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USE OF THE PRESSURE JUMP BOUNDARY CONDITION IN THE HIGH SPEED RAREFIED GAS FLOWS

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Abstract. The use of a new temperature jump condition considering the viscous heat generation due to sliding friction has been recently proposed in the literature. It gives a more accurate prediction w.r.t the DSMC results for temperature and heat flux. In this work, we study the case of hypersonic flow over a flat plate with inlet Mach number of 6.1, for which the experimental and the DSMC results are available in the literature. We have verified our formulation of various non-equilibrium boundary condition with the already published results. It is then shown that using the new temperature jump condition, pressure is over-predicted, especially at the leading edge of the plate. We have then demonstrated that the use of a previously-published pressure jump condition, which has been largely ignored in the literature, is a means to correct the over-prediction of pressure. The use of the new temperature jump with the pressure jump boundary condition circumvents the problem of over-prediction of pressure without affecting the other flow parameters. Also, we show the effect of the pressure jump condition with the "standard" non-equilibrium boundary condition.

1 INTRODUCTION

The simulation of rarefied gas flow in hypersonic aerodynamics is important for the design of space and re-entry vehicles. Computer simulations can provide the necessary aerodynamic data at less cost and for cases where experiments are difficult to conduct. Therefore, there is a constant effort to develop new numerical methods and to improve the

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existing ones based on appropriate physical modeling, so as to make the computer simulations closer to reality. CFD methods are preferred for rarefied flows in the continuum and slip flow regime.

In compressible flows, the regimes based on the rarefaction effect of gas molecules can be classified as continuum, slip, transition and free molecular flow. These different regimes are characterized by the Knudsen number(Kn), defined as [1]:

$$Kn = \frac{\lambda}{L} \tag{1}$$

where λ and L are the molecular mean free path and characteristic length scale of the flow, respectively.

The range $0.001 \leq Kn \leq 0.01$ is called the slip regime, where the no-slip conditions are no longer applicable. The no-slip boundary conditions are replaced in this regime with appropriate slip velocity and temperature-jump boundary conditions.

Recently, in the literature for high-speed non-equilibrium gas flows a new type of Smoluchowski temperature jump condition considering the viscous heat generation due to sliding friction has been proposed as an alternative jump condition for the prediction of the surface gas temperature at solid interfaces [2]. The effect of the new jump condition on temperature and heat flux has been reported for various flow situations. However, the jump condition seems to adversely affect the prediction of surface pressure. We have proposed to correct the anomaly by using a previously published pressure jump condition [3]. We show, by taking the case of rarefied gas flow over a flat plate, the benefits of this pressure jump boundary condition with the new temperature jump condition. We also use the pressure jump condition with the standard Maxwell velocity slip and Smoluchowski temperature jump condition. The results are compared with both the DSMC and experimental data.

2 Nonequilibrium Boundary Condition

2.1 Maxwell slip boundary condition

The Maxwell slip boundary condition [4], including the effect of thermal creep, can be written as a Robin (or mixed) boundary condition in the following way [5]:

$$\boldsymbol{u} + \Big(\frac{2-\sigma_u}{\sigma_u}\Big)\lambda\nabla_n(\boldsymbol{S}\cdot\boldsymbol{u}) = \boldsymbol{u_w} - \Big(\frac{2-\sigma_u}{\sigma_u}\Big)\frac{\lambda}{\mu}\boldsymbol{S}\cdot(\boldsymbol{n}\cdot\boldsymbol{\Pi_{mc}}) - \frac{3}{4}\frac{\mu}{\rho}\frac{\boldsymbol{S}\cdot\nabla T}{T} \tag{2}$$

In Equation 2 the right hand side consist of three terms that are associated with the wall velocity, the so-called curvature effect and the thermal creep, respectively. For the nomenclature of each term please refer [5].

