REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	**2. REPORT TYPE**	**3. DATES COVERED** *(From - To)*
11-12-2007	Technical Paper	

4. TITLE AND SUBTITLE

An Analytical Model of the Knudsen Layer with Thermal Conduction (Preprint)

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
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5d. PROJECT NUMBER

5e. TASK NUMBER
50260542

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/RZSA
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Edwards AFB CA 93524-7680

8. PERFORMING ORGANIZATION REPORT NUMBER

AFRL-RZ-ED-TP-2007-531

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/RZS
5 Pollux Drive
Edwards AFB CA 93524-7048

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S NUMBER(S)
AFRL-RZ-ED-TP-2007-531

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited (PA #07466A).

13. SUPPLEMENTARY NOTES
To be presented at CHT-8: Advances in Computational Heat Transfer, Marrakech, Morocco, 11-16 May 2008.

14. ABSTRACT

This work motivation is formulation of the boundary condition for numerical simulation of fluid dynamic with ablative boundaries. In this paper we develop an analytical model of the Knudsen layer by considering a kinetic formulation that takes into account the gas temperature gradient at a flat gas-wall interface. The main focus of this research is to study the effect of the thermal conductivity on the Knudsen layer formed near an ablating surface. This analysis is based on the premise that the thermal conductivity (the temperature gradient) in the bulk gas can be taken into account in the velocity distribution function at the outer boundary of the Knudsen layer. We use such a function obtained by Chapman-Enskog expansion method, based on the assumption that the molecular mean-free path is much smaller than the characteristic length scale of the temperature gradient. The model uses a bimodal velocity distribution function in the Knudsen layer which preserves the laws of conservation of mass, momentum and energy and converges to the Chapman-Enskog velocity distribution function at the outer boundary of the layer. The model allows obtaining the boundary conditions at the interface between the ablative surface and the bulk gas avoiding "micro" modeling of the evaporation process at the mean free path scale. Thus, our Knudsen layer model can be used as a "constructor" for boundary conditions between the bulk gas and ablative surface that is important for numerical simulation of evaporation processes and for fluid dynamics in general.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
					Dr. Jean-Luc Cambier
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**	SAR	13	**19b. TELEPHONE NUMBER** *(include area code)*
Unclassified	**Unclassified**	**Unclassified**			N/A

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. 239.18

Proceedings of CHT-08
ICHMT International Symposium on Advances in Computational Heat Transfer

May 11-16, 2008, Marrakech, Morocco

CHT-08-xx

AN ANALYTICAL MODEL OF THE KNUDSEN LAYER WITH THERMAL CONDUCTION (PREPRINT)

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ABSTRACT This work motivation is formulation of the boundary condition for numerical simulation of fluid dynamic with ablative boundaries. In this paper we develop an analytical model of the Knudsen layer by considering a kinetic formulation that takes into account the gas temperature gradient at a flat gas-wall interface. The main focus of this research is to study the effect of the thermal conductivity on the Knudsen layer formed near an ablating surface. This analysis is based on the premise that the thermal conductivity (the temperature gradient) in the bulk gas can be taken into account in the velocity distribution function at the outer boundary of the Knudsen layer. We use such a function obtained by Chapman-Enskog expansion method, based on the assumption that the molecular mean-free path is much smaller than the characteristic length scale of the temperature gradient. The model uses a bimodal velocity distribution function in the Knudsen layer which preserves the laws of conservation of mass, momentum and energy and converges to the Chapman-Enskog velocity distribution function at the outer boundary of the layer. The model allows obtaining the boundary conditions at the interface between the ablative surface and the bulk gas avoiding "micro" modeling of the evaporation process at the mean free path scale. Thus, our Knudsen layer model can be used as a "constructor" for boundary conditions between the bulk gas and ablative surface that is important for numerical simulation of evaporation processes and for fluid dynamics in general.

I. INTRODUCTION

The physics of the Knudsen layer, formed near the vaporizing (ablative) surface is of great interest for a number of applications such as capillary discharges [e.g., Seeger 2006 and Keidar 2006], plasma thrusters [e.g., Burton 1998 and Keidar 200], high-pressure discharges [e.g., Boulos 1995], vacuum arcs [e.g., Boxman 1995], electroguns [e.g., Raja, 1997] and laser ablation [e.g., Zhigilei 1998].

Anisimov [1968] was the first to consider details of the vaporization process for a case of vaporization of a metal exposed to laser radiation. He used a bimodal velocity distribution function in the kinetic layer, assuming no absorption of laser radiation in the ablated gas, the gas flow velocity at the external boundary of the Knudsen layer is equal to the sound velocity, and the temperature of the gas in the bulk region (beyond Knudsen Layer) is constant. The primary result

of his work was the calculation of the maximal flux of returned atoms to the evaporating surface, which was found to be about 18% of the flux of vaporized atoms. Ytrehus [1976] has used the Anisimov and Ansatz bimodal velocity distribution functions in the Knudsen layer to study the effect of bulk gas pressure on downstream vapor flow. He has calculated the gas flow velocity at the external boundary of the Knudsen layer (in the bulk gas), density and temperature jumps over the Knudsen layer, the evaporation mass flux, and other parameters of the Knudsen layer as functions of the ratio of the equilibrium vapor pressure to the gas pressure in the bulk region. In addition, Ytrehus has demonstrated that his analytical results are in substantial agreement with the experimental finding, DMCS and numerical solutions of the Boltzmann equations. He has also shown that the differences between the analytical solutions using the Anisimov approximation and the Ansats (more sophisticated) velocity distribution function are very small.

