{3}$$

Here q_i is the density of heat sources, due to which the surface of the drop is heated.

In the boundary conditions (3) away from the droplet, the temperature, the relative concentration of the diffusing component is set and the finiteness of the temperature in the center of the particle is taken into account. As for the boundary conditions for the diffusion equation on the surface of the evaporating drop itself, we do not give. They are determined by a specific physical problem, which allows us to obtain a solution of the equation (1) in general form. The problem is solved by the hydrodynamic method, i.e. the equations of gas dynamics with the corresponding boundary conditions are solved.

When describing the properties of a binary gas mixture, the power-law form of the dependence of the molecular transfer coefficients and the density of the medium on the temperature [2] is taken into account

$$\mu_e = \mu_\infty\left(\frac{T_e}{T_\infty}\right)^{\beta}, \quad \rho_e = \rho_\infty\frac{T_\infty}{T_e}, \quad \lambda_e = \lambda_\infty\left(\frac{T_e}{T_\infty}\right)^{\alpha},$$
$$D_{12} = D_\infty\left(\frac{T_e}{T_\infty}\right)^{1+\omega}, \quad \lambda_i = \lambda_{i0}\left(\frac{T_i}{T_\infty}\right)^{\gamma}, \tag{4}$$

where $\mu_\infty = \mu_E(T_\infty)$, $\rho_\infty = \rho_E(T_\infty)$, $\lambda_\infty = \lambda_E(T_\infty)$, $D_\infty = D_{12}(T_\infty)$, $\lambda_{i0} = \lambda_i(T_\infty)$, $0.5 \le \alpha, \beta, \omega \le 1$, $-1 \le \gamma \le +1$ [2].

Taking into account the power-law dependence of the molecular transfer coefficients and the density of the medium on temperature, we obtain a rather complex nonlinear system of gas-dynamic equations, and, naturally, the question arises about the method of solving this nonlinear system of equations and about the assumptions justified, for example, from a physical point of view, which need to be done to solve the problem. The study showed that for most gaseous media, the thermal conductivity coefficient of the particle (λ_i) is much larger in magnitude than the thermal conductivity coefficient of the gas (λ_e), i.e. $\lambda_e \ll \lambda_i$. There is a weak angular asymmetry of the temperature distribution in the "particle–gas" system. This leads to the fact that the viscosity is related only to the temperature $T_e^{(0)}(y)$: $\mu_e(T_e(y,\theta)) \approx \mu_e(T_e^{(0)}(y))$. At the same time, $T_e(y,\theta) = T_e^{(0)}(y) + \delta T_e(y,\theta)$, where $\delta T_e(y,\theta) \ll T_e^{(0)}(y)$; $T_e^{(0)}(y)$, $\delta T_e(y,\theta)$ are determined from the solution of the thermal problem. This assumption leads to the fact that the diffusion equations and the thermal conductivity equations make it possible to obtain analytical solutions.

3. SOLUTION OF THE DIFFUSION AND THERMAL CONDUCTIVITY EQUATIONS

The general solution of the first equation (2) satisfying the first boundary condition (3) taking into account (4) has the form

$$t_e(y,\theta) = \left[1 + \frac{N_0}{y} + \sum_{n=1}^{\infty}\left(\frac{N_n}{y^{n+1}} + D_n y^n\right)P_n(\cos\theta)\right]^{1/(1+\alpha)}, \quad t_e = T_e/T_\infty.$$

Here $P_n(\cos\theta)$ is Legendre polynomials; N_0, N_n, D_n are constant integrations that are determined from the boundary conditions on the surface of the evaporating droplet.

In our problem there is a small parameter $\varepsilon = Re_\infty$, i.e. when solving (1), (2), we can use the perturbation theory [1]. From the defining parameters of our problem, we can make the Reynolds number $Re_\infty = \left(\rho_\infty R U_\infty\right)/\mu_\infty \ll 1$. Here $U_\infty = |\mathbf{U}_\infty|$. The incoming flow has only a disturbing effect. Therefore, the function $t_e(y,\theta)$ is in magnitude proportional to the perturbation and hence

$$t_e(y,\theta) = t_{e0}(y) + \frac{t_{e0}^{-\alpha}(y)}{1+\alpha}\sum_{n=1}^{\infty}\left(\frac{N_n}{y^{n+1}} + D_n y^n\right)P_n(\cos\theta), \quad t_{e0}(y) = \left(1 + \frac{N_0}{y}\right)^{\frac{1}{1+\alpha}},$$

and accordingly

$$t_e^{\omega}(y,\theta) = t_{e0}^{\omega}(y) + \frac{\omega}{1+\alpha}t_{e0}^{\omega-\alpha-1}\sum_{n=1}^{\infty}\left(\frac{N_n}{y^{n+1}} + D_n y^n\right)P_n(\cos\theta). \tag{5}$$

