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LOW DENSITY GAS DYNAMIC WALL BOUNDARY CONDITIONS

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ABSTRACT

Low density nozzles or large expansion ratio nozzles used in space experience rarefaction effects near their exit in the form of velocity slip and temperature jump at the walls. In addition, the boundary layers become very thick and there is a very strong viscous/inviscid interaction. For these reasons no existing design technique has been found to accurately predict the nozzle flow properties up to the nozzle exit. The objective of this investigation was to examine the slip boundary conditions and formulate them in a form appropriate for use with a full Navier Stokes numerical code. The viscous/inviscid interaction would automatically be accounted for by using a compressible Navier Stokes code. Through examination of the interaction of molecules with solid surfaces a model for the distribution function of the reflected molecules has been determined and this distribution function has been used to develop a new slip boundary condition that can be shown to yield more realistic surface boundary conditions.

INTRODUCTION

As the density in a flow field diminishes the continuum description of that flow field begins to break down, first at the wall, and later in the interior of the flow field. The relevant parameter which describes the breakdown of the continuum description is the Knudsen number, defined as the ratio of a characteristic molecular mean free path to a relevant length that is descriptive of the flow field. The Knudsen number can be related to the Mach number and the Reynolds number, the simplest argument indicating that

$$Kn \sim \frac{M}{Re} \, .$$

The relevant mean free path and length scale depend upon the physical problem (see ref. 1–6).

If the Knudsen number is not considerably less than one, the flow is no longer a continuum. The most significant feature of the flow when there is slight rarefaction is a change in the boundary conditions at the wall. This regime is characterized by the fact that the rarefaction effects (i.e., changed wall boundary conditions) are small corrections to the continuum flow behavior. However, viscous effects become more important as Kn increases. Then the skin friction becomes comparable to the wall pressure and the heat transfer coefficient increases. The displacement effect of the thick boundary layer changes the surface pressure from its inviscid value. These are the dominant fluid mechanical effects in the slip flow regime, rather than the relatively small corrections introduced by the modified wall boundary conditions.

The transition regime occurs when the Knudsen number is of the order of one. In this regime molecular collisions with the surface and with the free-stream molecules are of more or less equal importance. The flow is no longer a slight correction to the continuum flow. At still larger values of the Knudsen number only collisions between the incoming molecules and the body surface need to be considered. This latter regime is called free-molecule. The delineation between the various regimes, i.e., continuum, slip, transition and free-molecule, is not sharp and depends upon the Mach number and the body geometry. References 1–6 should be consulted for more details.

Rarefied gas dynamics is the field that describes these flow regimes. NASA obviously has many applications for rarefied gas dynamics. These include the design of low density nozzles or large expansion ratio nozzles for use in space, the determination of contamination to spacecraft solar panels, optical sensor windows or temperature control surfaces, the estimation of drag and torque on satellites or the space station and of the heating and aerodynamics of vehicles entering or skip-

ping along the edge of the atmosphere. The present investigation concentrated on those applications that required slip flow boundary conditions.

The objectives of the present work are presented in the following section. This is followed by a brief review of kinetic theory, which is the tool used to solve rarefied gas dynamics problems, and of gas-surface interactions. The latter is required to understand the new formulation of the slip boundary condition that was accomplished for this study. The new slip condition is then presented and compared with previous slip boundary conditions. Evidence for the superiority of the present formulation is provided, but only incompletely. Finally, recommendations for additional work are made.

OBJECTIVES

NASA has a continuing need to improve nozzle contour design. Many of these nozzles are used under low density conditions but no design technique that is presently available can predict the flow field near the exit plane under these conditions. Accurate exit plane prediction is required to estimate thrust, as an input to contamination prediction codes and to accurately determine the back pressure on end plates of ultra-low thrust satellite control rockets.

With these applications in mind, the objective of this investigation was to devise an accurate means for the design of low density nozzles. To accommodate the strong viscous/inviscid interaction that will exist when the boundary layer becomes very thick near the nozzle exit, it will be necessary to use a full compressible Navier Stokes code and to add slip boundary conditions when the Knudsen number becomes sufficiently large. A second objective was to utilize recent gas surface interaction studies to develop a model for the distribution function of the molecules reflected from the surface that could be used to determine a slip boundary condition that can more accurately predict phenomena that are observed in slip flow, including some anomalous effects which have been observed in capillary flow.

PRINCIPLES OF KINETIC THEORY

Kinetic theory is the discipline that uses the molecular description of gases to determine the flow properties of a gas that is not in equilibrium. Because the number of molecules in any finite but small volume is very large, a statistical approach can be taken. The fundamental entity in kinetic theory is the distribution function, f, which is a function of position (x, y, z) , velocity (u, v, w) and time, t, such that

$$f(x, y, z, u, v, w, t) \, dx \, dy \, dz \, du \, dv \, dw \tag{1}$$

is the number of particles in the volume $dx \, dy \, dz$ about position (x, y, z) with velocity in the range $du \, dv \, dw$ about (u, v, w) at time t. If the distribution function is known then all flow properties can be obtained as integrals (moments) of the distribution function. For example, letting $d\boldsymbol{r} = dx \, dy \, dz$ and $d\boldsymbol{u} = du \, dv \, dw$

$$n(\boldsymbol{r}, t) = \int \int_{-\infty}^{\infty} \int f(\boldsymbol{r}, \boldsymbol{u}, t) d\boldsymbol{u}, \text{ number density} \tag{2}$$

$$\overline{\boldsymbol{u}} = \frac{1}{n} \int \int_{-\infty}^{\infty} \int f(\boldsymbol{r}, \boldsymbol{u}, t) d\boldsymbol{u}, \text{ mean (gas dynamics) velocity} \tag{3}$$

$$P_{ij} = m \int \int_{-\infty}^{\infty} \int U_i U_j f(\boldsymbol{r}, \boldsymbol{u}, t) d\boldsymbol{u} \tag{4}$$

P_{ij} is the flux of i-th momentum in the j-th direction. $\boldsymbol{U}$ is the peculiar or random velocity, defined as

$$\boldsymbol{U} = \boldsymbol{u} - \overline{\boldsymbol{u}} . \tag{5}$$

Other properties can be similarly defined; see reference 8.

