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Effect of Thermal Conductivity on the Knudsen Layer at Ablative Surfaces (Preprint)

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Abstract

In this paper we develop an analytical model of Knudsen layer at the ablative wall taking into account the temperature gradient in the bulk gas. The region of validity of the existing models and effect of the temperature gradient on the Knudsen layer properties are calculated.

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The formation of the Knudsen layer, the non-equilibrium (kinetic) layer, near the vaporizing surface and subsequent ablation is of great interest for a number of applications such as capillary discharges [1,2], plasma thrusters [3,4], high-pressure discharges [5], vacuum arcs [6], electroguns [7] and laser ablation [8].

Anisimov [9] 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 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. This result was obtained under the assumption that the atom flow velocity is equal to the sound velocity at the external boundary of the Knudsen layer and the temperature of the gas in the equilibrium region (beyond Knudsen Layer) is constant, i.e. no conductive heat flux to the ablative wall surface.

However, in many physical situations, the vapor leaving the non-equilibrium layer cannot be described by using a speed of sound approximation. For example, in ablative capillary discharges, the gas motion in the capillary chamber is not "free"; it is restricted by the capillary wall, leading to a more dense gas (plasma) in the discharge volume and therefore, larger backflux to evaporating surface and smaller flow velocity at the outer boundary of the Knudsen layer.

Beilis [10,11], was the first to consider ablation into a dense plasma. He studied the case of metal vaporization into discharge plasmas in a vacuum arc cathode spot. He concluded that the parameters at the outer boundary of the Knudsen layer are close to their equilibrium values and that the velocity at the outer boundary of the kinetic layer is much smaller than the sound velocity.

Later these models were applied for the case of dielectric ablation into the discharge plasma in the capillary discharge conditions [12, 13] and for the case of strong plasma acceleration [14]. 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. In particular, neglecting the conductive heat flux leads results in the calculated gas temperature at the outer boundary of the Knudsen layer to appears to be smaller than the temperature of the evaporating surface. This consequently leads to the heat flux through the Knudsen Layer being directed upward to the plasma chamber. Therefore, neglecting the conductive heat transfer in the Knudsen layer leads to an inconsistency in all the models [1-7] where the gas (plasma) temperature is larger than the surface temperature of the ablative wall.

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 temperature of the ablating surface might be larger than the gas temperature at the outer boundary of the Knudsen Layer. This is the case for the example in [9], where an externally applied laser radiation source heats the ablating surface but for which the gas (plasma) is transparent.

Recently many numerical models of evaporation processes were developed based on Monte Carlo simulation [15-17] and numerical solutions of the Boltzmann equations [18], describing the kinetic layer without any a prior approximation of gas velocity function distribution in that layer. However, as Rose [19] has demonstrated the models using his and Anisimov's bimodal velocity distribution functions in the kinetic layer give results virtually co-incident with numerical solutions of the Boltzmann-Krook-Welander equation for evaporation of a monatomic substance with condensation coefficient equal to unity. As shown in [15-17], analytical models also are in good agreement with Monte Carlo simulation.

Ideally Monte Carlo simulations 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. 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, and in improving our physical understanding of the Knudsen layer.

We would also like to point out the recent paper by Bond and Struchtrup [20] in which the authors have included the conduction heat flux in their analytical model of water evaporation. This is a generalized Hertz-Knudsen model, which does not consider the vapor velocity distribution function in the Knudsen layer but uses the condensation and evaporation coefficients (probabilities) at the boundaries of Knudsen layer to take into account backflux effect (due to collisions) in the Knudsen layer. However these coefficients can have a complex dependence on the evaporation conditions such as vapor pressure, temperature, surface conditions, incidence angle, etc., and are usually determined experimentally or by fitting the model with experimental data. In the case of dielectric ablation into plasma, where the ablation parameters vary among a wide range of temperatures and pressures, these coefficients are not experimentally measured. The analytical models using bimodal velocity distribution functions, such as the one described here, self-consistently calculate the backflux and implicitly assume a condensation coefficient of unity. As it has been mentioned above, they describe the ablation process with reasonable approximation, and the effect of variable condensation coefficient is not considered here.