2.2 Smoluchowski temperature jump boundary condition

In rarefied conditions the gas temperature of the surface is not equal to the surface temperature, and the corresponding difference it is called the “temperature jump”. It is dependent on the heat flux normal to the surface. The Smoluchowski model [6] expressed as a Robin (or mixed) boundary condition is shown below:

$$T + \Big(\frac{2-\sigma_T}{\sigma_T}\Big)\frac{2\gamma}{(\gamma+1)}\frac{\lambda}{Pr}\nabla_n T = T_w \tag{3}$$

2.3 The Le Temperature Jump boundary Condition [2]

This boundary condition for temperature at the wall is a modified form of the Smoluchowski temperature jump condition which also considers the viscous heat generation (sliding friction) due to the presence of a slip velocity of the fluid at the wall. The Le temperature jump condition as proposed in [2] is:

$$T + \Big(\frac{2-\sigma_T}{\sigma_T}\Big)\frac{2\gamma}{(\gamma+1)}\frac{\lambda}{Pr}\nabla_n T = T_w - \Big(\frac{2-\sigma_T}{\sigma_T}\Big) \times \frac{2\lambda(\gamma-1)}{\mu(\gamma+1)R}((\boldsymbol{S}\cdot(\boldsymbol{n}\cdot\boldsymbol{\Pi}))\cdot(\boldsymbol{u}-\boldsymbol{u_w}) \tag{4}$$

2.4 Pressure Jump Boundary Condition

The Maxwell-Smoluchowski boundary conditions given by Eqs. 2 and 3 are usually used with a homogeneous Neumann condition (zero normal gradient) for pressure [7, 8]. Using the Le temperature jump condition given by Eq. 4 with a homogeneous Neumann pressure condition at the wall, however, leads to over-prediction of the pressure for the hypersonic flow over the flat plate (as we shall see in Sec. 5). This is consistent with the notion that sliding friction, which is taken into account for temperature, should tend to lower the pressure and so would require consideration even in the pressure boundary condition. This observation motivated us to reconsider the pressure boundary condition at the wall.

Patterson [9] used an alternative derivation for non-equilibrium BCs using Grad's moment method [10]. It is based on the conservation laws for mass, momentum and energy for incident and reflected molecules at a surface. Vidal et al. [11] in their study of hypersonic flow over a flat plate have used this method for velocity slip and temperature jump and have mentioned the existence of a pressure jump. Recently, Greenshields and Reese [3] have revisited those formulations and have given a derivation for the non-equilibrium BCs following Patterson's derivations. The final form of the pressure jump boundary condition, as given in [3], is presented below.
Using the analysis of mass conservation, the expression for density at the wall is obtained as

$$\frac{\rho_w}{\rho} = \sqrt{\frac{T}{T_w}}(1+\zeta) \tag{5}$$

where ρ is the actual density of the fluid at the wall surface; ρ_w is the density of fluid obtained with an equilibrium distribution at the wall temperature T_w, and

$$\zeta = -\frac{\boldsymbol{\Pi} : \boldsymbol{nn}}{2p} \tag{6}$$

is the ratio of the normal viscous stresses to pressure. The normal unit vector ($\boldsymbol{n}$) is assumed to be pointing outward. Using, ρ_w we can obtain the wall pressure as $p_w =$

$\rho_w RT_w$, from the ideal gas relation. A point to note here (following [3]) is the subscript w denotes the presumed properties of the fluid for an assumed equilibrium distribution with the wall temperature T_w and those with no subscript denote the actual fluid property at the wall surface.
Using the analysis of normal-momentum conservation, the expression for the pressure jump is obtained as follows:

$$p\Big(1 + 2\zeta + \frac{2-\sigma}{\sigma}\frac{4}{5\sqrt{2\pi}}\mathbf{a}\cdot\mathbf{n}\Big) = p_w \tag{7}$$

or,

$$p = \frac{p_w}{\Big(1 + 2\zeta + \frac{2-\sigma}{\sigma}\frac{4}{5\sqrt{2\pi}}\mathbf{a}\cdot\mathbf{n}\Big)} \tag{8}$$

where using $\boldsymbol{q} = -k\nabla_n T$ we have:

$$\mathbf{a}\cdot\mathbf{n} = -\frac{1}{p\sqrt{RT}}\mathbf{q}\cdot\mathbf{n} = \frac{1}{p\sqrt{RT}}k\nabla_n T$$