To proceed further a molecular model must be developed. The simplest model is that of molecules composed of rigid elastic spheres of diameter σ which interact with one another only upon impact This is the model that will be assumed in this work while more realistic models are described in reference 8. Classical mechanics can then be used to show that the distribution function varies with time according to the equation

$$\frac{Df}{Dt} \equiv \frac{\partial f}{\partial t} + \boldsymbol{u} \cdot \frac{\partial f}{\partial \boldsymbol{r}} = C^{(+)} - C^{(-)} \equiv J(f, f_1) \tag{6}$$

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where $C^{(-)}$ $d\mathbf{r}$ $d\mathbf{u}$ dt is the total number of molecules having velocities in the range $\mathbf{u}$ to $\mathbf{u} + d\mathbf{u}$ which are lost in $d\mathbf{r}$ $d\mathbf{u}$ in time dt due to collisions with molecules having other velocities and $C^{(+)}$ $d\mathbf{r}$ $d\mathbf{u}$ dt is the total number of molecules gained to the range $\mathbf{u}$ to $\mathbf{u} + d\mathbf{u}$ in $d\mathbf{r}$ $d\mathbf{u}$ in time dt due to collisions between molecules having those initial velocities that lead to a final velocity of one of the molecules in the range $\mathbf{u}$ to $\mathbf{u} + d\mathbf{u}$. The specific form of the quantities $C^{(+)}$ and $C^{(-)}$ is given in reference 8. It has been assumed that the molecules are not acted upon by an external force field.

The above equation is called the Boltzmann equation and is considered to be the fundamental equation of rarefied gas dynamics. Many assumptions must be made to derive this equation, the two most important being that the equation as written applies only to a pure gas with no internal degrees of freedom (monatomic molecule). The equation can be generalized to eliminate these limitations (ref. 9) but even in this simplest case illustrated the functions $C^{(+)}$ and $C^{(-)}$ are so complex that the equation can be solved only for a few special circumstances.

Moments of the Boltzmann equation, i.e., equations of the form

$$\int \int_{-\infty}^{\infty} \int \left\{ \frac{Df}{Dt} - J(f, f_1) \right\} u^n \, d\mathbf{u} = 0, \tag{7}$$

play a special role in kinetic theory. These are the Maxwell equations of change. Since mass, momentum and kinetic energy are conserved in each molecular collision (monatomic molecules) the moments of the collision integral for $n = 0$, 1 and 2 are zero. The moments of the left hand convective term lead to the familiar continuity, momentum and energy equations of continuum mechanics. Each equation, however, contains a higher order moment and the system is not closed. The system can be closed for systems close to equilbrium in the limit as Kn goes to zero, leading to the Chapman-Enskog expressions for the stress tensor and heat flux vector.

A useful exact solution of the Boltzmann equation exists for a gas in a state of local equilibrium, called a locally Maxwellian distribution (ref. 8). It can be written as

$$f_0 = n \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left\{ - \frac{m}{2kT} U^2 \right\} ; U = \mathbf{u} - \bar{\mathbf{u}} \tag{8}$$

where n and $\bar{\mathbf{u}}$ depend upon $\mathbf{r}$ and t and T depends upon t. The collision integral is zero for the locally Maxwellian distribution, i.e., $J(f_0 f_{0_1}) = 0$, and the stress tensor and heat flux vector are zero. The conservation equations become the Euler equations of fluid mechanics.

A useful property of a gas is the mean free path, which is defined as the mean distance that a molecule travels between collisions. This concept has meaning only for a molecular model of hard elastic spheres. If the gas is described by a Maxwellian distribution then the mean free path is given by the expression

$$\lambda = \frac{1}{\sqrt{2}\, n\, \pi \sigma^2} .\tag{9}$$

More complicated situations are discussed in reference 8. It was assumed in the Introduction that a single mean free path described the flow but that is usually not the case.

The purpose of this brief introduction has been to indicate that boundary conditions must be provided on the distribution function itself to solve problems in rarefied gas dynamics. For problems of interest the most difficult boundary condition to specify is that at the wall. The interaction of molecules with solid surfaces will be reviewed in the next section and it will be shown that the experimental results can be described by a particularly useful model of the distribution function of the reemitted molecules. This model will then be used to develop a new boundary condition in the following section and this will yield a new slip regime boundary condition.

GAS-SURFACE INTERACTIONS

The study of gas-surface interactions provides the boundary conditions for the calculation of low density flows past wall boundaries. Our understanding of the molecule/wall interaction has evolved with time and is still presently incomplete. The range of relative energies between the molecule and the surface for applications of interest is very broad. Satellites operate in a free-molecule environment with a relative velocity between the satellite and the surrounding gas of around 26,000 ft/s (approximately 8000 m/s). This translates into a relative energy of $9.1eV$ for a nitrogen molecule or $5.2eV$ for an oxygen atom. The flow in low thrust or low density nozzles offer examples of the other extremes. The flow near the exit of a low density nozzle which is operating in space is in the slip regime on the wall. In this case the energy of the gas molecule relative to the wall is considerably lower, frequently below $0.1eV$, even though the wall and gas may be at a high temperature (the average molecular energy at $3000°K$ is $0.39eV$) This wide range of relative energy of interest has caused experimental problems with the study of the interaction of gases and surfaces because so many physical processes can occur over such a broad energy range (ref. 10) and because of the difficulty of producing relative energies greater than $0.3eV$; in fact, the satellite energy range has been reached only comparatively recently in laboratory experiments.

