

Boundary conditions for strongly perturbed rarefied gas

Yuriy E. Gorbachev, Ivan S. Nikitin

*St.-Petersburg State Polytechnical University, Polytechnicheskaya, 29, St.-Petersburg, 195251 Russia,
gorbachev@csa.ru*

Abstract. Boundary conditions for Navier-Stocks equations in the case of strong boundary effect are derived. The boundary function method is used to obtain the uniform asymptotic representation for distribution function in the Knudsen layer and outside. Kramers' kinetic problem for the boundary function inside the Knudsen layer is formulated. Derived hydrodynamic boundary conditions are applied to the film growth problem solution.

Keywords: Hydrodynamic Boundary Conditions, Heterogeneous Reactions

PACS: 51.10.+y, 68.43.-h

INTRODUCTION

The problem of boundary conditions for rarefied gas flow was previously studied both analytically on the base of Boltzmann equation [0] and numerically in the framework of DSMC approach. Correspondent publications are widely represented in the proceedings of RGD symposia. For high Mach number flows as well as for flows with intensive surface chemical reactions or evaporation the discrepancy of hydrodynamic parameters jumps on the surface obtained in DSMC and predicted from correspondent expressions derived from Boltzmann equations was disclosed. In paper [1] the hydrodynamic boundary conditions for the case of moderately strong evaporation/condensation and heterogeneous catalytic reactions were derived for the first time. Their principle distinction from the boundary conditions obtained for slightly perturbed gas consists in the values of the hydrodynamic parameters jumps. Generally used boundary conditions assumes those jumps to be of the order of the Knudsen number, while obtained in [1] assumes them to be of the order of unity.

The flow is described by the set of the Wang Chang-Uhlenbeck kinetic equations

$$\vec{\xi}_c \frac{\partial f_c}{\partial \vec{r}} = \frac{1}{\varepsilon} I(f_c, f_c), \quad (1)$$

where I and ε are collision integral and the Knudsen number, $\vec{\xi}_c$ is the velocity of the molecules. We suppose that the gas consists from the molecules of different sorts $c = 1, \dots, n$ with the correspondent distribution functions $f_c(\vec{\xi}_c, \vec{r}, t)$.

Following [2] the distribution function f_c will be represented in the form $f_c = f_c^0 + \Phi_c$. Here $f_c^0 \equiv f_c^{MB}$ is a Maxwell-Boltzmann distribution that is determined by hydrodynamic parameters of the flow outside the Knudsen layer. As in [2] the function Φ_c is expanded into series over small parameter ε : $\Phi_c = \sum_{k=0}^{\infty} \varepsilon^k \Phi_c^{(k)}$. Usually this expansion is assumed to begin from the term of the order of ε . If further to this perturbation of the distribution function caused by surface chemical reactions or by high-Mach-number flow is small enough ($\leq O(\varepsilon)$) one obtains the well known boundary conditions with gas dynamic parameter jumps of the order of ε . In our case we assume that the perturbation is not so small and therefore this expansion begins from the term with $k = 0$. Generally it will not allow to linearize the Boltzmann equation and to obtain the analytical solution necessary for hydrodynamic boundary condition derivation. Therefore we assume that $\Phi_c = O(\alpha)$, $\varepsilon \ll \alpha \ll 1$, $\alpha^2 \ll \varepsilon$. This allows to use the linear Boltzmann equation and at the same time to obtain strong jumps of hydrodynamic parameters on the surface. Since $\Phi_c^{(0)}$ is not of the order of unity more precisely this situation should be announced as moderately strong jumps. It should be mentioned that the same assumption towards the value of Φ_c was used for investigation of two component gas mixture with disparate mass ratio [3].