The general solution of the second equation (2) satisfying the second boundary condition (3), i.e. the extremity of temperature at $y \to 0$ has the form

$$t_i(y,\theta) = t_{i0}(y) + \frac{t_{i0}^{-\gamma}(y)}{1+\gamma}\sum_{n=1}^{\infty}\left[\frac{H_n}{y^{n+1}} + D_n y^n\right.$$

$$+\frac{1}{2n+1}\left(y^n\int\limits_1^y\frac{q_{in}}{y^{n-1}}dy-\frac{1}{y^{n+1}}\int\limits_1^y q_{in}y^{n+2}dy\right)\Bigg]P_n(\cos\theta),$$

$$t_{i0}(y)=\left(B_0+\frac{H_0}{y}+y\int\limits_1^y yq_{i0}dy-\frac{1}{y}\int\limits_1^y y^2q_{i0}dy\right)^{\frac{1}{1+\gamma}},$$

where

$$H_n=\frac{1}{2n+1}\int\limits_1^0 y^{n+2}q_{in}(y)dy,\quad q_{in}(y)=-\frac{1+\gamma}{\lambda_{i0}T_\infty}R^2\frac{2n+1}{2}\int\limits_{-1}^{+1}q_iP_n(x)d(x),\quad x=\cos\theta,$$

B_n are integration constants, which are determined from the boundary conditions on the surface of the evaporating droplet. Substituting the expression (1) into the diffusion equation (5) get

$$\operatorname{div}\left(t_{e0}^{\omega}\nabla C_1\right)=-\frac{\omega}{1+\alpha}\operatorname{div}\left[t_{e0}^{\omega-\alpha-1}\sum_{n=1}^{\infty}\left(\frac{N_n}{y^{n+1}}+D_ny^n\right)P_n(\cos\theta)\nabla C_1\right].\tag{6}$$

We will search for the solution of the equation (6) in the form

$$C_1(y,\theta)=\sum_{n=0}^{\infty}\frac{\psi_n(y)}{y^{n+1}}P_n(\cos\theta).$$

Function $C_1(y,\theta)$ is proportional in magnitude to the perturbation, i.e.

$$C_1(y,\theta)=C_{10}(y)+C_{11}(y,\theta),\quad C_{11}(y,\theta)\ll C_{10}(y),$$
$$C_{10}=\frac{\psi_0(y)}{y},\quad C_{11}(y,\theta)=\sum_{n=1}^{\infty}\frac{\psi_n(y)}{y^{n+1}}P_n(\cos\theta).\tag{7}$$

After substituting (7) into the equations (6) and using the orthogonality condition of Legendre polynomials, we obtain two equations in a spherical coordinate system

$$\frac{1}{y^2}\frac{d}{dy}\left(y^2t_{e0}^{\omega}(y)\frac{dC_{10}}{dy}\right)=0,\tag{8}$$

$$\frac{1}{y^2}\frac{d}{dy}\left[y^2t_{e0}^{\omega}\frac{d}{dy}\left(\frac{\psi_n}{y^{n+1}}\right)\right]-\frac{n(n+1)}{y^{n+3}}t_{e0}^{\omega}\psi_n$$
$$=-\frac{\omega}{y^1(1+\alpha)}\frac{d}{dy}\left[y^2t_{e0}^{\omega-\alpha-1}\left(D_ny^n+\frac{N_n}{y^{n+1}}\right)\frac{dC_{10}}{dy}\right].\tag{9}$$

