

Determination of Wall Boundary Conditions for High-Speed-Ratio Direct Simulation Monte Carlo Calculations

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A procedure for determining the velocity distribution function for the molecules that are reflected from an element of surface when a vehicle is moving in the transition or free-molecule flow regimes at high speed ratios is described. This distribution function could be used as the boundary condition for DSMC calculations. The method uses measurements of the momentum accommodation coefficients to determine the parameters for the Nocilla model of the reflected velocity distribution function. The use of this function as a boundary condition with the DSMC method would yield more accurate predictions of flow fields than are presently obtained using the assumption of diffuse scattering from the body surface. Several sets of Nocilla model parameters are determined as examples of the application of the procedure.

Nomenclature

B	= quantity given by Eq. (13)
E	= energy flux, $\text{J/m}^2\text{-s}$
f	= velocity distribution function: coefficient of momentum transfer introduced by Maxwell
k	= Boltzmann constant, J/K
$M_{\phi, f}$	= moment of the distribution function $f(\xi)$ with respect to the velocity function $\phi(\xi)$
m	= mass of a molecule, kg
n	= number density, m^{-3}
p	= normal momentum flux; pressure, N/m^2
R	= gas constant, N-m/kg-K
S	= speed ratio
T	= temperature, K
V	= macroscopic velocity, m/s
α_2	= partial thermal accommodation coefficient
α_{\max}	= maximum thermal accommodation coefficient, given by Eq. (23)
γ	= ratio of specific heats
δ	= angle of attack, deg
θ	= angle measured with respect to the local surface normal, deg
ξ	= molecular velocity, m/s
ρ	= density, kg/m^3
Σ	= quantity given by Eq. (5)
σ	= tangential momentum accommodation coefficient
σ'	= normal momentum accommodation coefficient
τ	= tangential momentum flux; shear stress, N/m^2
ϕ	= velocity function
χ	= quantity given by Eq. (6)

Subscripts

i	= incident
r	= reflected
w	= wall

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Introduction

FUTURE space flight may require using aeroassist for efficient orbital transfer. That technology requires further maturation before it can be successfully applied. In particular, accurate numerical prediction techniques must be developed. Continuum techniques, using the expanded Navier-Stokes equation set, can be used to predict aerodynamic performance at the lowest altitudes in the trajectory, but the higher-altitude portions are in the transition regime, where the molecular nature of the gas must be taken into account. Presently this regime can only be computed using the direct simulation Monte Carlo (DSMC) method. For example, Dogra et al.¹ used DSMC to compute the flowfield around a spherical body that passes from the free-molecule regime into the transition regime as its altitude decreases. Prediction of low-density aerodynamic performance requires a description of the collisional interaction between the incoming molecules and the vehicle surface. Maturation of the aeroassist orbit-transfer technology will require the incorporation of more realistic gas-surface collision models into the DSMC method before accurate predictions of performance can be made.

One of the most useful gas-surface interaction models is the Nocilla model.² This model has been widely used to analyze gas-surface scattering measurements. The advantage of the Nocilla model is that it gives the velocity distribution function of the molecules that are reflected from the body surface. The reflected velocity distribution function is required as the boundary condition for the DSMC method when it is used to calculate the transition-regime aerodynamics of a vehicle. This work will concentrate on the determination of the necessary parameters for the Nocilla model so that it will provide an accurate wall boundary condition for the DSMC computational method. Only very limited experimental information exists about the Nocilla model parameters for the conditions of interest.³ Thus, these parameters will be obtained using measurements of the momentum accommodation coefficients.

Gas-Surface Interactions

In free-molecule flow, the details of gas-surface interactions are important for accurately predicting vehicle aerodynamics; this topic was reviewed by Knox, Collins, and Liver.⁴ In addition, the details of the surface interactions have recently been shown to be important for predicting the wake region of an aeroassist orbit-transfer vehicle.⁵

It has long been known that the same gas-surface interaction mechanisms operate in all flow regimes, from the slip to the free-molecule regime,⁶ when due consideration is given to the energy of

collision relative to the surface. Details of the interaction that are obtained from measurements in the free-molecule regime can be used for DSMC computations in the transition regime.