Later the Anisimov bimodal velocity distribution function was used in modeling the vaporization into dense plasmas. Beilis [1985, and 1995] applied this function to study the case of metal vaporization into discharge plasmas in a vacuum arc cathode spot. He demonstrated that the parameters at the outer boundary of the Knudsen layer are close to their equilibrium values and that the flow velocity at the outer boundary of the kinetic layer is much smaller than the sound velocity. Then it was applied for the case of dielectric ablation into the discharge plasma in the capillary discharge conditions [e.g., Keidar 2001] and for the case of strong plasma acceleration [e.g., Keidar 2004]. All those analytical models neglected the conductive heat flux to the ablative surface. This can be significant because the temperature in the plasma core is assumed in the models to be much greater than the temperature of the ablative surface. However, it is worth noting, that in the case where the external heat flux to the ablating surface is larger than the conduction heat flux, the effect of the thermal conduction is small and can be dropped. This is the case for the example laser ablation [e.g., Anisimov 1968], where an externally applied laser radiation source heats the ablating surface but for which the gas (plasma) is transparent.

Ideally Monte Carlo simulations or numerical solutions of BGK equation describing the kinetic layer without any a prior approximation of gas velocity function distribution in that layer should be able to self-consistently describe the conductive heat flux to the ablating surface. However, this will require extending the analysis beyond the Knudsen layer region, making it computationally intensive. As shown in works of Ytrehus [1976], Sibold [1991], Sibold [1993], Morozov [2004], and Rose [2000], the models that utilize the Anisimov bimodal velocity distribution function, nevertheless, are in good agreement with DSMC simulations and numerical solutions of BGK equation. Thus, improving the analytical models by including heat conduction into consideration is an important step in developing practical (computationally efficient) solutions for modeling of evaporation processes and plasma discharges coupled to ablative processes.

We would also like to point out the paper by Bond [2004] in which the authors have included the conduction heat flux in their analytical model of water evaporation. This is a generalized Hertz-Knudsen model (Hertz [1882] and Knudsen [1915]) of the Knudsen layer. It worth noting that the classical Hertz-Knudsen model and all its generations assumes no collisions in the Knudsen layer (i.e. does not satisfy conservation of momentum through the Knudsen layer) preventing any “relaxation” in the kinetic (Knudsen) layer, where the velocity distribution function at the ablative surface has to relax (converge) to the bulk gas distribution function at the outer boundary of the Knudsen layer. The analytical models using bimodal velocity distribution functions, such as the Anisimov one, take into account the collisions in the Knudsen layer, satisfy the conservation of momentum through the Knudsen layer and self-consistently calculate the backflux.

In this paper we develop an analytical model of the Knudsen layer taking into account the gas temperature gradient at a flat gas-wall interface. The model is based on the premise that the thermal conductivity in the bulk gas can be taken into account in the velocity distribution function

at the outer boundary of the Knudsen layer. We use such a function obtained by Chapman-Enskog expansion method [e.g., Vincenti 1975] assuming that the molecular mean-free path is much smaller than the characteristic length scale of the temperature gradient. The model uses the Anisimov bimodal velocity distribution function in the Knudsen layer which converges to the Chapman-Enskog velocity distribution function at the outer boundary of the layer. The presented model allows obtaining the boundary conditions at the interface between the ablative surface and the bulk gas avoiding "micro" modeling of the evaporation process at the mean free path scale. Thus, our Knudsen layer model can be used as a "constructor" for boundary conditions between the bulk gas and ablative surface that is important for numerical simulation of evaporation processes and for fluid dynamics in general.

The model is applied to polyethylene ablation, for which two cases are considered: (a) the ablation process is due to pure heat conduction to the surface, with no external heating of the ablated surface, and (b) the ablation is due to both the thermal conduction and an external heating of the surface. The model formulation is presented in the next section. Numerical results and comparison of the presented model with the generalized collisionless Hertz-Knudsen model are presented in the Sections III and IV respectively. In Section V we review the results and present conclusions.

II. MODEL

Following Anisimov's method, the velocity distribution function in the kinetic layer with the evaporating surface can be written in the following form, Fig.1

$$f(x,\vec{V}) = \delta(x)\cdot f_b(\vec{V}) + \left[1-\delta(x)\right]\cdot f_a(\vec{V}) \quad , \tag{1}$$

$$f_b(\vec{V}) = \begin{cases} n_{sat}\cdot\left(\dfrac{1}{V_T\cdot\sqrt{\pi}}\right)^3\cdot\exp\left(-\dfrac{V^2}{V_T^2}\right), & V_x > 0 \\ \\ \beta\cdot n_a\cdot\left(\dfrac{1}{\sqrt{\pi}\cdot V_{T_a}}\right)^3\cdot\exp\left(-\dfrac{(V_x-u)^2+V_y^2+V_z^2}{V_{T_a}^2}\right), & V_x < 0 \end{cases} , \tag{2}$$

$$f_a(\vec{V}) = n_a\cdot f_M(\vec{V})\cdot\left\{1-\frac{V_{T_a}}{\nu}\cdot\left[\frac{(V_x-u)}{V_{T_a}}\cdot\left(\frac{(V_x-u)^2+V_y^2+V_z^2}{V_{T_a}^2}-\frac{5}{2}\right)\cdot\frac{d}{dx}(\ln T)\right]\right\} \quad , \tag{3}$$

$$f_M(\vec{V}) = \left(\frac{1}{\sqrt{\pi}\cdot V_{T_a}}\right)^3\cdot\exp\left(-\frac{\left[(V_x-u)^2+V_y^2+V_y^2\right]}{V_{T_a}^2}\right) \quad . \tag{4}$$