The study of gas-surface interactions has a long history that can only be highlighted here. The purpose of the discussion will be to justify the form of the distribution function of the reemitted molecules that will be used to obtain the slip flow boundary conditions

Early experiments indicated that there was some accommodation between the incident molecules and the wall properties. If molecules reflect specularly then there is no accommodation to the wall conditions and Maxwell reasoned that a portion must be reemitted diffusely after having come to complete accommodation with the wall. He introduced the reflection coefficient, f, which is the fraction of the molecules which reflect diffusely while the fraction $(1 - f)$ reflect specularly (ref. 11). Later it was recognized that different properties of the molecule-wall collision accommodate to a different degree and accommodation coefficients were introduced. The accommodation coefficients for normal momentum. tangential momentum and energy are defined by the equations (refs. 1 and 3).

$$\sigma^1 = \frac{p_i - p_r}{p_i - p_w} = \text{normal accommodation coefficient} \tag{10}$$

$$\sigma = \frac{\tau_i - \tau_r}{\tau_i} = \text{tangential accommodation coefficient} \tag{11}$$

$$\alpha = \frac{e_i - e_r}{e_i - e_w} = \text{thermal accommodation coefficient} \tag{12}$$

where p_i, τ_i and e_i are incident fluxes of normal and tangential momentum and energy, p_r, τ_r and e_r are the reemitted fluxes of these quantities from the surface while p_w and e_w $(\tau_w = 0)$ are the fluxes that would be reemitted by a gas in complete Maxwellian equilibrium with the surface. These expressions have significance only for conditions close to equilibrium.

Almost all rarefied gas dynamic problems have been solved using these accommodation coefficients with values that have been obtained from laboratory measurements. The measurements that correspond closest to the defined quantity are those of the thermal accommodation coefficient (refs. 12 to 14). Recently σ and σ' have been measured by measuring the forces exerted on a small plane surface, that is connected to a vacuum microbalance, by a stream of molecules (molecular beam) of known energy. Both of these quantities have been measured as a function of the energy of the incident molecules and of the angle between the surface normal and the incident molecular beam direction (E_i, θ_i).

The low energy and satellite energy behavior of σ and σ' have been found to be quite different (refs. 15–18). The low energy behavior was examined very completely by Seidl and Steinheil (ref. 17). In the ``as received''condition plus an ambient temperature desorption, the surface of all materials was found to be covered with adsorbed gases, primarily water vapor and hydrocarbons However, σ was found to depend greatly upon the bulk material even though the surface layers were the same. The tangential accommodation coefficient was greatly diminished for all values of θ_i by removing the adsorbed gases if the surface was atomically smooth but σ was greater than one at small θ_i for atomically rough surfaces due to back scattering.

The tangential accommodation coefficient was found to fall with increasing θ_i at low energies (ref. 17) but the opposite behavior was observed at satellite energies (ref. 18). Also, the integrated values of σ' (over all θ_i) decreased from their low energy value near unity to a minimum at an energy somewhere below satellite energy and then increased to values comparable to the low energy value at higher energies (refs. 10, 15 and 16).

The measurements of σ and σ' at satellite energies by Knechtel and Pitts (ref. 18) are of interest. They measured both coefficients as a function of θ_i and E_i for nitrogen on aluminum and then applied them to determine the torque and drag on a surface element in free molecule flow at satellite energy $(E_i = 9eV)$. A very large effect was shown to occur for the torque when compared to the assumption of full accommodation (see Fig 16 in ref. 15) The drag was also calculated for a spherical satellite as a function of E_i. For free-molecule flow in the limit $S \longrightarrow \infty$

it can be shown that the drag coefficient on a sphere reduces to (ref. 1)

$$C_D \longrightarrow (2 - \sigma' + \sigma).$$
(13)

In either the limit of full accommodation ($\sigma = \sigma' = 1$) or no accommodation ($\sigma - \sigma' = 0$) this gives the value $C_D = 2$, and in general $C_D > 2$. However, integration of the forces using the measured values of σ and σ' yielded values of C_D less that 2 at E_i less than $40eV$. This significant finding will be compared with calculations that do not use accommodation coefficients later.

The momentum accommodation coefficients were historically defined only for free molecule flow. But they are also important for the understanding of gas-surface boundary conditions in transition and slip flow (ref. 19). The velocity slip and the onset of rarefaction effects can be significantly influenced by the degree of accommodation (ref. 20).

The accommodation coefficients only allow integrated properties of the reflected molecules to be determined in terms of the incident properties (fluxes are integrals over the distribution function - see the next section). However, what is desired is a joint distribution function (ref. 1)

$$g(\boldsymbol{u}_r, \boldsymbol{u}_i),$$
(14)

which is the probability of a molecule incident upon a wall with velocity $\boldsymbol{u}_i$ being reflected with velocity $\boldsymbol{u}_r$. This distribution function would be a function of numerous parameters, such as the type of surface material, the microscopic surface state, the wall temperature and the presence or absence of adsorbed gases. Present knowledge of the gas-surface interaction process is insufficient to yield knowledge of the joint distribution function. However, molecular beam scattering experiments have given considerable information about the interaction process. The most useful experiments are those that impinge a surface of known state with a monoenergetic molecular beam at various θ_i and measure the reflected number density and velocity distribution as a function of reflected angle (ref. 21). These experiments have not yet produced enough information to give g, however they have assisted in the development of a parametric representation of the distribution function of the reflected molecules. This representation will be used in the next section to develop a new slip condition while the experiments themselves will be examined to estimate the values of the parameters in the representation.