Aeroassist orbit-transfer vehicles operate at very high speeds relative to the ambient atmosphere, the relative energy between the atmospheric molecules and the vehicle being in the range of 5 to 15 eV. In addition, the speed ratio, which is the ratio of the vehicle speed to the most probable speed of the random motion of the molecules in the ambient atmosphere (which is related to the local sound speed) is large, usually greater than 8. An improvement in the DSMC aerodynamic performance calculations of aeroassist orbit-transfer vehicles requires an accurate representation of the gas-surface interaction process that applies under these conditions.

Surface interactions are traditionally described by momentum and energy accommodation coefficients. The use of accommodation coefficients is adequate to describe the interaction of the incident molecular stream and the body under free-molecule conditions, when collisions between the reflected molecules and the incident molecules can be neglected. However, in the transition regime the re-emitted molecules collide with the incoming molecular stream to influence the momentum and energy of the molecules that impact the body, thereby influencing the body aerodynamics; these collisions can only be computed using the reflected velocity distribution function.

Accommodation Coefficients

The method to be presented utilizes measurements of momentum accommodation coefficients to determine the parameters in the Nocilla model. The Nocilla model will be described in the next section. First a short discussion of accommodation coefficients will prove useful.

Accommodation coefficients arose from the need to describe two sets of measurements. The first set measured the rate of damping of vanes and disks in rarefied gases, which was interpreted as due to a slip of the molecules over the surface (see Kennard⁷ and Hurlbut⁸). The slip phenomenon was described in terms of the coefficient of momentum transfer f (now called σ , the tangential momentum accommodation coefficient), which had been introduced by Maxwell.⁹ Accurate measurements of σ were made by Millikan¹⁰ and his students by measuring the drag on a cylinder under low-density conditions.

The second set measured the rate of conduction of thermal energy from a fine wire through a rarefied gas. These experiments were interpreted in terms of an accommodation coefficient α for the transfer of thermal energy. This is now called the thermal accommodation coefficient. Reviews of the techniques for measuring the thermal accommodation coefficient are given by Wachman¹¹ and Thomas.¹² Finally, Schaa¹³ introduced σ' , the normal momentum accommodation coefficient, by analogy with the tangential momentum accommodation coefficient. The exact definitions of these accommodation coefficients will be given in later sections.

The accommodation coefficients can be shown to be related to ratios of the differences of moments of the velocity distribution function $f(\xi)$ with respect to the appropriate velocity function $\phi(\xi)$, when the difference between the moments approaches zero. The standard definition of the accommodation coefficients can be written as¹⁴

$$AC = \frac{M_{\phi, f \text{ incident}} - M_{\phi, f \text{ reflected}}}{M_{\phi, f \text{ incident}} - M_{\phi, f \text{ wall}}} \quad (1)$$

where the limit $\Delta M \rightarrow 0$ is taken, that is, when the incoming molecules are in thermodynamic equilibrium with the surface. For the rotating-cylinder experiments this means that the measurements must be taken under the limit $V_{\text{gas}} - V_{\text{surface}} \approx 0$, and for the thermal conductivity cell experiments $T_{\text{gas}} - T_{\text{surface}} \approx 0$. The latter experiments strictly enforce this requirement, whereas the rotating-cylinder experiments satisfy the limit only approximately.

In usual practice the requirement $\Delta M \rightarrow 0$ is not observed and the accommodation-coefficient concept is used when the incoming molecules are not in thermodynamic equilibrium with the surface. Such is the case experienced by a vehicle in orbit, where the ambient molecules are not in thermal equilibrium with the vehicle

surface. The velocity of the molecules relative to an element of surface of an aeroassist orbit-transfer vehicle is of the order of 8 km/s, and the equivalent kinetic temperature of the ambient gas is greater than 25 times that of the surface temperature of the vehicle.³ This lack of thermodynamic equilibrium conditions will be important for later discussions. A review of applicable accommodation-coefficients measured under these conditions was made by Collins.³

In a recent paper, Collins and Knox¹⁵ showed that accommodation-coefficient measurements could be used to determine the Nocilla model parameters, thus alleviating the need for directly measuring the model parameters. This is important because the accommodation coefficients are much easier to measure than the Nocilla model parameters.³ The practical application of that method will be explored in this paper. In an independent work, Hurlbut¹⁶ showed that some limits could be placed on the Nocilla model parameters when the speed ratio is large. One of his limiting parameters was found to be very accurate when compared with the exact calculations of Collins and Knox.¹⁵ That approximation will be used here, to simplify the calculations. In addition, the Nocilla model as applied by Hurlbut and Sherman,¹⁷ called the HSN model,¹⁶ will be used. These points will be more carefully explored in the paragraphs to follow.