Here f_b is the gas distribution function at the inner boundary of Knudsen layer (at the ablative surface) with Maxwellian vaporization function for $V_x > 0$ [e.g., Knacke 1956] and a shifted "backflux" Maxwellian function distribution describing the particles falling to the surface from the gas, $V_x < 0$, where the x-axis is directed from gas chamber to the wall, Fig. 1; f_a is the Chapman-Enskog velocity distribution function [e.g., Vincenti 1975] at the outer boundary of the Knudsen layer that takes into account the temperature gradient and flow velocity above the Knudsen layer, in the gas bulk; $kT_0=V_T^2/(2m)$ is the temperature of the ablated surface, where V_T is the thermal vapor velocity at thermodynamic equilibrium; n_{sat} is the equilibrium vapor density corresponding to the surface temperature T_0; ν is the collision frequency depending of the temperature and density of the gas; $\delta(x)$ is an unknown function that satisfied the conditions $\delta(0) = 1$ and $\delta(\infty) = 0$. The parameter β is unknown variable that must be obtained in the solution; it represents essentially nonequilibrium effects caused by collisions in the Knudsen layer.

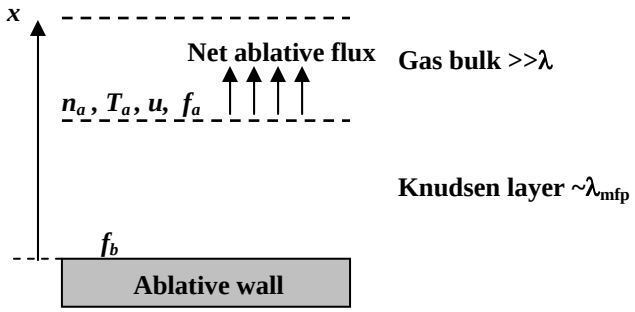

Figure 1. Schematic representation of the layer structure near the ablative surface

Assuming the laws of conservation of mass, momentum, and energy hold at all times within the Knudsen layer, as it has been assumed in all previous models of Anisimov [1968], Ytrehus [1976], Beilis [1985 and 1995], and Keidar [2001, 2004], the following integrals are defined:

$$C_1 = \int_{-\infty}^{+\infty} d\hat{V}_z \int_{-\infty}^{\infty} d\hat{V}_y \int_{-\infty}^{+\infty} \hat{f} \cdot \hat{V}_x \cdot d\hat{V}_x = \hat{n}_a \cdot \hat{u} \quad , \tag{5}$$

$$C_2 = \int_{-\infty}^{+\infty} d\hat{V}_z \int_{-\infty}^{\infty} d\hat{V}_y \int_{-\infty}^{+\infty} \hat{f} \cdot \hat{V}_x^2 \cdot d\hat{V}_x = \hat{n}_a \cdot \left(\hat{u}^2 + \frac{\hat{V}_{T_a}^2}{2} \right) \quad , \tag{6}$$

$$C_3 = \int_{-\infty}^{+\infty} d\hat{V}_z \int_{-\infty}^{\infty} d\hat{V}_y \int_{-\infty}^{+\infty} \hat{f} \cdot \hat{V}^2 \cdot \hat{V}_x \cdot d\hat{V}_x = \hat{n}_a \cdot \left[\hat{u} \cdot \left(\hat{u}^2 + \frac{5 \cdot \hat{V}_{T_a}^2}{2} \right) - \frac{\left(V_T \cdot \hat{V}_{T_a} \right)}{\nu} \cdot \frac{d(\ln T)}{dx} \cdot \frac{5 \cdot \hat{V}_{T_a}^3}{4} \right] , \tag{7}$$

where values of C_1, C_2, and C_3 are obtained at the outer boundary of the Knudsen layer (where δ is equal to zero), and mass, momentum, and energy fluxes are

$$M_x = m \cdot n_{sat} \cdot V_T \cdot C_1 \quad , \tag{5a}$$

$$P_x = m \cdot n_{sat} \cdot V_T^2 \cdot C_2 \quad , \tag{6a}$$

$$E_x = m \cdot n_{sat} \cdot \frac{V_T^3}{2} \cdot C_3 \quad . \tag{7a}$$

In Eqs. (5) – (7a) all number densities are normalized by the equilibrium vapor density $n_{sat}(T_0)$, and all velocities by V_T,

$$\hat{n}_a = \frac{n_a}{n_{sat}} \quad , \qquad \hat{V}_{T_a} = \frac{V_{T_a}}{V_T} \quad , \qquad \hat{u} = \frac{u}{V_T} \quad , \qquad \hat{V} = \frac{V}{V_T} \quad , \qquad \hat{f} = \frac{f}{n_{sat} \cdot V_T^3} \quad . \tag{8}$$