The asymptotic method of boundary functions [4] is used to obtain the uniform asymptotic representation for distribution function in the Knudsen layer and outside. Kramers' kinetic problem for the boundary function inside the Knudsen layer is formulated. Introduced function inside the layer is represented as $\Phi_c^{in}(z_1) = \Phi_c^{out}(0) + \Pi_c(z_1)$, where Φ_c^{out} is determined outside the layer using Chapman-Enskog method in the Navier-Stocks approximation; $z_1 = z/\varepsilon$ and

z is a co-ordinate, normal to the surface; Π_c is a boundary function that vanishes outside the Knudsen layer and gives the correction to the asymptotic behavior of the distribution function inside it. Since we assume that Φ_c is small enough we deal with the integral-differential equation for Π_c with linear collision integral. Using the model representation for the collision integral this equation is solved that allows to obtain the hydrodynamic boundary conditions and therefore determines the hydrodynamic parameter jumps.

Derived hydrodynamic boundary conditions are applied to the problem of film growth. The $\alpha - Si : H$ film formation from the silane (SiH_4) *rf* plasma is studied. The heterogeneous reactions of the silane and its radicals (SiH_3) with different surface sites are accounted following the model described in paper [5].

KINETIC BOUNDARY CONDITIONS

The kinetic boundary conditions for equation (1) have the following form:

$$f_c|_{z=\infty} = f_c^0, \quad f_c|_{z=0} = f_c^+, \quad (2)$$

where f_c^0 is the Maxwell-Boltzmann distribution function far from the surface (at the infinity):

$$f_c^0 = n_c \left(\frac{m_c}{2\pi k_B T_0} \right)^{3/2} e^{-\frac{m_c}{2k_B T_0} (\vec{\xi}_c - \vec{U}_0)^2}, \quad (3)$$

n_c is the numerical density of species c and \vec{U}_0 is hydrodynamic velocity. We will use boundary conditions for f_c with the diffusive model for non-reactive reflection processes

$$f_c^+ = (1 - \alpha_c) \hat{A}_c[f_c^-] + \gamma_c f_c^e, \quad (4)$$

where α_c is a sticking coefficient, γ_c is the probability of depletion ($\gamma_c < 0$) or production ($\gamma_c > 0$) of the particle of the c -th type. The linear operator \hat{A}_c conserve the mass flux of the component c and has the form:

$$\hat{A}_c[f_c^-] = \sum_{c'} P_{c'c} \hat{W}(\xi_{c'}, \xi_c)[f_c^-], \quad (5)$$

where $P_{c'c}$ is the probability of the reaction $c \rightarrow c'$, and operator \hat{W} is defined as:

$$\hat{W}(\xi_{c'}, \xi_c)[f_c^-] = \int_{\xi_c'^n < 0} d\vec{\xi}' \frac{|\xi_c'^n|}{\xi_c^n} W(\vec{\xi}' \rightarrow \vec{\xi}_c) f_c^-(\vec{\xi}'). \quad (6)$$

Here ξ_c^n is the component of the vector $\vec{\xi}_c$ normal to the surface. f_c^e is the equilibrium distribution function of the "evaporated" molecules c over the surface:

$$f_c^e = n_{ec} \left(\frac{m_c}{2\pi k_B T_w} \right)^{3/2} e^{-\frac{m_c}{2k_B T_w} (\xi_c - U_e)^2}, \quad (7)$$

where U_e is hydrodynamic velocity of the "evaporated" flux and T_w is the surface temperature.

Functions f_c^0 and f_c^e can be expanded over α that is the parameter of nonequilibrium, $1 \gg \alpha \gg \varepsilon$, $\alpha^2 \ll \varepsilon$ and expressed via the function f_c^w as follow:

$$f_c^0 = n_c f_c^w \left(1 + \alpha \tau \left(\frac{m_c}{2k_B T_w} v_c^2 - \frac{3}{2} \right) \right) + o(\varepsilon), \quad f_c^e = n_{ec} f_c^w (1 + 2v_c \alpha (v_{0c} - v_{ec})) + o(\varepsilon), \quad (8)$$

where $f_c^w = (m_c / (2k_B T_w \pi))^{3/2} e^{-m_c / (2k_B T_w) v_c^2}$, $\alpha \tau = (T_0 - T_w) / T_w$, $v_c = (\vec{\xi}_c - \vec{U}_0)$, $v_0 = \alpha U_0$, $v_e = \alpha U_e$.