Model for the Reflected Velocity Distribution Function

The Nocilla model assumes that the body is in the free-molecule flow regime. The formulas that are given in this section only apply to that regime. However, once the reflected velocity distribution function has been obtained, then it can be used for computations in the transition as well as the free-molecule regime. Additional remarks about the applicability of the model will be made at the end of the section.

Consider the free-molecule flow toward a surface element, as shown in Fig. 1. In this figure the flow is with respect to the surface element. The incident fluxes of momentum normal and tangential to the surface are given, respectively, by

$$p_i = \rho RT \left[\frac{\Sigma}{\sqrt{\pi}} \chi(\Sigma) + \frac{1}{2} (1 + \text{erf } \Sigma) \right] \quad (2)$$

$$\tau_i = \rho RT \frac{S \sin \theta_i}{\sqrt{\pi}} \chi(\Sigma) \quad (3)$$

Here S is the speed ratio, given by

$$S = \frac{V}{(2kT/m)^{1/2}} \quad (4)$$

and

$$\Sigma = S \cos \theta_i \quad (5)$$

$$\chi(\Sigma) = e^{-\Sigma^2} + \sqrt{\pi} \Sigma (1 + \text{erf } \Sigma) \quad (6)$$

These formulas are derived in standard rarefied-gas dynamics texts.¹³ In these formulas, ρ and T are the atmospheric density and temperature, respectively, and $k/m = R$ is the gas constant of the atmospheric gases.

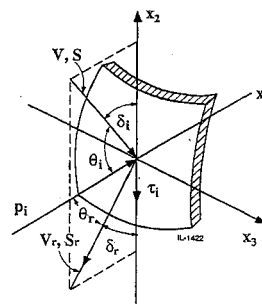


Fig. 1 Surface scattering coordinate systems.

Nocilla² assumed that the velocity distribution of the molecules reflected from the surface is in the form of a "drifting Maxwellian,"

$$f_r(\xi) = n_r \left(\frac{m}{2\pi k T_r} \right)^{\frac{1}{2}} \exp \left[-\frac{m(\xi - V_r)^2}{2k T_r} \right] \quad (7)$$

This distribution function contains three parameters: n_r , T_r , and V_r , which are the number density of the reflected molecules, their temperature, and their mean velocity, respectively.

The reflected velocity distribution function can be used to determine the reflected normal and tangential momentum fluxes. They are given by the formulas

$$p_r = \rho_r R T_r \left[\frac{\Sigma_r}{\sqrt{\pi}} \chi(\Sigma_r) + \frac{1}{2} (1 + \operatorname{erf} \Sigma_r) \right] \quad (8)$$

$$\tau_r = \rho_r R T_r \frac{S_r \sin \theta_r}{\sqrt{\pi}} \chi(\Sigma_r) \quad (9)$$

where

$$\Sigma_r = S_r \cos \theta_r \quad (10)$$

where $\chi(\Sigma_r)$ is given by Eq. (6) with Σ_r replacing Σ , and where S_r is the reflected speed ratio. Hurlbut and Sherman¹⁷ replaced the dependence of the model on T_r by introducing the partial thermal accommodation coefficient

$$\alpha_2(\theta_i) = \frac{E_i(\theta_i) - E_r}{E_i(\theta_i) - E_w} \quad (11)$$

In this equation the subscript i refers to the incident flux, r to the re-emitted flux, and w to the flux emitted after accommodation to the wall temperature. The density of the reflected molecules ρ_r can be obtained by equating the incident and reflected number fluxes. Hurlbut and Sherman¹⁷ have shown that $\rho_r R T_r$ may be written as

$$\rho_r R T_r = (\rho R T) S \sqrt{B} \frac{\chi(\Sigma)}{\chi(\Sigma_r)} \quad (12)$$