Taking into account that integrals C_1, C_2, and C_3 are preserved through the Knudsen layer and they should be independent on $\delta(x)$,

$$\int f(x,V) \cdot G_i(V_x) \cdot d^3\vec{V} = \int f_a(\vec{V}) \cdot G_i(V_x) \cdot d^3\vec{V} + \delta(x) \cdot \int [f_a(\vec{V}) - f_b(\vec{V})] \cdot G_i(V_x) \cdot d^3\vec{V} \, , \tag{9}$$

were $G_1 = m \cdot V_x$, $G_2 = m \cdot V_x^2$, and $G_3 = m \cdot V^2 \cdot V_x$, we obtain that second term in the right hand side of Eq. (9) should be equal to zero; it yields,

$$\frac{1}{2\cdot\sqrt{\pi}} = C_1 - \hat{n}_a\cdot\beta\cdot\left[\frac{\hat{u}}{2}\mathrm{erfc}\left(\frac{\hat{u}}{\hat{V}_{T_a}}\right) - \frac{\hat{V}_{T_a}}{2\cdot\sqrt{\pi}}\cdot\exp\left(-\frac{\hat{u}^2}{\hat{V}_{T_a}^2}\right)\right] \quad , \tag{10}$$

$$\frac{1}{4} = C_2 - \hat{n}_a\cdot\beta\cdot\left[\left(\frac{\hat{u}^2}{2}+\frac{\hat{V}_{T_a}^2}{4}\right)\cdot\mathrm{erfc}\left(\frac{\hat{u}}{\hat{V}_{T_a}}\right) - \frac{\hat{V}_{T_a}\cdot\hat{u}}{2\cdot\sqrt{\pi}}\cdot\exp\left(-\frac{\hat{u}^2}{\hat{V}_{T_a}^2}\right)\right], \tag{11}$$

$$\frac{1}{\sqrt{\pi}} = \beta\cdot\hat{n}_a\cdot\hat{V}_{T_a}^3\cdot\left[\frac{1}{2\cdot\sqrt{\pi}}\cdot\left(\frac{\hat{u}^2}{\hat{V}_{T_a}^2}+2\right)\cdot\exp\left(-\frac{\hat{u}^2}{\hat{V}_{T_a}^2}\right) - \frac{\hat{u}}{\hat{V}_{T_a}}\cdot\frac{1}{2}\left(\frac{5}{2}+\frac{\hat{u}^2}{\hat{V}_{T_a}^2}\right)\cdot\mathrm{erfc}\left(\frac{\hat{u}}{\hat{V}_{T_a}}\right)\right] + C_3 \ . \tag{12}$$

Equations (5), (6), (10) and (11) are identical to the corresponding mass and momentum conservation equations obtained in works of Beilis [1985 and 1995], Keidar [2001 and 2004], Sibold [1991 and 1993], and Morozov [2004] while Eqs. (7) and (12) differ from the corresponding energy conservation equations obtained in these works by the temperature gradient term, which is responsible for conduction heat flux to the ablative surface. Thus, Eqs. (10) – (12) are a system of boundary conditions that connects the ablative surface with the bulk gas.

Let us introduce a thermal conduction parameter τ_T

$$\tau_T = \frac{V_T\cdot\hat{V}_{T_a}}{\nu}\cdot\frac{d(\ln T)}{dx} = \frac{\lambda_{mfp}}{\delta x_T} << 1 \qquad , \quad \lambda_{mfp} = (V_T\cdot V_{T_a})/\nu \, , \qquad \delta x_T = [d\ln(T)/dx]^{-1} \tag{13}$$

where λ_{mfp} is the gas mean-free-path at the outer boundary of the kinetic layer and δx_T is the characteristic temperature gradient length. Condition (13) is needed for the Chapman-Enskog expansion method and Eq. (7) to be valid. Thus, our model is limited to relatively small values of the temperature gradients.

Let us illustrate the process of obtaining boundary conditions using as an example the case of boiling wall, the case of no heat loss in the bulk of the wall. In this approximation all heat coming into the wall is spent on vaporization. Let us also assume that the ablation process is due to only the gas thermal conduction (no external heat source is applied to ablative surface); then the additional boundary condition to Eqs. (10) – (12) can be written as

$$-E_x = M_x\cdot\Phi_{vap} \quad , \tag{14}$$

where Φ_{vap} is evaporation heat per unit mass of the wall material, $-E_x$ is the total energy flux through the Knudsen layer incoming into the ablative wall, Eq. (7a), and M_x is the mass ablation rate, Eq. (5a); the negative sign in front of E_x is due to the x-axis being directed from the wall into the gas chamber. Since τ_T is assumed to be small and, therefore $\hat{u} << 1$, Egs. (10) – (12) and (14) can be reduced to the following dimension form

$$T_a - T = -\frac{u}{8}\cdot\left(\frac{2\cdot\pi\cdot T\cdot m}{k}\right)^{1/2} + \frac{5}{4}\cdot\frac{1}{\nu}\cdot\frac{dT}{dx}\cdot\left(\frac{2\cdot k\cdot\pi\cdot T}{m}\right)^{1/2}, \tag{15}$$

$$n_a = n_{sat}\left[1 - u\cdot\left(\frac{m}{2\cdot k\cdot T}\right)^{1/2}\cdot\left(\frac{2}{\sqrt{\pi}}+\frac{5\cdot\sqrt{\pi}}{16}\right) - \frac{15\cdot\sqrt{\pi}}{16\cdot\nu}\cdot\left(\frac{2\cdot k}{m\cdot T}\right)^{1/2}\cdot\frac{dT}{dx}\right] \quad , \tag{16}$$

$$\frac{5\cdot T\cdot k^2}{2\cdot\nu\cdot m^2}\cdot\frac{dT}{dx} = u\cdot\left[\Phi + \frac{5\cdot k}{2\cdot m}\cdot T\right] \qquad . \tag{17}$$

As we can see, for $u = 0$ (in which case there is no ablation) and for $\tau_T > 0$, the temperature and density at the outer edge of kinetic layer are correspondingly larger and smaller than the wall

temperature and the equilibrium vapor density; it is as expected, since the gas bulk region has a higher temperature than the wall surface. This temperature jump is 1.136 times larger than the temperature jump calculated by using BGK simulation [e.g., Sharipov 2004].