In this paper we develop an analytical model of the Knudsen layer by considering an appropriate boundary condition in the kinetic formulation that takes into account the temperature gradient. The region of validity of the existing models and the effect of the temperature gradient on the Knudsen layer properties are calculated. The main impetus of this Communication is to study the effect of the thermal conductivity on the Knudsen layer formed near the ablated surface. This analysis is based on the premise that thermal conductivity (the temperature gradient) in the gas bulk can be taken into account in the velocity distribution function at the outer boundary of the Knudsen layer. In this paper we use such a function obtained by Chapman-Enskog expansion method for solving Boltzmann equation [21] based on assumption that the molecular mean-free-path is much smaller than characteristic scale of the temperature change. Thus, our model is limited to relatively small values of the temperature gradients.

Following Anisimov's method [9], let us write the velocity distribution function in the kinetic layer with the evaporating surface in the form, Fig.1

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

where

$$f_b(\vec{V}) = \begin{cases} \left(\dfrac{1}{\sqrt{\pi}}\right)^3 \cdot \exp\left(-V^2\right), & V_x > 0 \\ \\ \beta\cdot n_1 \cdot \left(\dfrac{1}{\sqrt{\pi}\cdot V_1}\right)^3 \cdot \exp\left(-\dfrac{(V_x-u)^2 + V_y^2 + V_z^2}{V_1^2}\right), & V_x < 0 \end{cases} \tag{2}$$

$$f_u(\vec{V}) = n_1 \cdot f_M(\vec{V}) \cdot \left\{ 1 - \frac{V_T \cdot V_1}{\nu} \cdot \left[\frac{(V_x - u)}{V_1} \cdot \left(\frac{(V_x - u)^2 + V_y^2 + V_z^2}{V_1^2} - \frac{5}{2} \right) \cdot \frac{d}{dx}(\ln T) \right] \right\} \quad , \quad (3)$$

$$f_M(\vec{V}) = \left(\frac{1}{\pi \cdot V_1^2} \right)^{3/2} \cdot \exp\left(- \frac{\left[(V_x - u)^2 + V_y^2 + V_y^2 \right]}{V_1^2} \right) \quad . \quad (4)$$

Here f_b is the velocity function distribution at the inner boundary of Knudsen layer (at the ablative surface) with Maxwellian vaporization function for $V_x > 0$ and a shifted "backflux" Maxwellian function of the particle for $V_x < 0$ describing the particles incoming to the surface from the gas, where *x*-axis is normal directed to the wall from the gas chamber; f_u is the Chapman-Enskog velocity distribution function at the outer boundary of the Knudsen layer that takes into account the temperature gradient and directed velocity [21] above the Knudsen layer, as shown in Figure 1; $T_0=V_T^2/(2m)$ is the temperature of the ablated surface; 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 number density is normalized on the equilibrium vapor number density corresponding to the surface temperature T_0 and all velocities are normalized on V_T. The expression for f_b takes into account the fact that the vaporized atoms have Maxwellian distribution at a temperature equal to the surface temperature [22] and also assumes that the number density of the evaporated atoms is equal to a half of the equilibrium vapor number density at this surface temperature that is a reasonable approximations used in all previous bimodal velocity distribution functions models [9 – 17]. It should be noted that the Anisimov's model [9] (as well as all other existing models) employed shifted Maxwellian function at the outer boundary of Knudsen Layer ignoring, as mentioned above, the conduction heat transfer to the ablative surface, i.e. temperature gradient at the edge of the Knudsen layer.