SiH₃ DEPOSITION

The main contribution to the deposition process is given by the SiH₃ radicals. According to [5] six types of surface sites are considered that are arranged into two types. The first one consists from Si atoms having one outward dangling bond and one or two Si–H bonds pointing outward from the surface. These dangling-bond sites will be marked as SiSi⁰, SiSiH⁰, SiSiH₂⁰ with correspondent coverage densities θ_0 , θ_1 and θ_2 .

The other type of the surface sites consists from the silicon atoms Si having at least one Si–Si bond with other atoms from the film and at least one Si–H bond pointing outward from the surface. The number of the Si–H bond can vary from 1 to 3. These hydrogenated sites will be marked as SiSiH, SiSiH₂ and SiSiH₃ and the correspondent coverage densities are θ_3 , θ_4 and θ_5 . The following surface reactions will be considered:

1) The direct chemisorption of SiH₃ radical on dangling-bond sites SiSi⁰, SiSiH⁰, SiSiH₂⁰ with the new Si–Si bond formation. The initial "sticking" probability P_0 for this reaction will be assumed to be equal to unity: $P_0 = 1$.

2) The thermal physisorption of SiH₃ with the probability P_{ph} . These reactions form the three new sites on the surface with the coverage densities: θ_6 , θ_7 and θ_8 corresponding to sites SiSiH, SiSiH₂ and SiSiH₃ respectively.

3) The reaction of dimerization (gas-phase hydrogen molecule formation from two atomic hydrogens from neighboring sites with released silicon dangling bonds saturation by each other) with the reaction probability P_{dim} .

4) The hydrogen abstraction giving one dangling bond and one silane molecule which goes back in the gaseous phase with the probability P_a .

5) The thermal desorption of SiH₃ with the probability P_{des} .

6) The diffusion reaction (hopping of SiH₃ on the neighboring sites) with the probability P_h .

The corresponding probabilities are written in the Arrhenius form.

Therefore three surface reaction channels can be distinguished:

1) Scattering reaction with the probability ($c = H_2 \equiv 1$, $c = SiH_3 \equiv 2$, $c = SiH_4 \equiv 3$) $P_c^1 = (1 - p_c^a)$, $c = 1, 2, 3$, where $p_c^a = v_c^a/v_c$ is the adsorption probability of the particle c , v_c^a is the adsorption rate, and $v_c = n_c k_B T_w / (2 \pi m_c k_B T_w)^{1/2}$. For the considered species the following expressions can be written $v_1^a = 0$, $v_2^a = P_0(\theta_0 + \theta_1 + \theta_2)n_3 + P_{ph}(\theta_3 + \theta_4 + \theta_5)n_3$, $v_3^a = 0$.

2) Desorption with the probability $P_c^2 = p_c^d p_c^a$, where $p_c^d = v_c^d/v_c$ is the desorption probability of the particles c , v_c^d is the desorption rate: $v_1^d = W_1 = P_{dim}(\theta_3^2 + \theta_4^2 + \theta_5^2)$, $v_2^d = P_{des}(\theta_6 + \theta_7 + \theta_8)$, $v_3^d = W_3 = P_a(\theta_6 + \theta_7 + \theta_8)$.

3) Probability of the reaction $c \rightarrow c'$ on the assumption of adsorption and diffusion is $P_{cc'}^3 = p_c^a p_{diff} p_{cc'}^r$, where $p_{cc'}^r = v_{cc'}^r/v_c$ is the reaction probability, $v_{cc'}^r$ is the reaction rate of the reaction $c \rightarrow c'$: $v_{23}^r = P_a(\theta_6 + \theta_7 + \theta_8)$, p_{diff} is taken as in [5].

