BOUNDARY CONDITIONS AT A SURFACE UNDERGOING SUBLIMATION INTO A RAREFIED MULTICOMPONENT GAS

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Boundary conditions have been found for flow of a rarefied multicomponent gas over a sublimating wall. For a multi-component gas the boundary conditions obtained are a generalization of the well-known conditions for slip and temperature jump in the case of a permeable surface.

It is well known that to solve the coupled problem in the case of sublimation of a wall washed by a stream of any thermally conducting gas, in order to have a single-valued transition through the wall-gas interface, besides the condition obtained from the laws of conservation, additional relations are required [1]. For a sufficiently dense mixture of gases, the assumption is made that the temperature and the tangential velocity components are equal on the two sides of the interface. The additional relation for the mixture composition at the interface depends on the kinetics of sublimation. In particular, if sublimation proceeds according to diffusion kinetics, the additional relation is the dependence of partial pressure of the vapor on temperature.

For sublimation of a wall into a stream of rarefied gas the additional relations must be different. Instead of the conditions for no slip and equality of temperature at the interface, discontinuities in velocity and temperature must be taken into account. In addition, lack of equilibrium in sublimation must be taken into account. It must be expected that, in the case of a nonzero vertical velocity component at the wall, the additional boundary conditions will differ from the conditions valid in the absence of flow of mass through the wall.

The derivation of these conditions for a gas-vapor mixture is analogous to that of similar conditions for a homogeneous gas given in [2]. The distribution function in the 13-moment approximation must be written for each component of the mixture. Some arbitrariness is possible in the choice of a local Maxwellian distribution function, about which we may carry out an expansion in terms of Hermite polynomials [3]. In the present paper we use the mean mass flow velocity in the local Maxwellian function, and all the components of the mixture have the same temperature. The distribution function for an individual component has the following form [4]:

$$f^{(r)} = \frac{\rho^{(r)}}{(2\pi R^{(r)} T)^{3/2}} \times$$

$$\times \left[1 + \frac{p_{ij}^{(r)} u_i u_j}{2p^{(r)} R^{(r)} T} - \frac{S_i^{(r)} u_i}{2p^{(r)} R^{(r)} T} \left(1 - \frac{u^2}{5R^{(r)} T} \right) + \right.$$

$$\left. + \frac{u_i V_i^{(r)}}{2R^{(r)} T} \left(7 - \frac{u^2}{R^{(r)} T} \right) \right] \exp\left\{ - \frac{u^2}{2R^{(r)} T} \right\}, \qquad (1)$$

where $r = 1, 2, 3 \ldots n$; $\vec{u} = \vec{\xi} - \vec{v}$; $p_{ij}^{(r)} = P_{ij}^{(r)} - p^{(r)} \delta_{ij} = \int u_i u_j f^{(r)} d\vec{\xi} - p^{(r)} \delta_{ij}$ is the viscous stress tensor of component r; $S_i^{(r)} = \int u_i u^2 f^{(r)} d\vec{\xi}$ is the binary heat flux of component r; and $V_i^{(r)} = \frac{1}{\rho^{(r)}} \int u_i f^{(r)} d\vec{\xi}$ is the diffusion velocity of component r.

The viscous stress tensor and the heat flux of the mixture are determined by summing the appropriate moments for the individual components:

$$p_{ij} = \sum_r p_{ij}^{(r)}, \quad S_i = \sum_r S_i^{(r)}.$$

We shall assume, as was done in [2, 5], that a definite fraction $\alpha^{(r)}$ of the molecules of the incident molecules of type r is reflected specularly, while the remaining molecules are absorbed by the wall and then emitted diffusely with the Maxwellian distribution corresponding to the wall temperature*:

$$f^{+(r)}(\xi_1, \xi_2, \xi_3) =$$

$$= \alpha^{(r)} f^{-(r)}(-\xi_1, \xi_2, \xi_3) + \beta^{(r)} \exp\left\{ - \frac{\xi^2}{2R^{(r)} T_0} \right\},$$

$$\xi_1 > 0, \qquad (2)$$

where

$$f^{(r)}(\vec{\xi}) = f^{+(r)}(\vec{\xi}) + f^{-(r)}(\vec{\xi});$$

$$f^{+(r)}(\vec{\xi}) = 0 \quad \text{for} \quad \xi_1 < 0, \quad f^{-(r)}(\vec{\xi}) = 0 \quad \text{for} \quad \xi_1 > 0.$$

The coefficient $\beta^{(1)}$ for a subliming component (r = = 1) is determined by the rate of sublimation, and the coefficients $\beta^{(2)}$, $\beta^{(3)} \ldots \beta^{(n)}$ for the remaining components of the gas mixture are determined by the conditions for absence of mass flux of these components through the wall.