Here, p is the pressure of the fluid at the wall. The pressure jump BC is incorporated using this value of p as Dirichlet condition at the wall, instead of giving pressure a homogeneous Neumann condition. Eq. 8 is usually ignored in simulation of rarefied gas flows. Greenshields and Reese [3] have written "its use is unclear" citing Gupta et al. [12]. We have however, chosen to examine the role of pressure jump condition with the Le temperature jump condition (Eq. 4) for various hypersonic flow situations over the flat plate cases considered in this work. In the numerical implementation, Eq. 6 is unphysical when $\zeta \le 1$ and almost impossible when $\zeta > 1$ [3]. The value of $|\zeta|$ is therefore assumed to be always less than 1 [9, 12], but this assumption may not hold true in the case of rarefied high speed flows [3]. To circumvent this problem researchers suggest clipping ζ when it falls below some level. Greenshields and Reese [3] have chosen to set $\zeta = 0$ for the cases considered in their work. We have, for our cases, clipped the values of ζ as follows:

$$\zeta = \begin{cases} 1, & \text{if } \zeta_o > 1 \\ -1, & \text{if } \zeta_o < -1 \\ \zeta_o, & \text{otherwise} \end{cases} \tag{9}$$

where, $\zeta_o = \frac{-\boldsymbol{\Pi}:\boldsymbol{nn}}{2p}$. In Eq. 8, based on the assumption of diffuse reflection everywhere, the accommodation coefficient (σ) is chosen as 1 [3].

3 Heat transfer in a rarefied gas flow simulations

With sliding friction being taken into the account in computing the heat transfer at the wall, Maslen [13] proposed a formulation for planar surfaces which was extended for curved surfaces by Le et al [14, 2] as follows:

$$\boldsymbol{q} = -k\nabla_n T - (\boldsymbol{S}\cdot(\boldsymbol{n}\cdot\boldsymbol{\Pi}))\cdot(\boldsymbol{u} - \boldsymbol{u_w}) \tag{10}$$

where the right hand side consists of two terms that respectively incorporate Fourier heat conduction and sliding friction (shear work per unit area).

4 Hypersonic Flat Plate Case

Several experimental and theoretical investigations have been carried out to study rarefied hypersonic flow over a flat plate with a sharp leading edge. These investigations, especially the striking experimental results obtained very near the leading edge, have generated a lot of interest in the problem [7]. In this work, we attempt a comprehensive analysis of different flat plate cases using the Le temperature jump condition [14] by not only studying the temperature and heat flux at the wall but also other flow properties such as pressure and slip-velocity. We compare the obtained results with DSMC results and the experimental data available in the literature [7, 3, 14, 2].

We first verify, in this section, our numerical implementation of the first order Maxwell Slip (Eq. 2), the Smoluchowski temperature jump (Eq. 3) and the Le temperature jump (Eq. 4) boundary condition with the results published in literature [2]. We then present our study of the flat plate case with different sets of non-equilibrium boundary conditions in the next section.

4.1 Boundary and initial conditions

Figure 1 also shows the boundaries of the flow domain for the flat plate problem. For the inlet and outlet, the characteristic boundary conditions based on Riemann invariants are used [15]. At the wall, nonequilibrium boundary conditions are applied (see Table 2). The uniform free-stream inflow condition is used to set the initial conditions throughout the flow-field, for the pseudo-transient solution.