Accommodation coefficients have significance only for conditions close to equilibrium (ref. 13) Frequently flows of interest are far from equilibrium and the results supplied by the accommodation coefficients are not adequate (ref. 21). The molecular beam simulates conditions far from equilibrium and should thus model

such conditions better than standard accommodation coefficients.

Considerable progress has been made toward determining the joint probability distribution. Recent molecular beam scattering experiments are described in references 22 to 29 while the earlier experiments are summarized in reference 13. Only certain aspects of these measurements are relevant to the present discussion and they can be summarized as follows.

1. Maxwellian diffusive reflection, with the molecules accommodated to the wall temperature, occurs at low beam energies if the energy of adsorption of the molecules is high or if the surface is covered with adsorbed gases.

2. Lobal rather than diffusive (cosine) reflection with incomplete thermal accommodation is observed at low energies if the surfaces are properly degassed or if the incident beam energy is increased such that the incident kinetic energy is greater than the wall temperature.

3. Lobal reflected distributions are always observed at higher energies whether the surfaces are degassed or not and from polyecrystalline or single-crystal materials.

4. The peak in the lobal distribution is at an angle θ_m from the surface normal which is less than the corresponding incident angle of the molecular beam, θ_i, at low energies. As the energy of the incident beam increases (for fixed θ_i), θ_m increases so that the lobe peak approaches the surface tangent, but at some energy less than $10eV$, θ_m reaches a maximum value and decreases toward the specular angle with further increases in the beam energy. This pattern is approximately the same for all θ_i.

5. The speed distribution of the reflected molecules is analyzed by fitting the data to a ``drifting''Maxwellian with parameters U_r and T_r. U_r is the mean velocity of the distribution. U_r, U_i and the surface normal are in the same plane. T_r is a measure of the spread of the distribution and is not usually equal to the wall temperature T_w. The parameters are usually combined to give a speed ratio $S_r = U_r/(2kT_r/m)^{1/2}$. Earlier experiments (ref. 30) indicated that a one-parameter distribution was insufficient to characterize the reflected speed distribution but most data can be adequately characterized using these two parameters.

6. At low energies, as $\theta_r \longrightarrow 90°$ (tangential reflection), S_r increases and T_r decreases for given S_i and θ_i (refs. 26 and 28).

Some years ago Nocilla (ref. 31) suggested that the reflected molecular distribution could be assumed to have the form of a ``drifting''Maxwellian of the

form

$$f_r(\boldsymbol{u}) = n_r \left(\frac{m}{2\pi k T_r} \right)^{3/2} \exp \left\{ \frac{-m(\boldsymbol{u} - \boldsymbol{U}_r)^2}{2kT_r} \right\} \tag{15}$$

where $\boldsymbol{u}$ is the molecular velocity, U_r is the macroscopic drift velocity attributed to the outgoing stream which is assumed to lie in the plane in the incident velocity and the surface normal, T_r is the effective temperature of the distribution (not necessarily the wall temperature T_w) and n_r must be found by balancing the incoming and outgoing number fluxes. The previous discussion indicates that this form of distribution function has been found to describe most of the molecular beam data.

Nocilla made a comparison between some of the scant angular flux data that were available at the time and determined a best fit using this distribution. The fit produced the parameters θ_r and S_r (the distributions were normalized to a unit value of $(2kT_r/m)^{1/2}$). The only measurements that existed were for the scattering of low energy nitrogen from lithium fluoride crystals. Polished crystal surfaces tests produced $\theta_r > 90°$ and small values of S_r. Cleaved crystal surface tests produced θ_r slightly greater than θ_i and S_r of the order of 1 0; an exception occurred for θ_i approaching 90°, for which $\theta_r > 90°$. All the measurements were adequately described by this function except the tests with θ_i near the surface tangent. In this case the data was adequately represented except in the quadrant that contained U_i, where the distribution underpredicted the scattering flux. In this case a greater number of molecules were rejected toward the source than the distribution function predicted.

This distribution function was used by Hurlbut and Sherman (ref. 32) to determine the drag on a spherical satellite. The value of T_r was determined from an angle-dependent thermal accommodation coefficient. Both S_r and α were assumed to vary linearly with θ_i ; U_r was assumed to be directed at θ_r, which was taken to be equal to θ_i. The results yielded the classical diffusive or specular reflection results for appropriate values of the parameters but notable among the results was a prediction that C_D could be less that 2 0 for $S_r \longrightarrow \infty$ for some values of the parameters. Recall that this result was also predicted by Knechtel and Pitts (ref. 18).

The Nocilla distributions will be assumed to be an accurate representation of the reflected distribution function for slip flow and a new slip boundary condition will be presented. The problem of the estimation of the parameters U_r, S_r and θ_r, will still remain, but the experimental results described in this section can be used as a guide.

SLIP WALL BOUNDARY CONDITIONS

Slip flow occurs when there is only slight rarefaction and the departure from the continuum behavior described by the Chapman-Enskog solution is small. The most rigorous way of solving this problem near the wall would be to solve the Boltzmann equation using an appropriate kinetic boundary condition (ref. 8). Instead an approximation due to Patterson will be used (refs. 6 and 33).

The molecular motion near a wall results from the interaction of the incident and reflected molecules. The incident molecules within a mean free path of the wall have a motion consistent with the external flow while the reflected molecules have come to some partial accommodation to the state of the wall, as discussed previously. The interaction of the incident and reflected molecules results in a deviation in the distribution of molecular velocities from a local Maxwellian. This distribution function next to the wall must be obtained by solving the Boltzmann equation, which is a very difficult task.