where

$$B = \frac{(1 - \alpha_2) \left[1 + \frac{\gamma + 1}{2(\gamma - 1)S^2} + \frac{\sqrt{\pi}\Sigma(1 + \operatorname{erf} \Sigma)}{2S^2\chi(\Sigma)} \right]}{S_r^2 + \frac{\gamma + 1}{2(\gamma - 1)} + \frac{\sqrt{\pi}\Sigma_r(1 + \operatorname{erf} \Sigma_r)}{2\chi(\Sigma_r)}} + \frac{\frac{\alpha_2 T_w}{S^2 T} \left[\frac{\gamma + 1}{2(\gamma - 1)} \right]}{S_r^2 + \frac{\gamma + 1}{2(\gamma - 1)} + \frac{\sqrt{\pi}\Sigma_r(1 + \operatorname{erf} \Sigma_r)}{2\chi(\Sigma_r)}} \quad (13)$$

The temperature of the reflected distribution is given by the equation

$$\frac{T_r}{T} = S^2 B \quad (14)$$

These equations can be used to determine the aerodynamic forces acting upon a surface element of a body. The total normal stress due to the incoming and reflected momentum fluxes is

$$p = p_i + p_r \quad (15)$$

and the total shear stress is

$$\tau = \tau_i - \tau_r \quad (16)$$

These stresses must be integrated over the entire body to yield the total lift, drag, and moments. The parameters S_r , θ_r , and α_2 must be known as functions of θ_i to carry out this integration. The available measured values of these quantities within the present energy range of interest are insufficient to perform these integrations with any accuracy.^{3,15} It will be shown, however, that the parameters and their

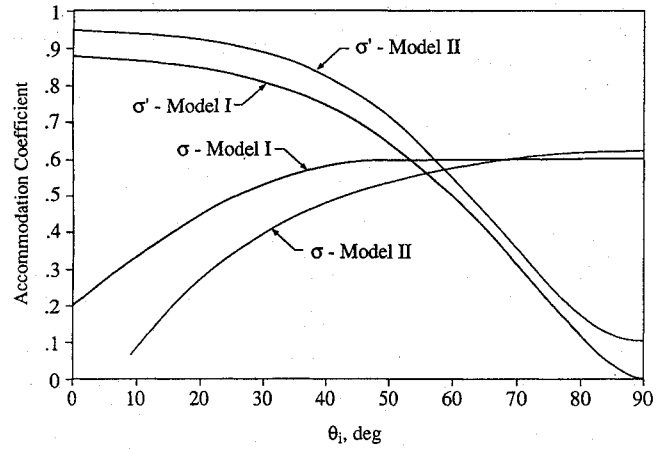


Fig. 2 Momentum accommodation coefficients given by models I and II.

angular dependence can be obtained from the measured values of the momentum accommodation coefficients as a function of angle. Justification for this procedure was discussed in Ref. 15.

The momentum accommodation coefficients are defined by the following equations:

$$\sigma' = \frac{p_i - p_r}{p_i - p_w} \quad (17)$$

$$\sigma = \frac{\tau_i - \tau_r}{\tau_i} \quad (18)$$

where σ' and σ are the normal and tangential accommodation coefficients, respectively. The values of p_i , τ_i , p_r , and τ_r are given by Eqs. (2), (3), (8), and (9), respectively. The normal momentum flux re-emitted at the wall temperature, p_w , is the same as the free-molecule flux emitted by an orifice in a chamber containing gas at the wall temperature and density, where the density is obtained by matching the incident and re-emitted number fluxes. The result is given by

$$p_w = \frac{\rho R T}{2} \left(\frac{T_w}{T} \right)^{\frac{1}{2}} \chi(\Sigma) \quad (19)$$

Collins³ thoroughly reviewed measurements of the momentum accommodation coefficients under the conditions of interest for aeroassist orbit-transfer vehicles. It was found that very few relevant laboratory and no space measurements had been made. However, sufficient data do exist so that a number of correlations of the data could be made and used to predict aerodynamic coefficients for several body shapes.³ Various correlations of the measurements were presented in Ref. 4. Correlation 17 from that reference will be used to illustrate the method of obtaining the Nocilla model parameters. That correlation is given by

$$\sigma' = 1 - \exp[-2.1(\cos \theta)^{1.6}] \quad (20)$$

$$\sigma = 0.6 - 0.4 \left(\frac{45 - \theta}{45} \right)^{1.6687}, \quad \theta \leq 45 \text{ deg} \quad (21)$$

$$= 0.6, \quad \theta \leq 45 \text{ deg} \quad (22)$$

and is plotted in Fig. 2. It is based upon the measurements of several investigators, who scattered neutral and ionized nitrogen and argon ions from surfaces of gold, aluminum, and copper over the energy range of 2 to 15 eV. The data are given in Ref. 15. In the present work θ is measured from the surface normal, whereas some other authors (e.g., Ref. 13) measure it from the surface tangent.