4.2 Numerical Verification and Validations

We have implemented the non-equilibrium boundary condition in our in-house 3D unstructured grid solver which has been previously validated for various configurations of flows [16, 17]. The first order Maxwell Slip (Eq. 2) and Smoluchowski temperature jump (Eq. 3) boundary condition has been implemented in our solver and verified for various configurations of the flow [18]. In this section, we present a numerical verification of our present code including the Le temperature jump condition (Eq. 4) with the results presented by Le et al [2] for a hypersonic flow over a flat plate. The flow domain is shown in Fig. 1. The inlet condition is the same as that of Metcalf et al [19, 2] with $T_w = 77$ K. The gas used is Nitrogen and its properties are given in Table 1. The accommodation coefficients σ_T and σ_u used in the nonequilibrium boundary conditions are taken to be unity, as in the reference [2]. The results are compared with the DSMC results presented in [2]. Fig. 2(a) and Fig. 2(b) shows the plot of surface gas temperature and heat flux over the flat plate surface along with the results obtained by Le et al. [2]. The results shows a good match with the reference study. However, the heat flux at the leading edge in the case of without sliding friction shows a over-prediction in comparison with the same reference's [2] CFD results but is close to their DSMC results. This is possibly because we have implemented gradient correction for obtaining the $\nabla_n T$ (used in heat flux computation) [15] which, hopefully, gives a more accurate result.

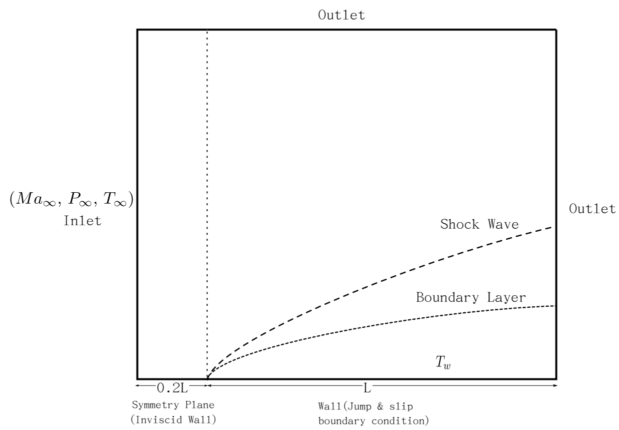
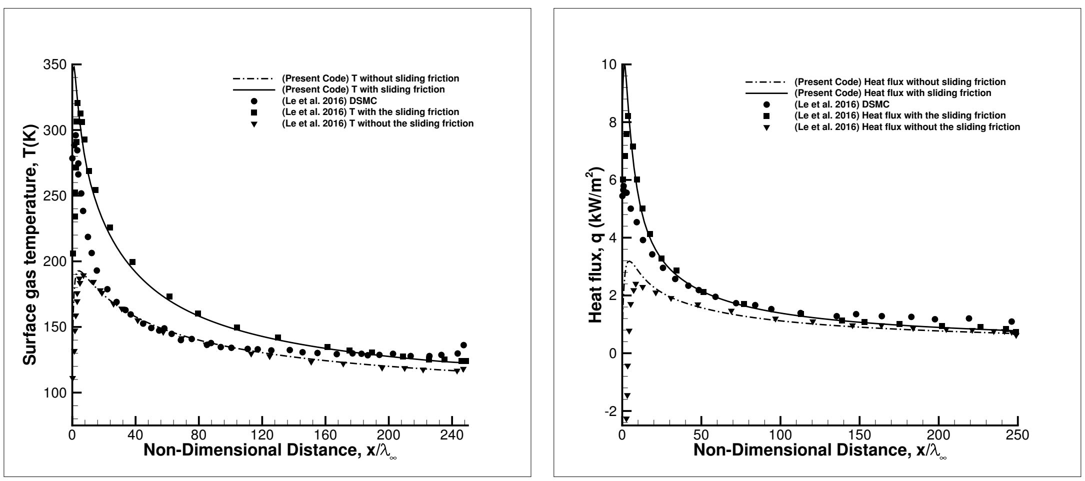


Figure 1: Flat plate problem.