Assuming the conservation laws of mass, momentum and energy hold at all times within the discontinuity region, through the Knudsen layer, as it has been assumed in all previous models [9-14] (quasi steady state approximation within the Knudsen layer), the following integrals are defined:

$$C_1 = \int_{-\infty}^{+\infty} dV_z \int_{-\infty}^{\infty} dV_y \int_{-\infty}^{+\infty} f \cdot V_x \cdot dV_x = n_1 \cdot u \quad , \quad (5a)$$

$$C_2 = \int_{-\infty}^{+\infty} dV_z \int_{-\infty}^{\infty} dV_y \int_{-\infty}^{+\infty} f \cdot V_x^2 \cdot dV_x = n_1 \cdot \left(u^2 + \frac{V_1^2}{2} \right) \quad , \tag{6a}$$

$$C_3 = \int_{-\infty}^{+\infty} dV_z \int_{-\infty}^{\infty} dV_y \int_{-\infty}^{+\infty} f \cdot V^2 \cdot V_x \cdot dV_x = n_1 \cdot \left[u \cdot \left(u^2 + \frac{5 \cdot V_1^2}{2} \right) - \frac{(V_T \cdot V_1)}{\nu} \cdot \frac{d(\ln T)}{dx} \cdot \frac{5 \cdot V_1^3}{4} \right] , \tag{7a}$$

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

$$M_x = m \cdot n_0 \cdot V_T \cdot C_1 \quad , \tag{5b}$$

$$P_x = m \cdot n_0 \cdot V_T^2 \cdot C_2 \quad , \tag{6b}$$

$$E_x = m \cdot n_0 \cdot \frac{V_T^3}{2} \cdot C_3 \quad . \tag{7b}$$

where E_x consists of the two parts: the conduction heat flux and the enthalpy flux of the gas moving with a directed velocity, Eq. (7a). Taking into account that integrals C_1, C_2, and C_3 are preserved through the Knudsen layer and they should be independent on $\delta(x)$, we obtain the following equations corresponding to C_1, C_2, and C_3:

$$\frac{1}{2 \cdot \sqrt{\pi}} = C_1 - n_1 \cdot \beta \cdot \left[\frac{u}{2} \operatorname{erfc}\left(\frac{u}{V_1} \right) - \frac{V_1}{2 \cdot \sqrt{\pi}} \cdot \exp\left(-\frac{u^2}{V_1^2} \right) \right] \quad , \tag{8}$$

$$\frac{1}{4} = C_2 - n_1 \cdot \beta \cdot \left[\left(\frac{u^2}{2} + \frac{V_1^2}{4} \right) \cdot \operatorname{erfc}\left(\frac{u}{V_1} \right) - \frac{V_1 \cdot u}{2 \cdot \sqrt{\pi}} \cdot \exp\left(-\frac{u^2}{V_1^2} \right) \right] , \tag{9}$$

$$\frac{1}{\sqrt{\pi}} = \beta \cdot n_1 \cdot V_1^3 \cdot \left[\frac{1}{2 \cdot \sqrt{\pi}} \cdot \left(\frac{u^2}{V_1^2} + 2 \right) \cdot \exp\left(-\frac{u^2}{V_1^2} \right) - \frac{u}{V_1} \cdot \frac{1}{2} \left(\frac{5}{2} + \frac{u^2}{V_1^2} \right) \cdot \operatorname{erfc}\left(\frac{u}{V_1} \right) \right] + C_3 \ . \tag{10}$$

Equations (5), (6), (8) and (9) are identical to the corresponding mass and momentum conservation equations obtained in [10-17] while Eqs. (7) and (10) differ from the corresponding energy conservation equations [10-17] by the temperature gradient term, which is responsible for conduction heat flux to the ablative surface.