We shall choose the axis x_1 and x_2 along the normal to the wall surface and along the surface, respectively, making the assumption that the shape of the

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*The sublimating wall is displaced in the direction of the x_1 axis with velocity D, and therefore the second term in the boundary condition (2) must have the following form:

$$\beta^{(r)} \exp\left\{ - \frac{(\xi_1 - D)^2 + \xi_2^2 + \xi_3^2}{2R^{(r)} T_0} \right\}.$$

But the velocity D is considerably less than the mass flow velocity of the vapor v_1, because the ratio of the density of the gas mixture to that of the solid is small. Therefore, we may neglect terms containing D in subsequent computations, which allows us to write the boundary condition in the form of (2).

body is maintained during sublimation. We shall find the boundary conditions in the same way as was done in [2, 5], i.e., we shall determine the moments of boundary condition (2) relative to ξ_1, u_1u_2, u_1^2, u_1u^2 for each component of the mixture, i.e., we shall multiply this condition respectively by ξ_1, u_1u_2, u_1^2, u_1u^2, and integrate with respect to $\vec{\xi}$. We shall determine $\beta^{(r)}$ from moments with respect to ξ_1. We shall sum over r the moments with respect to u_1u_2, u_1^2, u_1u^2. Here we shall assume that the mass flow velocity of vapor v_1 is considerably less than the mean velocity of thermal motion a. In addition, bearing in mind the Navier-Stokes approximation, we shall consider the quantities $p_{12}^{(r)}/p^{(r)}$, $S_i^{(r)}/p^{(r)}(R^{(r)}T)^{1/2}$, the relative slip velocity v_2/a, the relative temperature jump $(T - T_0)/T$, and the relative diffusion velocities $V_i^{(r)}/a$ to be small (because variation of velocity, temperature, and concentration is small in a mean free path). For simplicity of computation we shall assume also that the ratio $p_{11}^{(r)}/p_{12}^{(r)}$ is small (this is true for the boundary layer approximation and for Couette flow).

Neglecting derivatives of small quantities, we obtain

$$\frac{1}{2}\sum_r(1+\alpha^{(r)})p_{12}^{(r)}+\frac{1}{10(2\pi T)^{1/2}}\sum_r\frac{(1-\alpha^{(r)})S_2^{(r)}}{(R^{(r)})^{1/2}}+$$

$$+\frac{1}{(2\pi T)^{1/2}}\sum_r\frac{(1-\alpha^{(r)})p^{(r)}(v_2+V_2^{(r)}/2)}{(R^{(r)})^{1/2}}=0, \tag{3}$$

$$\frac{1}{2}\sum_r(1+\alpha^{(r)})S_1^{(r)}+4\left(\frac{T}{2\pi}\right)^{1/2}\left(1-\frac{T_0}{T}\right)\times$$

$$\times\sum_r(1-\alpha^{(r)})p^{(r)}(R^{(r)})^{1/2}+\frac{5}{2}v_1\sum_r(1+\alpha^{(r)})p^{(r)}-$$

$$-2(1+\alpha^{(1)})p^{(1)}(v_1+V_1^{(1)})=0, \tag{4}$$

$$\frac{1}{2}\left[1-\left(\frac{T_0}{T}\right)^{1/2}\right]\sum_r(1-\alpha^{(r)})p^{(r)}+$$

$$+\frac{1}{5(2\pi T)^{1/2}}\sum_r\frac{(1+\alpha^{(r)})S_1^{(r)}}{(R^{(r)})^{1/2}}+$$

$$+\frac{2-\pi}{2(2\pi T)^{1/2}}\sum_r\frac{(1+\alpha^{(r)})p^{(r)}V_1^{(r)}}{(R^{(r)})^{1/2}}+\left(\frac{2}{\pi T}\right)^{1/2}\times$$

$$\times v_1\sum_r\left[1-\frac{\pi}{4}-\alpha^{(r)}\left(1+\frac{\pi}{4}\right)\right]\frac{p^{(r)}}{(R^{(r)})^{1/2}}=0. \tag{5}$$

Condition (2) contains no assumptions relating to the kinetics of sublimation. However, the following assumptions are frequently made [6]:

1. The true velocity of evaporation (the mass of molecules leaving unit surface area in unit time) does not depend only on the partial pressure of the other components of the gas mixture, but also on the partial pressure of the sublimating component, i.e., it is the same as for equilibrium sublimation.
2. The fraction of incident molecules, condensing upon collision with the surface, does not depend on the partial pressure of the other components, nor on the true rate of evaporation of the given component.