(a) Surface gas temperature

(b) Heat flux

Figure 2: Code Verification: The profile of surface temperature and heat flux over the flat-plate surface.

5 RESULTS AND DISCUSSIONS

In this section, we investigate the behavior of pressure and other quantities along the flat plate surface in detail. To solve the Navier-Stokes equations at low speeds with a density-based solver we have used preconditioning with the ROE flux scheme, the details of which can be found in [16]. The time-stepping has been done implicitly using LU-SGS. We have considered the hypersonic flat plate case taken from Metcalf et al. [19] ($T_w = 77$). The flow domain is shown in Fig. 1. We plot the value of surface pressure, surface gas temperature, slip velocity and heat flux at the wall against $x/\lambda_\infty (= Kn^{-1})$. The value of $\sigma_u = 0.7$ (used in Eq. 2) and $\sigma_T = 1$ (used in Eq. 3 and 4) are taken, based on the study done by Le [7]. The grid spacing near the wall is taken to be the same as presented in the thesis of Le ([7]; Table 4.4, Pg. no 54). The first order Maxwell slip and Smoluchowski temperature jump along with the Le temperature jump boundary condition has been numerically verified in the previous section Sec. 4. Le et al. [2] have verified

Table 1: Coefficients of transport properties of the different gases considered [7].

Gas	R ($\mathrm{m^2s^{-2}K^{-1}}$)	γ	A_s ($\mathrm{Pa.sK^{-1/2}}$)	T_s (K)
Nitrogen	296.8	1.40	1.41×10^{-6}	111

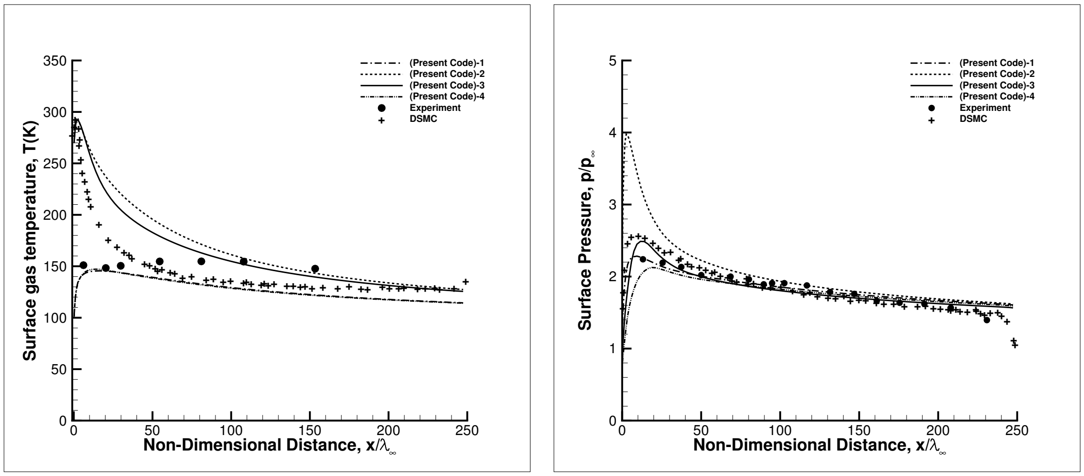
Table 2: Different studies performed based on the wall BC's for velocity, temperature and pressure.