Let us introduce a thermal conduction parameter τ_T

$$\tau_T = \frac{V_T \cdot V_1}{\nu} \cdot \frac{d(\ln T)}{dx} = \frac{\lambda_{mfp}}{\delta x_T} << 1 \quad , \tag{11}$$

where λ_{mfp} = $(V_T \cdot V_1)/\nu$ is the gas mean-free-path at the outer boundary of the kinetic layer and δx_T = $[d(lnT)/dx]^{-1}$ is the characteristic gradient length. Condition (11) is needed for the Chapman-Enskog expansion method and Eq. (7a) to be valid, as explained earlier. In the case of small u, Equations (8) - (10) can be simplified to the following form

$$V_1 = 1 - u \cdot \frac{\sqrt{\pi}}{8} + \frac{5 \cdot \sqrt{\pi} \cdot \tau_T}{8} \quad , \tag{12}$$

$$\beta = 1 + u \cdot \left(\frac{2}{\sqrt{\pi}} - \frac{9 \cdot \sqrt{\pi}}{16} \right) + \frac{5 \cdot \sqrt{\pi} \cdot \tau_T}{16} \quad , \tag{13}$$

$$n_1 = 1 - u \cdot \left(\frac{2}{\sqrt{\pi}} + \frac{5 \cdot \sqrt{\pi}}{16} \right) - \frac{15 \cdot \sqrt{\pi} \cdot \tau_T}{16} \quad . \tag{14}$$

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 1; it is as expected, since the gas bulk region has a higher temperature than the wall surface and the total conduction heat flux is assumed to be directed to the wall ($\tau_T > 0$). This temperature jumps between the solid surface and the Maxwellian gas at the outer edge of the kinetic layer is a very well known phenomenon in gas dynamics, see for example review [23].

Assuming that ablation process is due to only by the gas thermal conduction (no external heat source is applied to the ablative surface), the boundary condition at the ablative surface can be written as

$$-E_x - \kappa_{wall} \cdot \frac{dT_{wall}}{dx} = M_x \cdot \Phi_{vap} \quad , \tag{15}$$

where κ_{wall} is thermal conductivity of the wall, and Φ_{vap} is evaporation heat of the wall material, $-E_x$ is the total energy flux through the Knudsen layer incoming into the ablative wall, Eq. (7b), and M_x is the mass ablation rate, Eq. (5b); the negative sign in front of E_x is due to the x-axis being directed from the wall into the gas chamber. Assuming no heat loss in the bulk of the wall[2], the boundary condition at the ablative surface is reduced to:

$$-E_x = M_x \cdot \Phi_{vap} \quad . \tag{16}$$

Thus, for a given ablative surface temperature and corresponding equilibrium vapor pressure and number density, and given heat conduction parameter τ_T, Eqs. (8) – (10) and (15) can be solved relative to variables n_1, V_1, u, and β. The total ablation rate and the heat flux to the ablative wall (Eqs. (5b) and (7b) can then be computed. The dependences of n_1, V_1, and backflux (the total flux of particles incoming to the ablative surface from the gas) on the τ_T and for a specific example of polyethylene wall are presented below.

Figure 2 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. (8) – (10) and (16); the evaporation heat has been taken as $3.6 \cdot 10^6$ [J/kg] and equilibrium vapor pressure equal as $P = 10^5 \cdot \exp(5565.22 \cdot [1/453 - 1/T])$ [24], where the pressure is in Pascal and temperature is in Kelvin. One can see that u, T, backflux, and n_1 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 2 for higher τ_T, because the Chapman-Enskog expansion method is valid only for $\tau_T << 1$. In this limit, Eq. (16) can be simplified to the following form

$$-u \cdot \left(\frac{\Phi_{vap} \cdot m}{k \cdot T_s} \right) = \frac{5}{2} \cdot u - \frac{5}{4} \cdot \tau_T \quad , \tag{17}$$

where m is the average atomic mass of polyethylene composition, and T_s is the polyethylene surface temperature. Expressing u as a function of τ_T, Eq. (17), and substituting it into Eqs. (12) and (14) and then into equation for normalized backflux at the ablative wall,

$$F_{b-flux} = 1 - u \cdot n_1 \cdot 2 \cdot \sqrt{\pi} \approx 1 - u \cdot 2 \cdot \sqrt{\pi} \quad , \tag{18}$$

yields the explicit relationships between n_1, $T = V_1^2$, u, $F_{b\text{-}flux}$ and τ_T. Comparison of this approximate solution and the "exact" solution obtained from the solution of Eqs. (8)-(10) is shown in Fig. 3, leading to the conclusion that approximate solution gives satisfactory results for $\tau_T < 0.05$.