A few mean free paths from the surface the gradients of the macroscopic velocity and temperature can be considered to be constant. These gradients cease to be constant only in the immediate vicinity of the wall where the collisions between the incident and reflected molecules have their effect (see figure 1). The extrapolation of the gradient to the surface yields the slip velocity or extrapolated wall temperature. Note that this does not yield either the gas velocity or the gas temperature at the surface. But as far as the velocity and temperature fields in the bulk of the flow are concerned, these quantities can be used as boundary conditions for the Navier Stokes equations (second term of the Chapman-Enskog expansion) to yield accurate solutions everywhere except within a few mean free path lengths of the wall.

Patterson assumed that the gas near the wall was not in equilibrium but was close to equilibrium. The distribution function was assumed to be of the form

$$f_i = f_0 \left[1 + F(H) \right]$$

$$(16)$$

$$H_1 = \left(\frac{m}{kT} \right)^{1/2} U_x \,;\; H_2 = \left(\frac{m}{kT} \right)^{1/2} U_y \,;\; H_3 = \left(\frac{m}{kT} \right)^{1/2} U_z$$

f_0 is the local Maxwellian.

$$f_0 \, dU_x \, dU_y \, dU_z = (2\pi)^{-3/2} \, e^{-\frac{1}{2} \sum_1^3 H_i^2} \, dH_1 \, dH_2 \, dH_3 \qquad (17)$$

$$F(H) = \sum_1^3 a_i \, H_i + \frac{1}{2} \sum_1^3 \sum_1^3 a_{ij} \, H_i \, H_j + \frac{1}{6} \sum_1^3 \sum_1^3 \sum_1^3 a_{ijk} \, H_i \, H_j \, H_k \qquad (18)$$
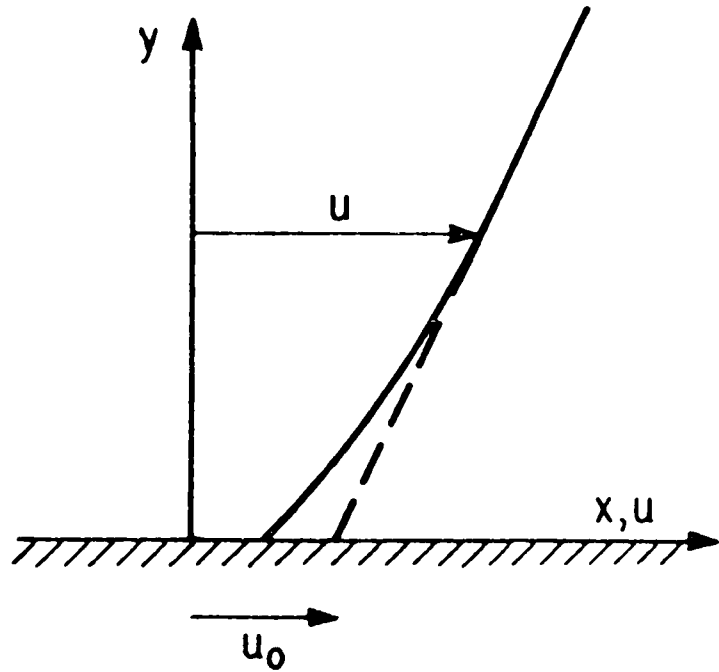
Figure 1. Coordinate geometry for slip flow boundary condition $u_{,j} = u_{,i}$
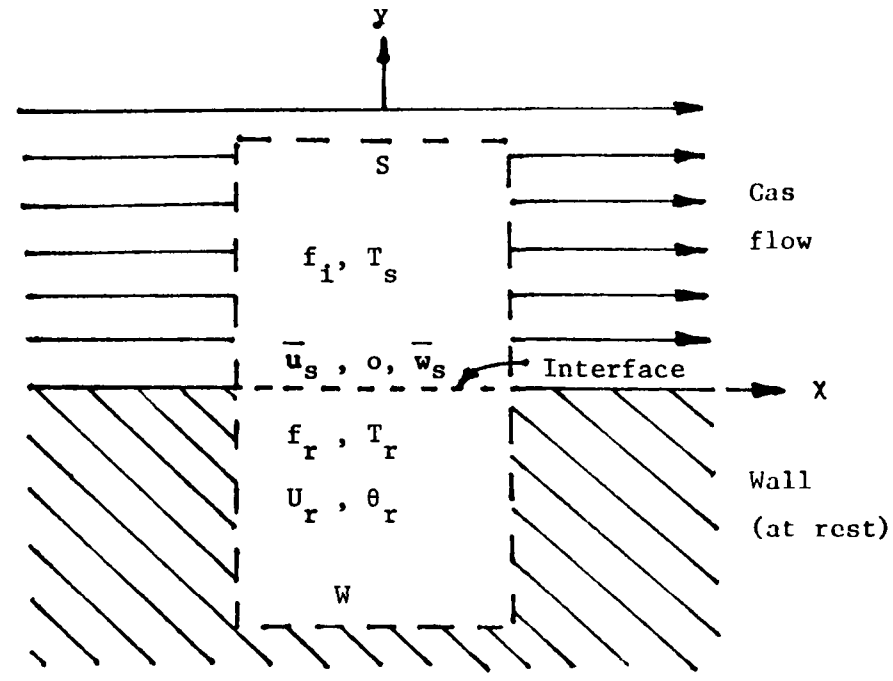

Figure 2. Integration volume for determining slip conditions

where the order of the subscripts is immaterial, e.g., $a_{12} = a_{21}$ and $a_{122} = a_{212} = a_{221}$. n, T and $\overline{U^2}$ are defined by integrals of f_0.

Certain conditions must be satisfied by the coefficients, namely (ref. 33).

$$a_{11} + a_{22} + a_{33} = 0 \qquad (19)$$

and

$$2a_i + a_{i\,11} + a_{i\,22} + a_{i\,33} = 0 \ (i = 1, 2 \text{ or } 3) \qquad (20)$$

Patterson demonstrated how to relate the remaining coefficients to integrals involving properties of the intermolecular collisions which were evaluated for hard elastic spheres.