Now let us obtain the system of equations describing the bulk gas at the ablative surface in the parabolic CFD approximation that satisfies Eqs. (15) – (17). Figure 2 shows two sells above the ablated surface and one ghost sell underneath the surface, where x_1, x_2 , x_{-1}, are the coordinates of the centers of the sells, T_1, n_1, u_1, and T_2, n_2, u_2 are the temperature, density, and flow velocity, at x_1 and x_2 correspondingly, T is the surface temperature, and T_{-1}, n_{-1}, u_{-1} are the approximated parameters of the bulk gas in the center of the ghost cell used for modeling the ablative surface in CFD code.

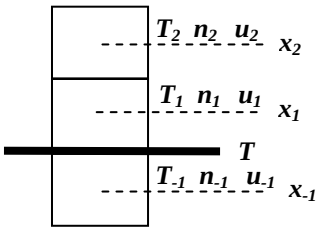

Figure 2. Schematic of CFD cells at ablated surface, where cells *1* and *2* are above the wall and the ghost cell *-1* is underneath the ablative surface.

In parabolic approximation the temperature, density and flow velocity in vicinity of the cells can be written as

$$T_a(x) = \theta_2^T \cdot x^2 + \theta_1^T \cdot x + \theta_0^T, \quad n_a(x) = \theta_2^n \cdot x^2 + \theta_1^n \cdot x + \theta_0^n, \quad u(x) = \theta_2^u \cdot x^2 + \theta_1^u \cdot x + \theta_0^u, \tag{18}$$

where functions $T_a(x)$, $n_a(x)$, $u(x)$ have to satisfy the following conditions at $x = x_1$ and $x = x_2$

$$T_1 = \theta_2^T \cdot x_1^2 + \theta_1^T \cdot x_1 + \theta_0^T, \quad n_1 = \theta_2^n \cdot x_1^2 + \theta_1^n \cdot x_1 + \theta_0^n, \quad u_1 = \theta_2^u \cdot x_1^2 + \theta_1^u \cdot x_1 + \theta_0^u, \tag{19}$$

$$T_2 = \theta_2^T \cdot x_2^2 + \theta_1^T \cdot x_2 + \theta_0^T, \quad n_2 = \theta_2^n \cdot x_2^2 + \theta_1^n \cdot x_2 + \theta_0^n, \quad u_2 = \theta_2^u \cdot x_2^2 + \theta_1^u \cdot x_2 + \theta_0^u, \tag{20}$$

and following Eqs. (15) – (17) the following conditions at $x = 0$

$$\theta_0^T - T = -\frac{\theta_0^u}{8} \cdot \left(\frac{2 \cdot \pi \cdot T \cdot m}{k} \right)^{1/2} + \frac{5}{4} \cdot \frac{1}{\nu} \cdot \theta_1^T \cdot \left(\frac{2 \cdot k \cdot \pi \cdot T}{m} \right)^{1/2}, \tag{21}$$

$$\theta_0^n = n_{sat}(T) \cdot \left[1 - \theta_0^u \cdot \left(\frac{m}{2 \cdot k \cdot T} \right)^{1/2} \cdot \left(\frac{2}{\sqrt{\pi}} + \frac{5 \cdot \sqrt{\pi}}{16} \right) - \frac{15 \cdot \sqrt{\pi}}{16 \cdot \nu} \cdot \left(\frac{2 \cdot k}{m \cdot T} \right)^{1/2} \cdot \theta_1^T \right], \tag{22}$$

$$\frac{5 \cdot T \cdot k^2}{2 \cdot \nu \cdot m^2} \cdot \theta_1^T = \theta_1^u \cdot \left[\Phi + \frac{5 \cdot k}{2 \cdot m} \cdot T \right]. \tag{23}$$

Thus, the system of Eqs (19) – (23) is complete, all θ-parameters can be calculated and, consequently T_{-1}, n_{-1}, u_{-1} are determined. A similar method can be used for other physical situations and approximations.

III. NUMERICAL RESULTS

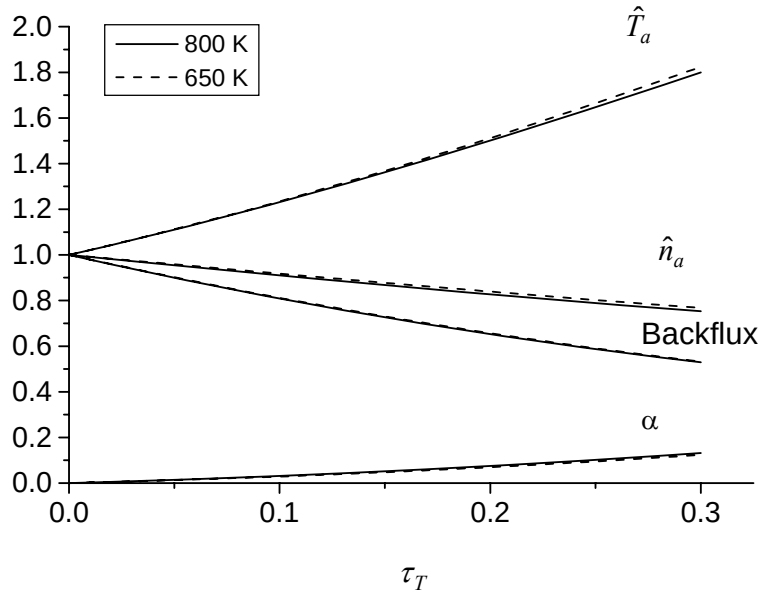

Figure 3. $\hat{T}_a$, $\hat{n}_a$, $\alpha = u / V_{T_a}$, and backflux at the polyethylene ablative surface vs. τ_T