[2]This can be the case of a "boiling wall", where all heat incoming into the wall is spent on vaporization.

We also would like to point out that in the case of thermal conduction, u is small and cannot reach sonic condition. Otherwise, E_x would be positive, Eqs. (7a) and (7b), meaning that the total energy flux would be directed not to the ablative surface but upward into the gas chamber, contradicting the model assumptions.

In the case where the ablating surface is heated by an additional (external) heat source, for example by laser radiation [9], Eq. (16) can be rewritten as

$$-E_x - E_{ext} = M_x \cdot \Phi_{vap} \quad , \qquad (16')$$

where E_{ext} is an external heat flux to the ablative 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 [9-14]. Figure 4 shows V_1 and 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 $\gamma = 5/3$. As one can see with a decrease in τ_T and an increase in q, the distributions of V_1 and u are converging to the case of $\tau = 0$.

The effect of heat conduction in the case of an external heat flux can also be calculated, following [10-14], as functions of of $\alpha = u/V_1$ for different τ_T, Eqs. (8) – (10); here, the variation of α indicates the magnitude of the external heat flux compared to the conduction heat flux (as α and the flow velocity increase up to sonic condition, there can be no heat conduction to the wall). The results of these calculations are shown in Figure 5. As one can see at small α the effect of thermal conduction is important, and with an increase in α, the effect of thermal conduction decrease, E_x increases and changes sign (becomes positive meaning that the total energy flux is directed upward, Fig. 1, into the gas chamber, see Eqs. (7a) and (7b)) and the temperature and density plots are converging to the case of $\tau_T = 0$. As one can see, T_1 and n_1 decreases with an increase in α (with an increase in directed velocity u), Fig. 5, that can be explained by expansion of the dense ablated gas stream in less dense gas surrounding. It is worth noting, that such a decrease in T_1 and n_1 leads to a decrease in the thermal heat conduction at a given τ_T too, see Eqs. (7a) and (11).

In summary, a model of the Knudsen layer near the ablated surface in the case of surface heating by the adjacent gas by virtue of thermal conductivity was developed. Previously existing models were not able to describe this physical situation due to neglecting effect of the temperature gradient on the velocity distribution function in the gas and thus leading to temperature gradient directed outwards the surface. In contrast, the developed model predicted existence of the temperature gradient towards the surface. It should be pointed out that this model is limited to relatively small temperature gradients due to the limitation of the Chapman-Enskog expansion for solving the Boltzmann equation. In a case of a larger temperature gradient a more rigorous model is required and only numerical simulations such as DSMC would be able to solve the problem.

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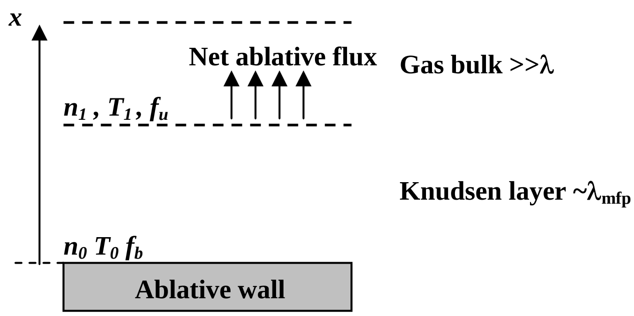

Fig. 1. Schematic representation of the layer structure near the ablative surface