As a result one can write the following expressions for these three channels of reactions:

1) For H_2 : $P_1^1 = 1$, $P_1^2 = 0$, $P_1^3 = 0$

2) For SiH₃: $P_2^1 = (1 - p_2^a) = \left(1 - (P_0(\theta_0 + \theta_1 + \theta_2) + P_{ph}(\theta_3 + \theta_4 + \theta_5))n_3/v_2\right)$,

$$P_2^2 = (P_0(\theta_0 + \theta_1 + \theta_2) + P_{ph}(\theta_3 + \theta_4 + \theta_5))P_{des}(\theta_6 + \theta_7 + \theta_8)n_3/v_2^2,$$

$$P_2^3 = \frac{(P_0(\theta_0 + \theta_1 + \theta_2) + P_{ph}(\theta_3 + \theta_4 + \theta_5))B(1 - \theta_H)\theta_H P_a(\theta_6 + \theta_7 + \theta_8)n_3}{(1 - \theta_H P_h)v_2^2}.$$

3) For SiH₄: $P_3^1 = 1$, $P_3^2 = 0$, $P_3^3 = 0$.

Taking into consideration the previous expressions, the boundary condition at the surface for SiH₃ can be written as following:

$$f_c^+ = (1 - p_c^a)\hat{A}_c + (P_c^2 + P_{cc'}^3)f_c^e, \quad (9)$$

where operator $\hat{A}_c[f_c^-]$ is determined by (5) and (6) and the kernel $W(\vec{\xi}'_c \rightarrow \vec{\xi}_c)f_c(\vec{\xi}'_c)$ has the following form:

$$W(\vec{\xi}'_c \rightarrow \vec{\xi}_c) = \frac{2}{\pi} \left(\frac{m_c}{2k_B T_w} \right)^2 \xi_c^n e^{-\frac{m_c}{2k_B T_w} \xi_c^2}.$$

Taking into consideration expression (4) we can find the following relationships for α_c and γ_c :

$$\alpha_c \equiv p_c^a; \quad \gamma_c \equiv P_c^2 + P_{cc'}^3 \quad (10)$$

KRAMER'S PROBLEM

In order to distinguish the intensive processes the semilinearization is performed by Chapman-Enskog expansion. We look for the distribution function in the form:

$$f_c(\xi_c) = f_c^0(\xi_c)(1 + \alpha\varphi_c(\xi_c)), \quad (11)$$

where $\varepsilon \ll \alpha \ll 1$. After substituting this expansion into (1) and (2) one obtains the following set of equations for φ_c :

$$\vec{\xi}_c \frac{\partial \varphi_c}{\partial z} = \frac{1}{\varepsilon} L[\varphi_c] + \Lambda(\varphi_c), \quad L[\varphi_c] = 2f_{0c}^{-1} J(f_{0c}, f_{0c}\varphi_c), \quad \Lambda(\varphi_c) = \vec{\xi}_c f_{0c}^{-1} \frac{\partial f_{0c}}{\partial r} (1 + \alpha\varphi_c), \quad (12)$$

$$\varphi_c|_{z=\infty} = 0, \quad \varphi_c|_{z=0} = (1 - \alpha_c) \left(\tilde{A}_c[\varphi_c]^- + \frac{A_c^0}{\alpha} \right) + \frac{n_{ec}/n_c \gamma_c - 1}{\alpha} + \gamma_c \frac{n_{ec}}{n_c} \left[2v_c(v_0 - v_e) - \tau(a_{wc}v_c^2 - 3/2) \right], \quad (13)$$

where

$$A_c^0 = \frac{n_c (a_{wc}a_{0c})^{3/2}}{v_c^n f_{02} \sqrt{\pi} (a_{wc} + a_{0c})^2}, \quad \tilde{A}_c[\varphi_c]^- = f_{0c}^{-1} \hat{A}_c[\varphi_c f_{0c}]^-; \quad a_{wc} = \frac{m_c}{2k_B T_w}, \quad a_{0c} = \frac{m_c}{2k_B T_0}. \quad (14)$$

To solve the equation (12) the boundary function method is used. Function φ is divided into the outside (of the Knudsen layer) part and the internal function inside the Knudsen layer. The external decomposition of the distribution function has the form $\varphi_c^{ext} = \varphi_c^0 + \varepsilon\varphi_c^1$, while the internal one has the form $\varphi_c^{int} = \varphi_c^{ext} + \Pi_c(z_1)$, $z_1 = z/\varepsilon$. The internal decomposition can be rewritten as

$$\varphi_c^{int} = \varphi_c^0(0) + \varepsilon \frac{\partial \varphi_c^0(0)}{\partial z_1} z_1 + \Pi_c^0(z_1) + \varepsilon(\varphi_c^1(0) + \Pi_c^1(z_1)) = \varphi_c^0(0) + \Pi_c^0(z_1) + \varepsilon \left[\frac{\partial \varphi_c^0(0)}{\partial z} z_1 + \varphi_c^1(0) + \Pi_c^1(z_1) \right]. \quad (15)$$