Now consider the interaction of the incoming and reflected molecular streams in the vicinity of the wall. The motion of the gas on the surface depends on the transfer of mass, momentum and energy by the gas molecules to and from the surface. Consider figure 2 with the axis fixed relative to the body. The volume S in the flowing gas contains gas molecules with mean velocity components $\bar{u}_s$, 0, $\bar{w}_s$ and a random motion described by f_i. The reflecting molecules are assumed to act as though they emerged from an adjacent volume W with a Nocilla distribution with U_r lying in the $(x - y)$ plane. The molecular motions in the volumes S and W are mutually compatible if the total mass, momentum and energy transferred upward by the molecules from W to S are respectively equal to the total mass, momentum and energy which would be transported upward if the molecules in W moved with the same mass velocity and random motion as the molecules in S.

Compatibility of the mass flux yields

$$m\,n_s \int\limits_{-\infty}^{\infty} \int\limits_{0}^{\infty} \int\limits_{-\infty}^{\infty} v\,f_i(T_s)du\,dv\,dw = m\,n_r \int\limits_{-\infty}^{\infty} \int\limits_{0}^{\infty} \int\limits_{-\infty}^{\infty} v\,f_r(T_r)du\,dv\,dw \qquad (21)$$

with

$$f_r = \left(\frac{2\pi\,k\,T_r}{m}\right)^{-3/2} \exp\left[-\frac{m(\mathbf{u} - \mathbf{U}_r)^2}{2\,k\,T_r}\right] \qquad (22)$$

Integration and the use of the conditions on the a coefficients yields

$$\frac{m\,n_s}{4\sqrt{\pi\beta_s}}\left[2 + a_{22}\right]_s = \frac{m\,n_r}{2\sqrt{\pi\beta_r}}\,\chi\,(\sigma_r) \qquad (23)$$

where $\beta = \frac{m}{2kT}$

$$\chi(\sigma_r) = \exp\left(-\sigma_r^2\right) + \sqrt{\pi}\,\sigma_r\left[1 + \operatorname{erf}(\sigma_r)\right] \qquad (24)$$

$$\sigma_r = S_r\cos\theta_r \ ; \ S_r = U_r\left(\frac{m}{2k\,T_r}\right)^{1/2} \qquad (25)$$

This result can be written as

$$\frac{n_r}{n_s} = \sqrt{\frac{T_s}{T_r}} \frac{[1 + a_{22}/2]_s}{\chi(\sigma_r)} \tag{26}$$

In the hard sphere approximation used by Patterson,

$$a_{22} = \frac{5}{6} \left[\frac{\lambda}{\overline{\overline{U}}} \left(\frac{\partial \overline{u}}{\partial x} + \frac{\partial \overline{w}}{\partial z} - 2 \frac{\partial \overline{v}}{\partial y} \right) \right]_s \tag{27}$$

The balance of the transport of the tangential component of momentum at the interface yields an equation for the slip velocity.

$$m \, n_s \int\limits_{-\infty}^{\infty} \int\limits_{0}^{\infty} \int\limits_{-\infty}^{\infty} u v f_i(T_s) du \, dv \, dw = m \, n_w \int\limits_{-\infty}^{\infty} \int\limits_{0}^{\infty} \int\limits_{-\infty}^{\infty} u v f_r(T_r) du \, dv \, dw \tag{28}$$

$$\frac{m \, n_s}{(2\pi)^{3/2}(2\beta_s)} \left\{ \pi \left[\sqrt{2\pi} \, a_{12} + a_{122} \right] \right\}_s + \frac{m \, n_s}{2^{3/2}\sqrt{2\pi\beta_s}} \left[\overline{u}(2 + a_{22}) \right]_s \tag{29}$$

$$= -\frac{n_r m}{2\sqrt{\pi}} \frac{U_r^2}{S_r} \chi(\sigma_r) \sin \theta_r$$

Using the previous result for n_r/n_s and dropping higher order terms yields

$$\overline{u}_s = -2 S_r \sqrt{\frac{kT_r}{m}} \sin \theta_r - \frac{\sqrt{\frac{kT_s}{m}}}{2} \left[\sqrt{2\pi} \, a_{12} + a_{122} \right]_s \tag{30}$$

$$a_{12} = -\frac{5}{4} \frac{\lambda}{\overline{\overline{U}}} \left(\frac{\partial \overline{u}}{\partial y} + \frac{\partial \overline{v}}{\partial x} \right) \tag{31}$$

$$a_{122} = -\frac{15}{16} \left(\frac{\pi}{2} \right)^{1/2} \frac{\lambda}{T} \frac{\partial T}{\partial x} \tag{32}$$

Similarly,

$$\overline{w}_s = -\frac{\sqrt{\frac{kT_s}{m}}}{2} \left[\sqrt{2\pi} \, a_{32} + a_{322} \right]_s \tag{33}$$

$$a_{32} = -\frac{5}{4} \frac{\lambda}{\overline{\overline{U}}} \left(\frac{\partial \overline{w}}{\partial y} + \frac{\partial \overline{v}}{\partial z} \right) \tag{34}$$

$$a_{322} = -\frac{15}{16} \left(\frac{\pi}{2} \right)^{1/2} \frac{\lambda}{T} \frac{\partial T}{\partial z} \tag{35}$$

The balance of the transport of the normal component of momentum at the interface yields a relation between p_s and p_w.

$$m n_s \int\limits_{-\infty}^{\infty} \int\limits_{0}^{\infty} \int\limits_{-\infty}^{\infty} v^2 f_i(T_s) du\, dv\, dw = m n_r \int\limits_{-\infty}^{\infty} \int\limits_{0}^{\infty} \int\limits_{-\infty}^{\infty} v^2 f_r(T_r) du\, dv\, dw \qquad (36)$$