Figure 3 shows the calculated parameters of the Knudsen layer vs. τ_T for the case of thermal conduction heating of the ablative polyethylene wall with the polyethylene surface temperatures of 650 and 800 K, Eqs. (10) – (12) and (16); the evaporation heat has been taken as $3.6 \cdot 10^6$ [J/kg] and equilibrium vapor pressure equal as $P = 10^5 \cdot \exp(5565.22 \cdot [1/453 - 1/T])$ [e.g., Keidar 2006], where the pressure is in Pascal and temperature is in Kelvin. One can see that $\hat{u}$, $\hat{T}_a$, backflux, and $\hat{n}_a$ are weak functions of temperatures in this temperature region, although their equilibrium vapor pressures differ almost in five times. As it has been mentioned above, we cannot extend the obtained results of Figure 3 for higher τ_T, because the Chapman-Enskog expansion method is valid only for $\tau_T << 1$. In this limit, the normalized backflux at the ablative wall given by

$$\hat{F}_{b-flux} = 1 - \hat{u} \cdot \hat{n}_a \cdot 2 \cdot \sqrt{\pi} \tag{24}$$

reduces to

$$\hat{F}_{b-flux} = 1 - \hat{u} \cdot 2 \cdot \sqrt{\pi} \tag{25}$$

yielding the explicit relationships between $\hat{n}_a$, $\hat{T}_a$, $\hat{u}$, $\hat{F}_{b-flux}$ and τ_T. Comparison of this approximate solution and the "exact" solution obtained from the solution of Eqs. (10)-(12) is shown in Fig. 4, leading to the conclusion that approximate solution gives satisfactory results for $\tau_T < 0.05$.

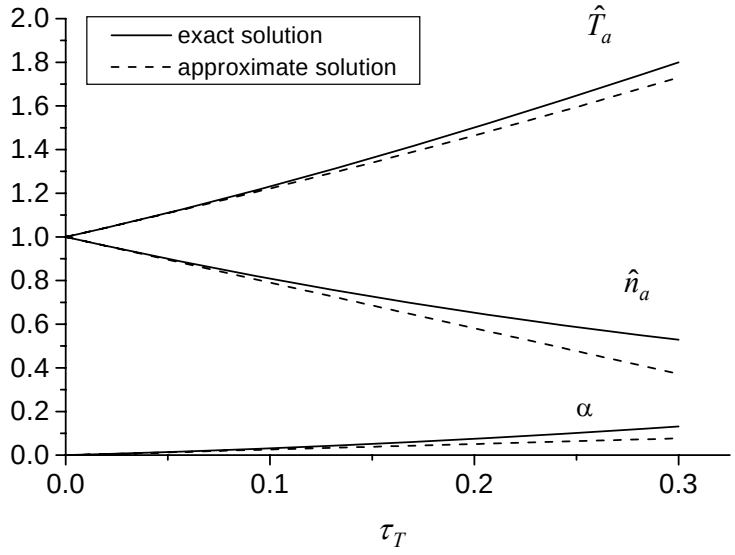

Figure 4. Comparison of exact and approximate solutions.
Polyethylene with the surface temperature of 800 K.

In the case where the ablating surface is heated by an additional (external) heat source, for example by laser radiation [e.g., Anisimov 1968], Eq. (14) can be rewritten as

$$-E_x - E_{ext} = M_x \cdot \Phi_{vap} \quad , \tag{26}$$

where E_{ext} is an external heat flux to the ablative surface. It is worth noting that in the case where thermal conduction in the wall is not equal to zero, see Eq. (26), the E_{ext} is the net external heat flux at the wall equal to the external heat flux to the wall "above" the surface minus conduction heat into the wall "behind" the surface. With an increase in E_{ext} the ablation rate increases and, if E_{ext} becomes much larger than conduction heat flux, we may drop the conduction heat term from the velocity distribution function (Eq. (3)), recovering the previous models [9-15].

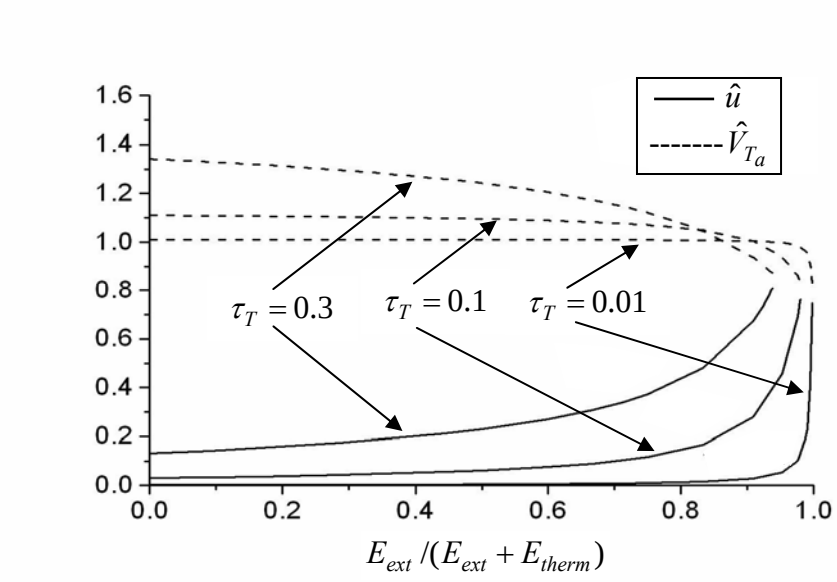

Figure 5. Parameters of the Knudsen layer as functions of ratio of external heat flux to the total heat flux at the ablating polyethylene surface