The boundary functions $\Pi_c^{0,1}$ should satisfy the following asymptotic condition: $\lim_{z_1 \rightarrow \infty} \Pi_c^{0,1}(z_1) = 0$. After substituting the internal decomposition (15) into the kinetic equation (12) one obtains the following equations for $\Pi_c^{0,1}$:

$$\xi_{zc} \frac{\partial \Pi_c^0}{\partial z_1} = L[\Pi_c^0(z_1)], \quad \xi_{zc} \frac{\partial \Pi_c^1}{\partial z_1} = \frac{1}{\varepsilon} L[\Pi_c^1(z_1)]. \quad (16)$$

For the functions $\Pi_c^{0,1}$ the following boundary conditions are used

$$\begin{aligned} \hat{R}_c[\Pi_c^0] &= (1 - \alpha_c) \frac{A_c^0}{\alpha} + \frac{n_{ec}/n_c \gamma_c - 1}{\alpha} + \gamma_c \frac{n_{ec}}{n_c} \left[2v_c(v_0 - v_e) - \tau(a_{wc}v_c^2 - 3/2) \right] - \hat{R}_c[\varphi_c^0(0)], \quad z_1 = 0 \\ \hat{R}_c[\Pi_c^1] &= -\hat{R}_c[\varphi_c^1(0)], \quad z_1 = 0, \quad \hat{R}_c[\Pi] \equiv \Pi^+ - (1 - \alpha_c) \tilde{A}_c^+[\Pi]^-, \quad \varphi_c^0(0) = \sum_j a_j \Psi_{ci}, \end{aligned} \quad (17)$$

where $a_n = \tilde{n}_c$, $a_{u_i} = \tilde{u}_{ic}$, $a_\theta = \theta$, and $\tilde{n}_c, \tilde{u}, \theta$ are the deviations from the equilibrium values of the numerical density n_c , hydrodynamic velocity \vec{u} and the temperature T respectively (index 0 denotes the equilibrium values): $n_c = n_0 + \tilde{n}_c$, $\vec{U} = \vec{U}_0 + \tilde{u}$, $T = T_0 + \theta$. These deviation-macroparameters can be expressed via the following invariants:

$$\begin{aligned} \Psi_{ci} &= \left\{ \delta_{ck}; (\xi_{ci} - U_i); \frac{(\vec{\xi}_c - \vec{U})^2 - 3}{\sqrt{6}} \right\}, \quad i = 0 \dots 4 \\ \tilde{n}_c &= \langle \Psi_{c0}, \varphi_c \rangle; \quad \tilde{u}_i = \langle \Psi_{ci}, \varphi_c \rangle, \quad i = 1, 2, 3; \\ \theta &= \langle \Psi_{c4}, \varphi_c \rangle; \quad \langle a_c, b_c \rangle = \int d\vec{\xi}_c a_c(\vec{\xi}_c) b_c(\vec{\xi}_c) f_{c0}(\vec{\xi}_c). \end{aligned} \quad (18)$$

Function $\varphi_c^1(0)$ has a Navier-Stocks form

$$\begin{aligned} \varepsilon \varphi_c^1(0) &= \vec{A}_c \cdot \nabla \ln T - \mathbf{B}_c \nabla \vec{v}_c + n^{-1} \sum_i \vec{D}_c^i \cdot \vec{d}_i, \\ \vec{d}_i &= \nabla x_i + (x_i - y_i) \nabla \ln(p), \quad x_i = n_i/n, \quad y_i = \rho_i/\rho, \end{aligned} \quad (19)$$

where \vec{D}_c^i is the diffusion coefficient and \vec{d}_i are the diffusion thermodynamic forces, p is the total pressure. Vectors \vec{D}_c^i and \vec{A}_c and tensor \mathbf{B}_c are functions of ξ .