These assumptions allow us to write down the boundary condition for the distribution function (1) in the form

$$f^{+(r)}(\xi_1,\ \xi_2,\ \xi_3)=$$

$$=\alpha^{(r)}f^{-(r)}(-\xi_1,\ \xi_2,\ \xi_3)+(1-\alpha^{(r)})f^{0(r)}(\xi_1,\ \xi_2,\ \xi_3), \tag{6}$$

where

$$f^{0(r)}=\frac{\rho^{0(r)}}{(2\pi R^{(r)}T)^{3/2}}\exp\left\{-\frac{\xi^2}{2R^{(r)}T_0}\right\};$$

$\rho^{0(1)}$ is the density of saturated vapor of component 1 at the wall temperature T_0. By determining the same moments of expression (6), we obtain a somewhat different form of boundary conditions. In particular, computation of the moment of condition (6) relative to ξ_1 for the sublimating component gives

$$\rho^{(1)}(v_1+V_1^{(1)})=\rho v_1=$$

$$=\frac{2(1-\alpha^{(1)})}{1+\alpha^{(1)}}\left(\frac{p_0^{(1)}}{\sqrt{2\pi R^{(1)}T_0}}-\frac{p^{(1)}}{\sqrt{2\pi R^{(1)}T}}\right)=$$

$$=\frac{2f^*}{2-f^*}\left(\frac{p_0^{(1)}}{\sqrt{2\pi R^{(1)}T_0}}-\frac{p^{(1)}}{\sqrt{2\pi R^{(1)}T}}\right).$$

The relation obtained for the mass rate of evaporation differs from the analogous relation presented in [7] by a coefficient on the right ahead of the brackets.

We shall now express the moments $p_{12}^{(r)}$, $V_i^{(r)}$, $S_i^{(r)}$ for a binary mixture (r = 1, 2) in the Navier-Stokes approximation, in terms of the corresponding appropriate gradients (see shall neglect thermodiffusion and pressure diffusion):

$$p_{12}^{(r)}=-\mu^{(r)}\frac{\partial v_2}{\partial x_1}\ \text{in the boundary layer and in Couette flow,}$$

$$\rho^{(r)}V_i^{(r)}=-\rho D_{12}\frac{\partial c^{(r)}}{\partial x_i},$$

$$S_i^{(r)}=-2\lambda^{(r)}\frac{\partial T}{\partial x_i}+5\rho^{(r)}R^{(r)}TV_i^{(r)}=-2\lambda^{(r)}\frac{\partial T}{\partial x_i}-$$

$$-5\rho TR^{(r)}D_{12}\frac{\partial c^{(r)}}{\partial x_i}.$$

Here

$$p_{12}=\sum_{r=1,2}p_{12}^{(r)}=-(\mu_{12}^{(1)}+\mu_{12}^{(2)})\frac{\partial v_2}{\partial x_1}=-\mu\frac{\partial v_2}{\partial x_1},$$

$$\mu=\mu_{12}^{(1)}+\mu_{12}^{(2)};$$

$$S_i=\sum_{r=1,2}S_i^{(r)}=$$

$$=-2(\lambda_{12}^{(1)}+\lambda_{12}^{(2)})\frac{\partial T}{\partial x_i}-5T\rho D_{12}(R^{(1)}-R^{(2)})\frac{\partial c}{\partial x_i}=$$

$$=-2\lambda\frac{\partial T}{\partial x_i}-5T\rho D_{12}(R^{(1)}-R^{(2)})\frac{\partial c}{\partial x_i},$$

$$\lambda=\lambda_{12}^{(1)}+\lambda_{12}^{(2)},$$

i.e., the coefficients $\mu_{12}^{(r)}$, $\lambda_{12}^{(r)}$ are not the corresponding coefficients for transfer of component r, but depend on collisions of molecules of a given component both with molecules of the same type r, and with molecules of the other component.

Starting from the approximate formulas for the viscosity and thermal conductivity of the mixture given in [7], we may write the coefficients $\mu_{12}^{(1)}$ and $\mu_{12}^{(2)}$, $\lambda_{12}^{(1)}$ and $\lambda_{12}^{(2)}$ in the following form:

$$\mu_{12}^{(1)} = \frac{\mu_1}{1 + G_{12}(1-c)/c}, \quad \mu_{12}^{(2)} = \frac{\mu_2}{1 + G_{21}c/(1-c)},$$

$$\lambda_{12}^{(1)} = \frac{\lambda_1}{1 + G'_{12}(1-c)/c}, \quad \lambda_{12}^{(2)} = \frac{\lambda_2}{1 + G'_{21}c/(1-c)},$$

where G_{12}, G_{21}, G'_{12}, G'_{21} are functions of the ratio of the molecular weights of the components and quantities describing the collision process.