Figure 5 shows $\hat{V}_{T_a}$ and $\hat{u}$ as functions of the ratio of an external heat flux to the total heat flux, $q = E_{ext}/(E_{ext} + E_{thermal})$ for the ablative polyethylene wall with the polyethylene surface temperatures of 800 K and for τ_T = 0.01, 0.1, and 0.3; the calculations have been performed up to sonic conditions with γ = 5/3. As one can see with a decrease in τ_T and an increase in q, the distributions of $\hat{V}_{T_a}$ and $\hat{u}$ are converging to the case of τ = 0.

IV. COMPARISON WITH HERTZ-KNUDSEN THEORY

One commonly used analytical model of the Knudsen layer is the classical Hertz-Knudsen model, Hertz [1882] and Knudsen [1915], which assumes no collisions in the gas kinetic layer at the wall, no thermal conductivity in the bulk gas. Bond and Struchtrup [2004] have shown that in the case of non-zero thermal conduction to the wall, as long as the vapor is not too rarefied, the thermal conduction parameter $\tau_T << 1$, and the Mach number is small, $u << V_{T_a}$, the Chapmen-Enskog theory gives the same equations for mass and energy fluxes through the discontinuity region as does the classical Hertz-Knudsen theory,

$$M_x = \frac{m \cdot n_{sat} \cdot V_T}{\sqrt{\pi}} - \frac{m \cdot n_a \cdot V_{T_a}}{\sqrt{\pi}} \quad , \tag{27}$$

$$E_x = \frac{m \cdot n_{sat} \cdot V_T^{3/2}}{\sqrt{\pi}} - \frac{m \cdot n_a \cdot V_{T_a}^{3/2}}{\sqrt{\pi}} \quad , \tag{28}$$

However, their model, as well as the classical Knudsen layer model, ignores collisions in the Knudsen layer and, therefore, the law of conservation of momentum does not hold through the Knudsen layer. As mentioned in the Introduction, the Hertz-Knudsen assumption of no collisions in the Knudsen layer is inconsistent because it assumes no "relaxation" in the kinetic (Knudsen) layer, where the velocity distribution function at the ablative surface has to relax (converge) to the bulk gas distribution function at the outer boundary of the Knudsen given, in our case, by Eq. (1). That is why a comparison between a Hertz-Knudsen model and our model is important. Since our model as well as all others, including the Bond-Schruchtrup-Hertz-Knudsen model, give the right asymptotical solution at thermodynamic equilibrium, where the mass and energy fluxes are equal to zero, we can expect differences in the Knudsen layer models in the region far from the equilibrium.

We can derive a Hertz-Knudsen model of Bond-Struchtrup [2004] in the case of the wall absorption coefficient equal to one from our model, Eq. (10) - (12) by dropping the momentum conservation law equation, Eq. (11), and taking $\beta = 1$, literally using Eq. (2) with $\beta = 1$ for preserving the mass and energy conservation laws within the Knudsen layer,

$$\frac{1}{2 \cdot \sqrt{\pi}} = C_1 - \hat{n}_a \cdot \left[\frac{\hat{u}}{2} \mathrm{erfc}\left(\frac{\hat{u}}{\hat{V}_{T_a}} \right) - \frac{\hat{V}_{T_a}}{2 \cdot \sqrt{\pi}} \cdot \exp\left(- \frac{\hat{u}^2}{\hat{V}_{T_a}^2} \right) \right] \quad , \tag{29}$$

$$\frac{1}{\sqrt{\pi}} = \hat{n}_a \cdot \hat{V}_{T_a}^3 \cdot \left[\frac{1}{2 \cdot \sqrt{\pi}} \cdot \left(\frac{\hat{u}^2}{\hat{V}_{T_a}^2} + 2 \right) \cdot \exp\left(- \frac{\hat{u}^2}{\hat{V}_{T_a}^2} \right) - \frac{\hat{u}}{\hat{V}_{T_a}} \cdot \frac{1}{2} \left(\frac{5}{2} + \frac{\hat{u}^2}{\hat{V}_{T_a}^2} \right) \cdot \mathrm{erfc}\left(\frac{\hat{u}}{\hat{V}_{T_a}} \right) \right] + C_3 , \tag{30}$$

where C_1 and C_3 are given by Eqs. (5) and (7). Our generalized Hertz-Knudsen model differs from the Bound and Struchtrup model [2004], where they have used first-order Taylor expansion of Eq.

(3) about zero in u/V_{T_a} ; thus, the Bond-Struchtrup model cannot be used for relatively large Mach numbers.