Functions $\Pi_c^{0,1}$ can be represented as a sum of two ones depending on co-ordinates tangential and the perpendicular to the surface respectively: $\Pi_c^{0,1} = h_{cx}^{0,1} \otimes h_{cz}^{0,1}$, $h_{cx}^{0,1} = P_x \Pi_c^{0,1}$, $h_{cz}^{0,1} = P_z \Pi_c^{0,1}$. Operators P_x, P_z are the projectors to the corresponding subspaces $P_x = \frac{1}{4}(I - \wp_x)(I - \wp_y)$, $P_z = \frac{1}{2}(I + \wp_x \wp_y)$, $\wp_x f(x, y, z) = f(-x, y, z)$. Operators P_x, P_z commute with the operator L therefore we obtain two equations for each function Π_c in their own subspaces

$$\xi_{zc} \frac{\partial h_{zc}^0}{\partial z_1} = L_c[h_{zc}], \quad \xi_{zc} \frac{\partial h_{xc}^0}{\partial z_1} = L_c[h_{xc}], \quad \xi_{zc} \frac{\partial h_{zc}^1}{\partial z_1} = \frac{1}{\varepsilon} L_c[h_{zc}^1], \quad \xi_{zc} \frac{\partial h_{xc}^1}{\partial z_1} = \frac{1}{\varepsilon} L_c[h_{xc}^1]. \quad (20)$$

The boundary condition for h_{zc}^0 then has the form

$$\begin{aligned} \hat{R}_c[h_{zc}^0] &= \left(\frac{n_{ec}/n_c \gamma_c - 1}{\alpha} + (1 - \alpha_c) \frac{A_c^0}{\alpha} - \alpha_c \tilde{n}_c^0 \right) \tilde{\Psi}_1 + \left(\gamma_c \frac{n_{ec}}{n_c} (v_{0z} - v_{ez}) + \alpha_c v_{0z} \right) \tilde{\Psi}_2 \\ &\quad - \tau \gamma_c \frac{n_{ec}}{n_c} \frac{1}{k_B T_w} \tilde{\Psi}_3 - \tilde{u}_z^0 \tilde{\Psi}_4 - \theta \tilde{\Psi}_4, \\ \hat{R}_c[h_{xc}^0] &= \left(\gamma_c \frac{n_{ec}}{n_c} (v_{0x} - v_{ex}) v_{xc} + \alpha_c v_{0x} \right) - \tilde{u}_x^0 \hat{R}_c[\Psi_{c1}], \\ \tilde{\Psi}_1 &= 1, \quad \tilde{\Psi}_2 = \Psi_{c3}, \quad \tilde{\Psi}_3 = \Psi_{c4}, \quad \tilde{\Psi}_4 = \hat{R}_c[\Psi_{c3}], \quad \tilde{\Psi}_5 = \hat{R}_c[\Psi_{c4}]. \end{aligned} \quad (21)$$

where relationships $(h_{cz}, v_z \tilde{\Psi}_i) = 0$, $i = 0, 4$; $(h_{cx}, v_x \tilde{\Psi}_i) = 0$ are used. For functions h_{cx}^1 and h_{cz}^1 one has

$$\hat{R}_c[h_{cz}^1] = -\hat{R}_c[\pi_{cz}], \quad \hat{R}_c[h_{cx}^1] = -\hat{R}_c[\pi_{cx}], \quad (22)$$

where

$$\begin{aligned} \pi_{cz} &= \left(A_{cz} \frac{1}{T} \left(\frac{\partial T}{\partial z_1} \right) - \theta \right) \tilde{\Psi}_3 + \left(B_{cz} \left(\frac{\partial v_{cz}}{\partial z} \right) - \tilde{u}_{cz}^1 \right) \tilde{\Psi}_2 + (n^{-1} \sum_i D_{cz}^i \cdot d_{zi} - \tilde{n}_c^1) \tilde{\Psi}_1. \\ \pi_{cx} &= \left(B_{cx} \left(\frac{\partial v_{cx}}{\partial x} + \frac{\partial v_{cy}}{\partial y} \right) - \tilde{u}_{cx}^1 \right) \hat{R}_c[\Psi_{21}]. \end{aligned} \quad (23)$$