Integration yields

$$\frac{p_s}{2}\left[1 + a_{22} + \frac{2}{3\sqrt{2\pi}}\right]_s = \frac{p_r}{\sqrt{\pi}}\left\{\sigma_r \chi(\sigma_r) + \frac{\sqrt{\pi}}{2}(1 + \mathrm{erf}\,\sigma_r)\right\} \qquad (37)$$

where the perfect gas law

$$p = n\,kT$$

has been used. This can be written as

$$\frac{p_s}{p_r} = \left[1 - a_{22} - \frac{2a_{222}}{3\sqrt{2\pi}}\right]_s \left[1 + \mathrm{erf}\,\sigma_r + \frac{2}{\sqrt{\pi}}\sigma_r \chi(\sigma_r)\right] \qquad (38)$$

$$a_{222} = -\frac{45}{16}\left(\frac{\pi}{2}\right)^{1/2} \frac{\lambda}{T}\frac{\partial T}{\partial y} \qquad (39)$$

The temperature jump between the gas and the wall can be determined by the flow of translational energy of the molecules across the interface.

$$\frac{1}{2} m n_s \int\limits_{-\infty}^{\infty} \int\limits_{0}^{\infty} \int\limits_{-\infty}^{\infty} v(u^2 + v^2 + w^2) f_i(T_s)\, du\, dv\, dw$$

$$(40)$$

$$= \frac{1}{2} m n_r \int\limits_{-\infty}^{\infty} \int\limits_{0}^{\infty} \int\limits_{-\infty}^{\infty} v(u^2 + v^2 + w^2) f_r(T_r) du\, dv\, dw$$

Integration yields the following result

$$\frac{m n_s}{4\sqrt{\pi}\beta_s}\left[1 + \frac{a_{22}}{2}\right]_s (\bar{u}^2 + \bar{w}^2)_s + \frac{m n_s}{4\sqrt{2\pi}\,\beta_s}\left[\left(\sqrt{2\pi}\,a_{12} + a_{122}\right)\bar{u}\right.$$

$$+ \left(\sqrt{2\pi}\,a_{23} + a_{322}\right)\bar{w}\right]_s + \frac{m n_s}{\sqrt{\pi}\,(4\beta_s)^{3/2}}\left[4 + 3a_{22} - (2\pi)^{1/2}\,2\,a_2\right]_s \qquad (41)$$

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$$= m\,n_r\,\frac{kT_r}{m}\left(\frac{kT_r}{2\pi m}\right)^{\frac{7}{2}}\left\{(S_r^2 + 2)\chi(\sigma_r) + \frac{\sqrt{\pi}}{2}\,\sigma_r(1 + \text{erf }\sigma_r)\right\}$$

Only keeping higher order terms, assuming S_r is small, gives

$$\frac{T_s}{T_r} = \left[1 - \frac{1}{4}\,a_{22} + \frac{1}{2}\sqrt{\frac{\pi}{2}}\,a_2\right]_s \left\{\left(1 + \frac{S_r^2}{2}\right) + \sqrt{\frac{\pi}{2}}\,\frac{\sigma_r\,(1 + \text{erf }\sigma_r)}{\chi(\sigma_r)}\right\} \quad (42)$$

$$a_2 = \frac{75}{32}\left(\frac{\pi}{2}\right)^{1/2}\frac{\lambda}{T}\frac{\partial T}{\partial y} \quad (43)$$

These results can be compared with the results of other investigators by writing the expressions in the form used by Kogan (ref. 34.). He wrote, for diffuse reflection

$$\overline{u_s} = A\,\frac{\mu}{n}\sqrt{\frac{2}{mkT}}\,\frac{\partial \overline{u}}{\partial y} + B\,\frac{2\mu}{n\,m}\frac{1}{T}\frac{\partial T}{\partial x} \quad (44)$$

$$\Delta T_s = C\,\frac{K}{2kn}\sqrt{\frac{\pi m}{2kT}}\,\frac{\partial T}{\partial y} \quad (45)$$

where μ is the coefficient of viscosity and K is the coefficient of thermal conductivity. The magnitude of the coefficients A, B and C depend upon the equation used for their determination and the molecular model assumed.

The present results can be written in this form by using the transport coefficient relations derived by Patterson for a hard sphere molecular model, namely,

$$\lambda = \frac{1}{\sqrt{2}\,n\pi\,\sigma^2} \quad ; \quad \mu = \frac{5m}{16\,\sigma^2}\left(\frac{kT}{\pi m}\right)^{1/2}$$

$$\overline{U} = \left(\frac{8}{\pi}\frac{kT}{m}\right)^{1/2} \quad ; \quad K = \frac{15}{4}\,\mu\,\frac{k}{m} \quad (46)$$

Then, the results can be compared as follows:

1. Patterson, hard spheres, diffuse reflection.

$$\overline{u_s} = \left\{0.8862\,\frac{\mu}{n}\sqrt{\frac{2}{mkT}}\left(\frac{\partial \overline{u}}{\partial y} + \frac{\partial \overline{v}}{\partial x}\right) + 0.3750\,\frac{2\mu}{nm}\frac{1}{T}\frac{\partial T}{\partial x}\right\}_s \quad (47)$$

$$\frac{T_s}{T_w} = \left\{1 + \frac{K}{2kn}\sqrt{\frac{\pi m}{2kT}}\,\frac{\partial T}{\partial y} - 0.1667\,\frac{\mu}{p}\left(\frac{\partial \overline{u}}{\partial x} + \frac{\partial \overline{w}}{\partial z} - 2\frac{\partial \overline{v}}{\partial y}\right)\right\}_s \quad (48)$$

or $A = 0.8862$, $B = 0.3750$ and $C = 1.000$.