The general solution of the equation (8) satisfying the second boundary condition (2) has the form

$$C_{10}(y)=C_{1\infty}+M\left(t_{e0}^{1+\alpha-\omega}-1\right).\tag{10}$$

Here M is a constant determined from the boundary conditions on the drop surface. Substituting (10) into (9), we obtain the following equation for finding the function $\psi_n(y)$

$$y^2\frac{d^2\psi_n}{dy^2}-y(2n+s\ell)\frac{d\psi_n}{dy}+s\ell(n+1)\psi_n$$
$$=\frac{\omega(1+\alpha-\omega)}{(1+\alpha)^2}M\frac{\ell}{t_{e0}^{\omega}}\left[D_ny^{2n+1}(n+\ell)+N_n(\ell-n-1)\right].\tag{11}$$

Here $s = \omega/(1+\alpha)$, $\ell = N_0/(N_0 + y)$. The partial solution of the equation (11) has the form

$$\Phi_n(y) = \frac{1+\alpha-\omega}{1+\alpha} M \frac{\ell}{t_{e0}^{\omega}} \Big[D_n y^{2n+1} + N_n \Big].$$

Let's find a solution to the homogeneous equation (11), for this we go to the new variable $z = y/N_0$, we get

$$(1+z^2)z^2 \frac{d^2\psi_n}{dz^2} - z\,[2nz + 2n + s]\,\frac{d\psi_n}{dz} + (n+1)z\psi_n = 0,$$

and we are seeking for a solution to this equation in the form

$$\psi_n(z) = \left(1 + \frac{1}{z}\right)^{\delta n} f_n(z),$$

here $\delta_n = -\frac{1}{2}(2n+1+s) + \frac{1}{2}\sqrt{(2n+1)^2 - 2s + s^2}$. The function f_n is determined from the solution of the equation

$$t(t-1)f_n''(t) - \big[2(n+1) + t(2\delta_n + s - 2)\big] f_n'(t) - (n+1)(2\delta_n + s) f_n(t) = 0, \quad t = \frac{1}{1+z}. \quad (12)$$

If in the equation (12) enter the notation $\gamma_n = 2(n+1)$, $\alpha_n = -\delta_n$, $\beta_n = 1 - \delta_n - s$, then the equation (12) takes the form

$$t(1-t)f_n''(t) + \big[\gamma_n - (\alpha_n + \beta_n + 1)t\big] f_n'(t) - \alpha_n \beta_n f_n(t) = 0,$$

and its solution is the hypergeometric function $F_n(\alpha_n, \beta_n; \gamma_n; t)$ [3].

Theorem. *The general solution of the equation (1) satisfying the boundary conditions (3) has the form*

$$C_1(y,\theta) = C_{10}(y) + \sum_{n=1}^{\infty} \frac{P_n(x)}{y^{n+1}} \left[\Phi_n(y) + L_n \left(1 + \frac{N_0}{y}\right)^{\delta_n} F_n(\alpha_n, \beta_n; \gamma_n; \ell) \right],$$

$$C_{10}(y) = C_{1\infty} + M\left(t_{e0}^{1+\alpha-\omega} - 1\right), \quad t_{e0}(y) = \left(1 + \frac{N_0}{y}\right)^{\dfrac{1}{1+\alpha}},$$

$$\Phi_n(y) = \frac{1+\alpha-\omega}{1+\alpha} \frac{M}{t_{e0}^{\omega}} \Big[D_n y^{2n+1} + N_n \Big],$$

$$\delta_n = -\frac{1}{2}\big(2n+1+s\big) + \frac{1}{2}\sqrt{(2n+1)^2 - 2s + s^2}, \quad \alpha_n = -\delta_n,$$

$\beta_n = 1 - \delta_n - s$, $\gamma_n = 2(n+1)$, $\ell = \frac{N_0}{N_0+y}$, $s = \frac{\omega}{1+\alpha}$, $F_n(\alpha_n, \beta_n; \gamma_n; \ell)$ *is hypergeometric function.*

4. CONCLUSIONS

Assuming a weak temperature inhomogeneity in the angular part (the thermal conductivity coefficient of a particle is much larger in magnitude than the thermal conductivity coefficient of a gas), which is the case for most physical applications, a general solution of the stationary diffusion equation has been found with a power-law dependence of the molecular transfer coefficients (viscosity, thermal conductivity, diffusion) and the density of a binary non-isothermal gas mixture on temperature.

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