Functions $h_{cz}^{0,1}$ can be represented as $h_{cz}^{0,1} = -\sum_{k=1}^4 g_{ck}^{0,1} \rho_{ck}^{0,1}$. When using the asymptotic stipulation $\lim_{z_1 \rightarrow \infty} h_{cz}^{0,1} = 0$ one finds the following gas-dynamic boundary conditions $\sum_{k=1}^4 m_{ks}^{0,1} \rho_{ck}^{0,1} = 0$, $s = 1, 2$. Finally the hydrodynamic variables entering the Navier-Stocks equation that are n_{0c} , T_0 and \vec{U}_0 can be connected with true (in sense of [1]) boundary values $n_c(0)$, $\vec{U}(0)$ and $T(0)$ by the following equations:

$$\begin{aligned} m_{1s}^0 (n_{ce}/n_c \gamma_c - 1 + (1 - \alpha_c) A_c^0) + m_{2s}^0 (m_c/k_B T_0)^{1/2} (\gamma_c n_{ce}/n_c (U_{0z} - U_{ez}) + \alpha_c U_{0z}) - m_{3s}^0 (1 - T_0/T_w) \gamma_c n_{ce}/n_c \\ + m_{3s}^0 m_{5s}^0 T(0)/T_0 + m_{2s}^0 m_{4s}^0 (m_c/k_B T_0)^{1/2} (U_z(0) - U_{0z}) + m_{1s}^0 n_0/n (\sum_i D_{cz}^i \cdot d_{zi} - \alpha_c n_c(0)/n_0) = 0, \quad s = 1, 2, \\ \beta_1^0 (\gamma_c n_{ce}/n_c (U_{0x} - U_{ex}) + \alpha_c U_{0x}) + \beta_2^1 (U_x(0) - U_{0x}) - \beta_1^1 l_{c0} B_{cx} \nabla_{x,y} U_{0x} = 0, \end{aligned} \quad (24)$$

where \vec{U}_e is the parameter of f_c^e function and in the case of the chemical reaction it should be set to zero, l_{0c} is the mean free path for c -th particle: $l_{c0} = (\sqrt{2} n \pi \sigma_c^2)^{-1}$

The expression for the velocity $U_{0z}(0)$ can be derived from the boundary condition (9) by integration over ξ

$$\begin{aligned} n_0(0) U_0^n(0) &= \sum_c \int d\vec{\xi}_c \xi_c f_c(\xi_c) = \sum_c \alpha_c \sum_{c'} P_{c'} \int_{\xi_c'^n < 0} d\vec{\xi}_c' \xi_c'^n f_c^-(\xi_c') \\ &+ \sum_c \gamma_c n_{ec} \sqrt{\frac{k_B T_w}{2\pi m_e}} \left[\exp\left(\frac{m_e U_e^{n2}}{2k_B T_w}\right) + U_e^n \sqrt{\frac{\pi m_e}{2k_B T_w}} \operatorname{erfc}\left(-U_e^n \sqrt{\frac{m_e}{2k_B T_w}}\right) \right]. \end{aligned} \quad (25)$$

In the case of BGK model for the collision integral $L[h_{2z}^{0,1}, f_0] \approx -h_{2z}^{0,1} + \Lambda[h_{2z}^{0,1}]$ one obtains the following equations for functions $g_k^{0,1}$

$$\xi_{2z} \frac{\partial g_k^0}{\partial z_1} + g_k^0 = \Lambda[g_k^0], \quad \xi_{2z} \frac{\partial g_k^1}{\partial z_1} + \frac{1}{\varepsilon} g_k^1 = \frac{1}{\varepsilon} \Lambda[g_k^0] \quad (26)$$

can be rewritten as the integral ones

$$g_k^{0+}(s) = \Psi_k \exp^{-s/v_z} + \frac{1}{v_z} \int_0^s ds' \Lambda_k(s') \exp \frac{-(s-s')}{v_z}, \quad g_k^{0-}(s) = -\frac{1}{v_z} \int_s^\infty ds' \Lambda_k(s') \exp \frac{-(s-s')}{v_z}. \quad (27)$$