The experimental data on the accommodation coefficients f^* are very conflicting. Therefore, for simplicity of calculation, we shall consider that $f^{*(1)} = f^{*(2)}$, i.e., $\alpha^{(1)} = \alpha^{(2)}$. Allowing for the assumptions made, the boundary conditions (3)–(5) may be represented in the form

$$-\frac{2-f^*}{f^*}\mu\frac{\partial v_2}{\partial x_1} - \frac{1}{5(2\pi T)^{1/2}}\left[\frac{\lambda_{12}^{(1)}}{(R^{(1)})^{1/2}} + \frac{\lambda_{12}^{(2)}}{(R^{(2)})^{1/2}}\right]\times$$

$$\times\frac{\partial T}{\partial x_2} - \rho D_{12}\left(\frac{T}{2\pi}\right)^{1/2}[(R^{(1)})^{1/2} - (R^{(2)})^{1/2}]\frac{\partial c}{\partial x_2} +$$

$$+\rho\left(\frac{T}{2\pi}\right)^{1/2}[c(R^{(1)})^{1/2} + (1-c)(R^{(2)})^{1/2}]v_2 = 0, \tag{7}$$

$$-\frac{2-f^*}{f^*}\lambda\frac{\partial T}{\partial x_1} + 4\rho\left(\frac{T}{2\pi}\right)^{1/2}(T-T_0)[c(R^{(1)})^{3/2} +$$

$$+(1-c)(R^{(2)})^{3/2}] + \frac{2-f^*}{2f^*}\rho D_{12}T[5R^{(2)} - R^{(1)}]\frac{\partial c}{\partial x_1} +$$

$$+\frac{2-f^*}{2f^*}\rho T[cR^{(1)} + 5(1-c)R^{(2)}]v_1 = 0, \tag{8}$$

$$-\frac{2(2-f^*)}{5(2\pi T)^{1/2}f^*}\left[\frac{\lambda_{12}^{(1)}}{(R^{(1)})^{1/2}} + \frac{\lambda_{12}^{(2)}}{(R^{(2)})^{1/2}}\right]\frac{\partial T}{\partial x_1} +$$

$$+\frac{\rho T}{2}\left[1 - \left(\frac{T_0}{T}\right)^{1/2}\right][cR^{(1)} + (1-c)R^{(2)}] -$$

$$-\frac{2-f^*}{2f^*}\left(\frac{T}{2\pi}\right)^{1/2}\rho D_{12}(4-\pi)[(R^{(1)})^{1/2} - (R^{(2)})^{1/2}]\times$$

$$\times\frac{\partial c}{\partial x_1} + \rho\left(\frac{2T}{\pi}\right)^{1/2}\left[1 - \frac{\pi(2-f^*)}{4f^*}\right][c(R^{(1)})^{1/2} +$$

$$+(1-c)(R^{(2)})^{1/2}]v_1 = 0. \tag{9}$$

Conditions (7) and (8) are a generalization of the well-known boundary conditions for slip and temperature jump in the case of a binary mixture and a permeable surface.

For a multicomponent gas (sublimation of a flat plate into a vapor of the same composition, or outgassing in a boundary layer), taking into account the well-known relations $\mu = \rho l(2RT/\pi)^{1/2}$, $\lambda = (15/4)R\mu$, conditions (7)–(9) take the following form:

$$v_2 = \frac{2-f^*}{f^*}l\frac{\partial v_2}{\partial x_1} + \frac{3}{4}l\left(\frac{2R}{\pi T}\right)^{1/2}\frac{\partial T}{\partial x_2}, \tag{10}$$

$$T - T_0 = \frac{2-f^*}{f^*}\left[\frac{15}{8}l\frac{\partial T}{\partial x_1} - \frac{v_1}{8}\left(\frac{2\pi T}{R}\right)^{1/2}\right], \tag{11}$$

$$T\left[1 - \left(\frac{T_0}{T}\right)^{1/2}\right] - \frac{3(2-f^*)}{\pi f^*}l\frac{\partial T}{\partial x_1} +$$

$$+2\left(\frac{2T}{\pi R}\right)^{1/2}\left[1 - \frac{\pi(2-f^*)}{4f^*}\right]v_1 = 0. \tag{12}$$

It should be noted that the slip condition (10) does not contain the velocity v_1 in the approximation adopted, i.e., it coincides with the analogous condition in the case when mass flow through the wall is absent.

NOTATION

$\rho^{(r)}$ is the density of component r; $p^{(r)}$ is the partial pressure of component r; T is gas temperature; T_0 is wall temperature; $R^{(r)}$ is the gas constant of component r; $\vec{\xi}$ is the velocity of the molecule in a fixed coordinate system; $\vec{v}$ is the mean mass velocity of the gas mixture; $f^{*(r)} = 1 - \alpha^{(r)}$ is the accommodation coefficient of component r; D_{12} is the binary diffusion coefficient; μ_1 and μ_2 are viscosities of components 1 and 2; λ_1 and λ_2 are thermal conductivities of components 1 and 2; c is the concentration of the vapor of the sublimating wall; l is the mean free path length.

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