Label	Abbreviation	Velocity	Temperature	Pressure
(Present Code)-1	PC1	Maxwell, Eq. 2	Smoluchowski, Eq. 3	Zero Normal Gradient
(Present Code)-2	PC2	Maxwell, Eq. 2	Le temperature jump, Eq. 4	Zero Normal Gradient
(Present Code)-3	PC3	Maxwell, Eq. 2	Le temperature jump, Eq. 4	Pressure Jump, Eq. 8
(Present Code)-4	PC4	Maxwell, Eq. 2	Smoluchowski, Eq. 3	Pressure Jump, Eq. 8

their temperature jump condition with the DSMC results of temperature and heat flux. Here we attempt a more detailed analysis of their temperature jump boundary condition by studying the behavior of pressure, temperature, slip velocity and heat flux along the wall. We perform studies for the hypersonic flow over a flat plate and compare them with the DSMC and the experimental results available in the literature. We use four different numerical models, labeled in Table 2, differing in the wall boundary conditions used for the governing equations. It can be noted that PC1 corresponds to the "standard" model [4, 6, 7], PC2 to the Le temperature jump proposed in [2], PC3 has the Le temperature jump *and* the new pressure jump condition [3] and PC4 is the "standard" model, except for pressure, for which we use the pressure jump condition. For PC1 and PC4, the heat flux is computed using only the Fourier law of heat conduction; while for PC2 and PC3 it is computed including the sliding friction component i.e. Eq. 10.

5.1 Metcalf *et al.*'s, $T_w = 77$K

In this case of hypersonic flow over a flat plate [19], we have considered the flow of Nitrogen with the free-stream Mach number of $Ma = 6.1$, free-stream presure $P_\infty = 2.97$ Pa and temperature $T_\infty = 83.4$ K. The corresponding free-stream mean free path and Knudsen number are 0.35 mm and 0.004, respectively. The wall temperature is given as $T_w = 77$ K. The various constants for Nitrogen are listed in Table 1. The corresponding DSMC and experimental results are obtained from [20, 2]. In this case the Mach number is at the lower end of the hypersonic regime and the wall temperature is close to (and less than) the free-stream temperature. The calculated surface gas temperature and surface pressure are shown in Fig. 3(a) and Fig. 3(b) respectively. We can see that the surface gas temperature in Fig. 3(a) using the Le temperature jump boundary condition (PC2) comes closer to the DSMC results than the standard approach (PC1), but for the pressure (Fig. 3(b)) it clearly shows an over-prediction (the peak pressure being nearly 66% over-predicted w.r.t DSMC), especially at the leading edge, in comparison to both the experiment and the DSMC results. Using the Le temperature jump with the pressure jump condition (PC3) corrects this unusual rise in the pressure, showing a much closer match with the DSMC and experimental results at the leading edge (the peak pressure being merely 2.8% under-predicted w.r.t DSMC). The reason for this is probably that the calculation of pressure is based on the conservation of normal momentum which is



(a) Surface gas temperature.

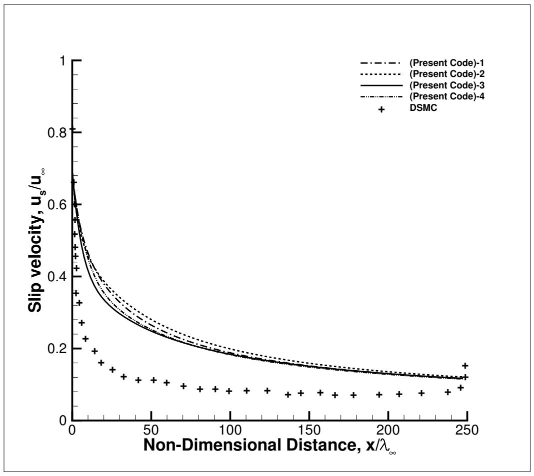
(b) Surface pressure

Figure 3: Metcalf et al.'s case [19] T_w = 77K. Comparison of temperature and pressure over the flat plate surface.