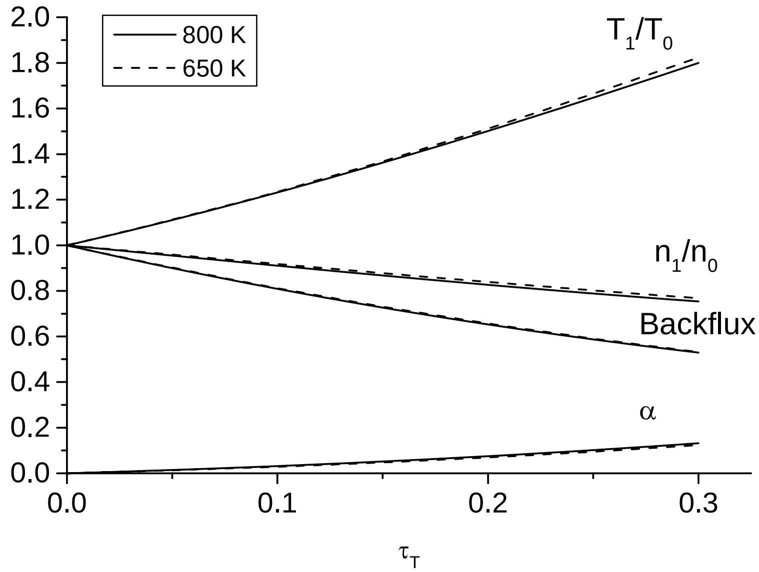

Fig. 2. Normalized u, T_1=V_1^2, and Backflux at the ablative surface vs. τ_T.

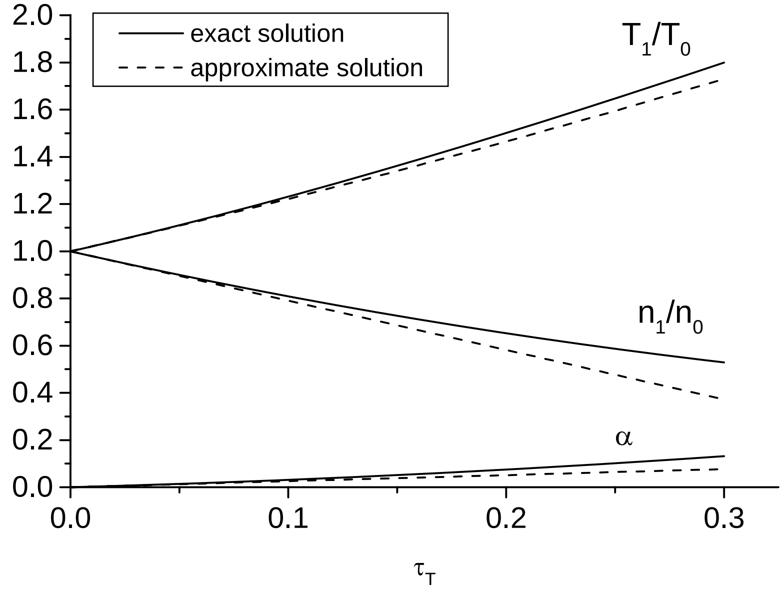

Fig. 3. Comparison of exact and approximate solutions. Polyethylene with the surface temperature of 800 K.