In our case the BGK model has the following form

$$\Lambda_k = \omega_k + \theta_k \left(\frac{m_2 v_z^2 - 3}{\sqrt{6}} \right), \quad \omega_k = (g_k^0, \Psi_0), \quad \theta_k = \left(g_k^0, \frac{m_2 v_z^2 - 3}{\sqrt{6}} \right). \quad (28)$$

By calculating the scalar product (g_k^0, Ψ_i) , $i = 0, 4$ the following integral equations for ω_k and $\tau_k \equiv \sqrt{\frac{2}{3}} \theta$ are obtained

$$\begin{aligned} \omega_k &= \Xi_k(s) + \int_0^\infty ds' \left[(K_{00}(|s-s'|) + W_{00}(s, s')) \omega_k(s') + (K_{04}(|s-s'|) + W_{04}(s, s')) \tau_k(s') \right], \\ \tau_k &= T_k(s) + \int_0^\infty ds' \left[(K_{40}(|s-s'|) + W_{40}(s, s')) \omega_k(s') + (K_{44}(|s-s'|) + W_{44}(s, s')) \tau_k(s') \right], \end{aligned} \quad (29)$$

where

$$\begin{aligned} \Xi_k(s) &= \langle \Psi_0, \tilde{\Psi}_k e^{-(s-s')/v_z} \rangle, \quad T_k(s) = \langle \Psi_4, \tilde{\Psi}_k e^{-(s-s')/v_z} \rangle, \\ K_{ij} &= \langle \Psi_i, \Psi_j \frac{1}{v_z} e^{-(s-s')/v_z} \rangle, \quad W_{ij} = -(1-p_2^a) \langle \Psi_i e^{-(s-s')/v_z}, \tilde{A}_2 \left[\frac{\Psi_j}{v_z} e^{-(s-s')/v_z} \right] \rangle. \end{aligned} \quad (30)$$

The expressions for the moments ω_k^1 and τ_k^1 have the same view. The coefficients in the gas-dynamic boundary conditions are related with the solution of the integral equations as

$$m_{k1}^0 = \lim_{s \rightarrow \infty} \omega_k s, \quad m_{k2}^0 = \lim_{s \rightarrow \infty} \tau_k s. \quad (31)$$

CONCLUSION

The boundary conditions problem for rarefied gas flow has been considered and the boundary conditions for Navier-Stocks equations in the case of strong boundary effect were derived. The boundary function method was used to obtain the uniform asymptotic representation for distribution function in the Knudsen layer and outside. Kramers' kinetic problem for the boundary function inside the Knudsen layer was formulated. Derived hydrodynamic boundary conditions are applied to the film growth problem solution. The obtained result shows that in the case of the strongly perturbed rarefied gas flow the boundary function in the zero order approximation should be taken into account. It gives an appreciable correction into the hydrodynamic boundary conditions and therefore into the hydrodynamic parameter jumps.

ACKNOWLEDGMENTS

The research was supported by the Dutch National Science Foundation NWO and the Russian Foundation for Basic Research, grant #047.016.018.

REFERENCES

1. M. N. Kogan, *Dynamics of Rarefied Gases*, Nauka, Moscow, 1967, 440 p. (in Russian)
2. D. A. Shapiro, in *Proc. of the 17th International Symposium on RGD*, VCH, Weinheim, NY, Basel, Cambridge, 1990, pp. 400–407
3. E. G. Kolesnichenko, *Mechanics of fluid and Gas*, **3**, 96–105 (1981) (in Russian)
4. Yu. E. Gorbachev, *Math. Methods*, **15**, pp.120–124 (2003)
5. A.H. Nayfen, *Introduction to the Perturbation Techniques*, Wiley, New York (1981)
6. J.-L. Guizot, K. Nomoto, A. Matsuda, *Surface Science*, **244**, pp.22–38 (1991)