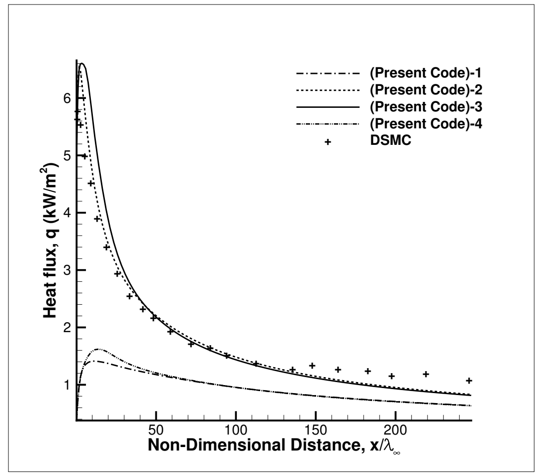
ignored in the standard non-equilibrium BC's (i.e. Maxwell and Smoluchowski). PC3 also gives a somewhat closer match with the DSMC result for the surface gas temperature in comparison with PC2. Both PC2 and PC3 are closer to experiment for temperature far from the leading edge, while at the tip both (and DSMC) over-predict the temperature. Figure 4(a), 4(b) and 4(c), respectively show the slip velocity, computed heat flux and the friction heating rate (wall shear stress × slip velocity) for the three models. In these figures only the DSMC results are used for comparison, as experimental data are unavailable. It is observed that all three models give close results, but far from the DSMC, for the slip velocity. But for the most important wall heat flux, PC2 and PC3 both give results very close to DSMC while PC1 is unexpectedly quite erroneous. All three models give close results (except at the leading edge) for the friction heating rate in Fig. 4(c). The region ($x/\lambda_\infty \geq 100$) corresponds to $Kn \leq 0.01$ where CFD and DSMC are expected to give close results [3, 2]. Indeed, we see the four models better match the DSMC results in this range. PC4 gives almost the same results as PC1 except for pressure and heat flux at the wall, where there is a small deviation at the leading edge. This shows that the pressure jump boundary is most effective with the Le temperature jump condition, i.e., with PC3 conditions. We can clearly see the Le temperature jump with the pressure jump condition (PC3) is able to model the flow in a more comprehensive way than the use of merely the temperature jump (PC2). PC3 ensures a good prediction of pressure at the leading edge without deterioration in the prediction of other quantities.

6 CONCLUSIONS

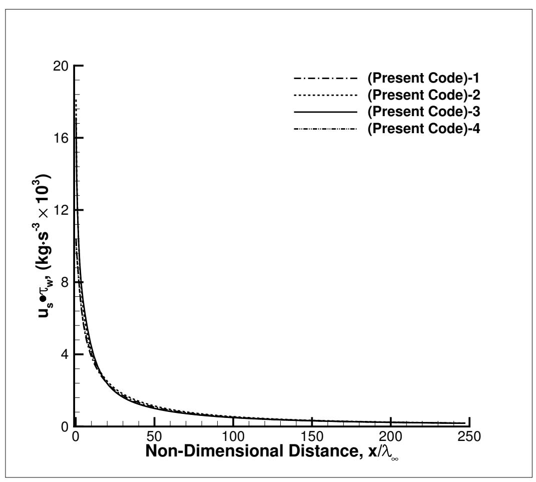
1. We have verified our numerical implementation of the Maxwell velocity slip, Smoluchowski and Le temperature jump condition with similar numerical implementations in the literature.



(a) Slip velocity



(b) Heat flux



(c) Inner product of wall shear stress and slip velocity

Figure 4: Metcalf et al.'s case [19] $T_w = 77$K. Slip velocity, wall heat flux and shear work per unit area (measure of sliding friction) distribution over the flat plate surface.

2. The Le temperature jump condition over-predicts the pressure, especially at the leading edge, while correcting the temperature profile near the wall w.r.t. to the DSMC results. This anomaly can be removed by the use of the pressure jump condition which corrects the pressure prediction without significantly changing the prediction of the other flow properties.

3. The pressure jump condition, which was previously ignored in the literature when used with the standard non-equilibrium boundary condition, has been shown to be a useful complement to the Le temperature jump condition.

4. A more detailed study should be performed with these boundary conditions for different cases to obtain a more comprehensive understanding of their capabilities and limitations.

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