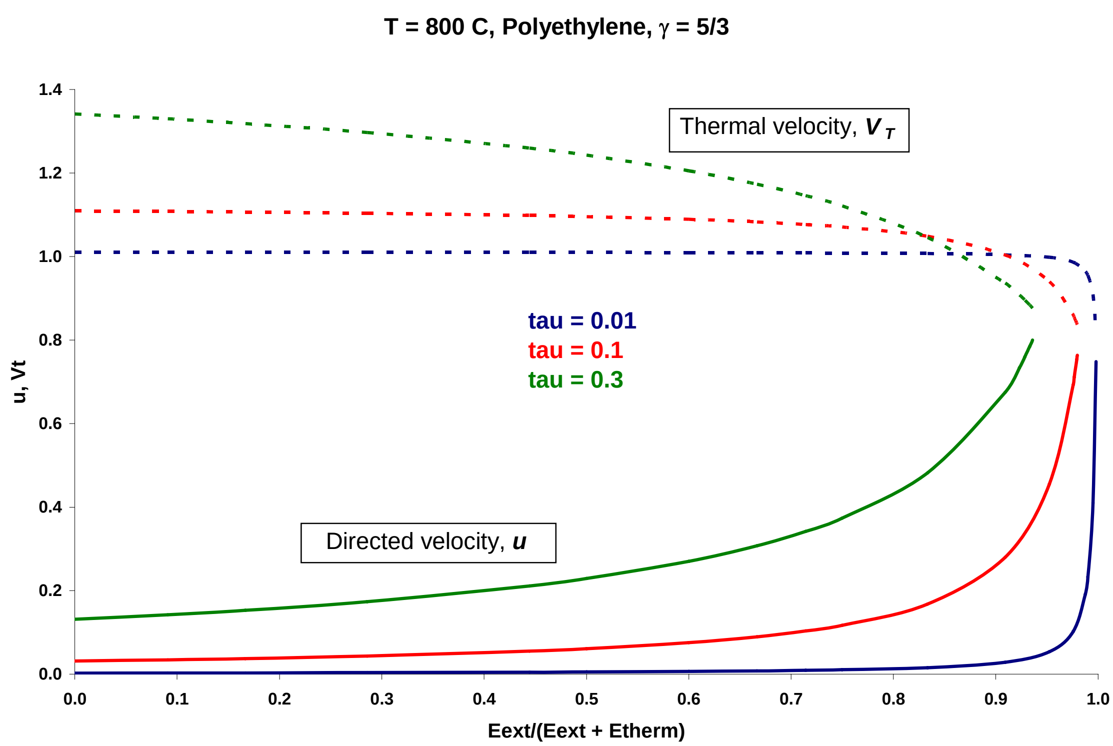

Fig. 4. Normalized thermal and directed velocities at the outer boundary of the Knudsen layer as functions of ratio of external heat flux to the total heat flux at the ablating polyethylene surface.

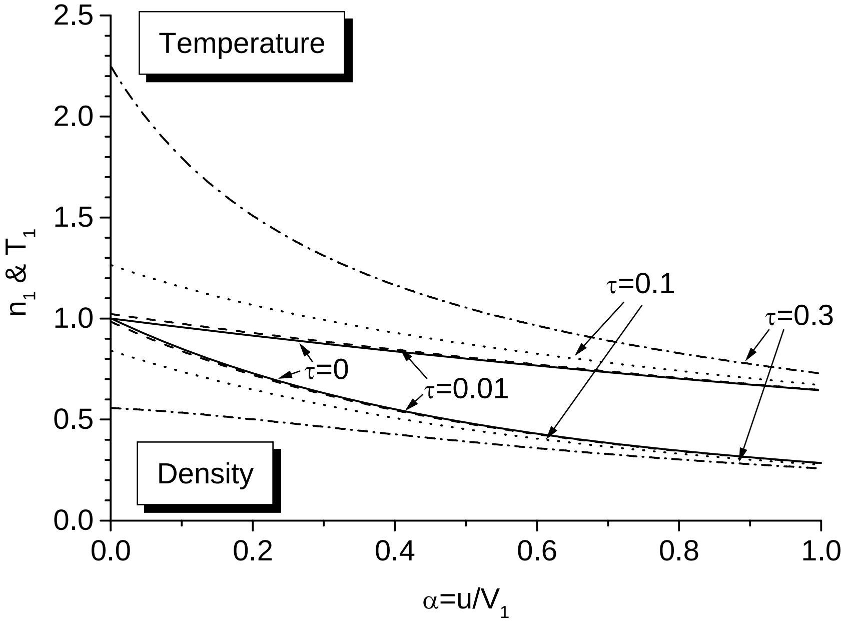

Fig. 5. Normalized temperature and density at the outer boundary of Knudsen layer as a function of $\alpha = u/V_1$ with temperature gradient at the Knudsen layer edge as a parameter.