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2. Present results, using Nocilla reflection model and hard spheres.

$$\bar{u}_s = -2S_r\sqrt{\frac{kT_r}{m}}\,\sin\theta_r + \left\{0.8862\,\frac{\mu}{n}\,\sqrt{\frac{2}{mkT}}\left(\frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x}\right)\right.$$

$$\left.+0.3750\,\frac{2\mu}{nm}\,\frac{1}{T}\,\frac{\partial T}{\partial x}\right\}_s \tag{49}$$

$$\frac{T_s}{T_w} = \left\{1 + \frac{K}{2km}\sqrt{\frac{\pi m}{2kT}}\,\frac{\partial T}{\partial y} - 0.1667\,\frac{\mu}{p}\left(\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{w}}{\partial z} - 2\frac{\partial \bar{v}}{\partial y}\right)\right\}_s \times \tag{50}$$

$$\left\{\left(1 + \frac{S_r^2}{2}\right) + \sqrt{\frac{\pi}{2}}\,\frac{\sigma_r(1 + \mathrm{erf}\,\sigma_r)}{\chi(\sigma_r)}\right\}$$

3. The traditional approach using accommodation coefficients and Patterson's technique is given by Shidlovskiy (ref. 6). θ = percentage of diffusely reflected molecules and α is the thermal accommodation coefficient.

$$\bar{u}_s = \left\{0.8862\left(\frac{2-\theta}{\theta}\right)\frac{\mu}{n}\sqrt{\frac{2}{mkT}}\left(\frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x}\right) + 0.3750\,\frac{2\mu}{nm}\,\frac{1}{T}\,\frac{\partial T}{\partial x}\right\}_s \tag{51}$$

$$\frac{T_s}{T_w} = \left\{1 + \frac{2-\alpha}{\alpha}\,\frac{K}{2kn}\sqrt{\frac{\pi m}{2kT}}\,\frac{\partial T}{\partial y} - 0.1667\,\frac{\mu}{p}\left(\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{w}}{\partial z} - 2\frac{\partial \bar{v}}{\partial y}\right)\right\}_s \tag{52}$$

These results are identical to those of Chrusciel, et al. (ref. 18) except that their results were nondimensionalized.

Kogan summarized other determinations of the coefficients A, B and C. This is repeated in Table I.

The new slip formulation (equations (38), (39), (27), (49) and (50)) contains the parameters S_r, U_r or T_r and θ_r that must be specified before a problem can be solved. The parameters used will depend upon the problem being solved. That is, flow in a nozzle has the free stream flow tangent to the surface at all locations and it would be expected that θ_r would be close to 90° or greater, S_r would be large and T_r would be less than T_w. On the other hand, for the flow over a blunt body, the parameters would be a function of θ_i and various forms could be assumed, much as

Hurlbut and Sherman did (ref. 32) for sphere drag, and ranges of the values could be examined for comparison with experiments. Notice that the form of the boundary conditions is somewhat different from those that include the accommodation coefficients. The slip velocity contains an subtractive term which is of the order of U_r. The scattering experiments have shown that U_r is never larger than the mean thermal velocity of the reemitted gas. For tangential flow over a surface this is small compared to the mean thermal velocity of the gas at the wall temperature. Since this term is negative it diminishes the magnitude of the usual slip boundary condition. This was also found by Chrusciel, et al. (refs. 21 and 35) using Monte Carlo methods to solve the flow over a blunt-nosed body in hypersonic flow. The temperature jump expression is multiplied by an expression that goes between the values 0.82 at $\sigma_r = -0.20$ to 1.44 for $\sigma_r = 0.50$. Values less than 1.0 would be required to match the results of Chrusciel, et al.

Table I

Coefficient	Value	Method of Determination
A	1.012	Krook equation
B	0.383	Krook equation
C	1.173	Krook equation
A	1.047	Boltzmann equation Maxwell molecules
A	1.015	``
B	0.383	``
B	0.402	``
A	1.103	Boltzmann equation, hard spheres
B	0.4456	``
B	0.3292	``
C	1.113	``
A	0.8862	Present results
B	0.3750	Present results
C	1.000	Present results

CONCLUSIONS AND RECOMMENDATIONS

A new form of the slip flow boundary conditions has been developed which appears to have characteristics that can improve the agreement between the computations and measurements. However, the boundary conditions have been obtained in an approximate manner and they contain unknown parameters. Therefore, the following steps should be taken to complete the task of obtaining useful slip flow boundary conditions.

1. The analysis of the previous section should be repeated using the Chapman-Enskog expansion rather than the approximate solution of Patterson.

2. Since the Chapman-Enskog expansion assumes that the flow is close to equilibrium, the analysis should be repeated by solving the Boltzmann equation close to the wall. It is not anticipated that this could be done exactly but a series expansion would be required. The boundary condition would then apply for flows arbitrarily far from equilibrium (ref. 21).

3. The boundary condition should be used on a simple flow, such as Poiseville flow through a circular capillary. This problem is well understood theoretically (ref. 36) and has an extensive data base (refs. 37 and 38). Therefore, it would be a good test case for the new boundary conditions and would help develop a rational for determining the parameters in the equations.

4. Once the parameters have been obtained then the equations can be applied to the calculation of low density nozzle flows. For low throat Reynolds numbers $(Re^* < 100)$ the interaction of the wall viscous region with the nozzle core is so great that only the full Navier Stokes equations can be used to adequately solve the flow field. Therefore, an axisymmetric Navier Stokes code, such as that of Lombard (ref. 39), will be used with the new slip boundary conditions to calculate nozzle flow fields and compare the properties with any existing measurements that can be found (ref. 38).

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