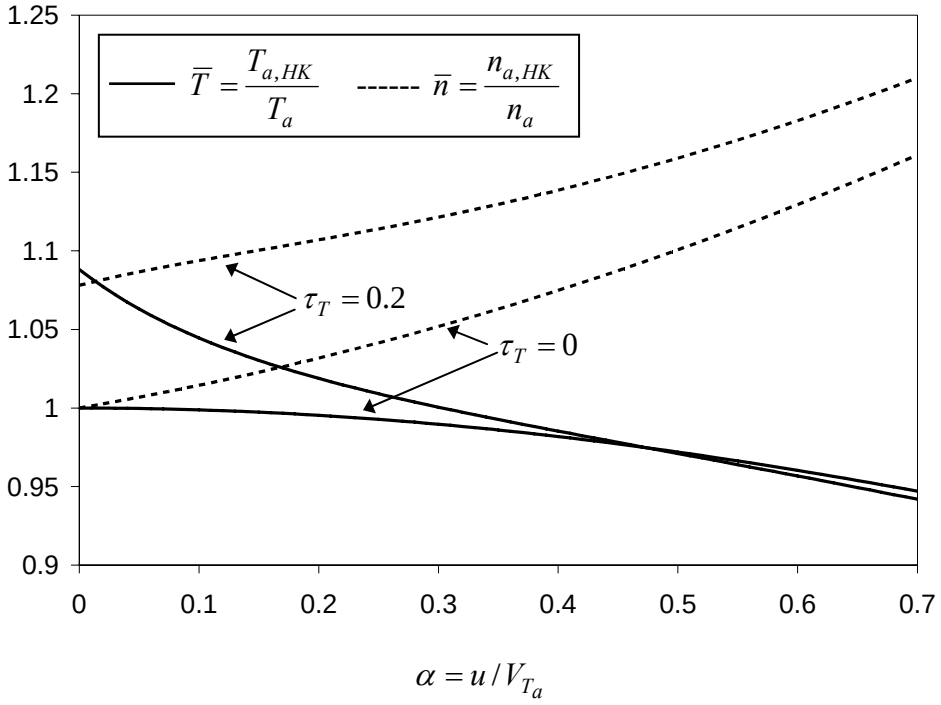

Figure 6. Comparison of the bimodal-collisional model with a generalized Hertz-Knudsen model.

Fig. 6 represents a comparison of our general model, Eqs. (10) – (12) and the generalized collisionless Hertz-Knudsen model, Eqs. (29) – (30), for $\tau_T = 0,\ 0.2$. This figure shows the distributions of $\overline{T} = T_{a,H-K}/T_a$ and $\overline{n} = n_{a,H-K}/n_a$ vs. $\alpha = u/V_{T_a}$, where $T_{a,H-K}$ and $n_{a,H-K}$ are the temperature and number density at the outer boundary of the Knudsen layer calculated using the generalized Hertz-Knudsen model. As one can see, in the case of no conduction heat ($\tau_T = 0$), the ratios $\overline{T}$ and $\overline{n}$ converge to unity as $\alpha \to 0$; this is expected since the case of $\tau_T = \alpha = 0$ corresponds to thermal equilibrium. However, with an increase in α (non-thermodynamic region) the temperature and density distributions calculated by the two models begin to diverge, and $\overline{T}$ and $\overline{n}$ for $\alpha = 0.7$ reach up to -5% and 16%, respectively. In the case of thermal conduction, with an increase in τ_T, the differences in the models rise: for $\tau_T = 0.2$ and $\alpha = 0$, the case of thermal heat conduction to the wall with no ablation, $\overline{T}$ and $\overline{n}$ reach 9% and 8%, respectively, and for $\tau_T = 0.2$ and $\alpha = 0.7$, they are -5% and 20% respectively. Thus, it has been demonstrated that our model of the Knudsen layer gives very different results than the Hertz-Knudsen model.

V. CONCLUDING REMARKS

We presented an analytical model of the Knudsen layer near the ablative surface, taking into account the thermal conductivity in the adjusted bulk gas. This model employs a bimodal velocity distribution function in the Knudsen layer. The gas mean-free-path in the model is assumed to be much smaller than the characteristic temperature gradient length in the bulk gas. This condition is needed for the Chapmen-Enskog expansion method to solve the Boltzmann equation used in the

paper. Thus, this model is limited to relatively small temperature gradients. In the case of a larger temperature gradient a more rigorous model is required and only numerical simulation such as DSMC would solve the problem.

The model allows obtaining the boundary conditions at the interface between the ablative surface and the bulk gas avoiding "micro" modeling of the evaporation process at the mean free path scale. Thus, our Knudsen layer model can be used as a "constructor" for boundary conditions between the bulk gas and ablative surface that is important for numerical simulation of evaporation processes and for fluid dynamics in general.

The widely used Hertz-Knudsen model and its generalizations assume no collisions in the Knudsen layer and, therefore, do not preserve the law of conservation of momentum within the Knudsen layer; they preserve only the mass and energy conservation laws. In comparison, our model preserves all three conservation laws. However, both models give the right asymptotical solution at thermodynamic equilibrium (where the mass and energy fluxes are equal to zero). That is why it was important to compare these models in cases that are far from thermodynamic equilibrium. Our calculations show significant differences between the two models. With an increase in the thermal conductive heating of the ablated surface or/and in the flow velocity, the differences between the two models dramatically increase; for $\tau_T = 0.2$ and $\alpha = 0.7$ the differences in temperatures and density calculated at the outer boundary of the Knudsen layer reach up to almost 20%.

Finally, the presented analytical model can be verified by comparison with direct Monte Carlo or ES-BGK simulations.

The authors wish to thank M. Kapper for helpful discussions and important remarks.

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