Although this is not a discussion on the merits or limitations of the Nocilla model, nevertheless, since it is the basis of this work, some comments about them are appropriate. The model is particularly suited for use with Monte Carlo computations, since it is

continuous in velocity space. Hurlbut and Sherman¹⁷ showed that it reproduced the classical limits for diffuse scattering, $S_r = 0$, and for specular scattering, $S_r = S_i$, $\alpha_2 = 0$. The Nocilla model can be used to describe gas-surface interactions under thermodynamic equilibrium conditions when $\Delta M \rightarrow 0$, which is not necessarily classical diffuse scattering.

The parameters T_r and V_r are empirical functions of the incident velocity distribution function and its moments and of the nature of the surface. Onji¹⁸ measured the scattered intensity distributions of Kr scattered from Ni over the energy range 0.06 to 3.8 eV. At an incident energy of 0.06 eV, when the incident gas was essentially in thermodynamic equilibrium with the surface, the measured intensity distribution was very nearly diffuse. At 1.0 eV, the intensity distribution had developed a distinct lobular pattern. The lobe peak moved closer to the specular direction, away from the normal, as the energy increased to 3.8 eV. The Nocilla model parameters appropriate to these experimental results depend strongly on the relative energy of the incident molecules; at low energy, when the incident molecules are essentially in equilibrium with the surface, S_r is nearly zero, and the scattering is close to diffuse.

The Nocilla model does not satisfy the principle of reciprocity. The principle of reciprocity was formulated by Tolman,¹⁹ who called it the principle of microscopic reversibility at equilibrium, and was later used by Onsager²⁰ to develop the reciprocal relations. However, the principle of microscopic reversibility was used in the derivation of the reciprocal relations, and thus they cannot be expected to hold far from equilibrium. The free-molecule conditions met by an orbital transfer vehicle are far from equilibrium, in the sense that the incoming stream is far from being in thermodynamic equilibrium with the surface, and there is no reason to believe that the principle of microscopic reversibility at equilibrium should hold. The fact that the Nocilla model does not satisfy the principle is not a fundamental limitation, however, and it should generate a useful representation of the velocity distribution function of the re-emitted molecules for the conditions appropriate to an orbit-transfer vehicle.

Note that the Nocilla model cannot be used to model all observed scattering patterns, especially those that have a pronounced backscattering lobe as well as a quasispecular lobe. As an example, Alcalay and Knuth²¹ scattered argon, in the energy range of 0.6 to 1.2 eV, from surfaces of mica, glass, and brass. A common feature of the measurements was the observation of three scattering lobes, one close to the specular direction, one in the normal direction, and one in a backscattering direction. Such multiple-lobed patterns cannot be described using the Nocilla model as presented in this paper. It is not known whether any accommodation-coefficient measurements have been made under conditions that would produce multiple scattering lobes, because simultaneous measurements of the scattering patterns and the accommodation coefficients have never been made, although measurements have been made simultaneously of the scattered density distribution and the velocity distribution of the scattered molecules.

Computation of Nocilla Model Parameters

The procedure for computing the Nocilla model parameters will now be described. First, values of σ' and σ are computed for a given value of θ_i using an appropriate correlation of the measurements, in the present case given by Eqs. (20–22). The parameters in the Nocilla model, i.e., S_r , θ_r , α_2 , and T_r , must now be adjusted until the model predicts these values of σ' and σ when Eqs. (2), (3), (8), (9), (12), (13), and (19) are substituted into the equations defining σ' and σ [Eqs. (17) and (18), respectively]. This complete equation set was used in Ref. 15, where it was found that a simplification could be made using an expression for the maximum value of α_2 derived by Hurlbut.¹⁶ The previous exact calculations in Ref. 15 indicated that the value of α_2 was always within 1.5% of the maximum value from Ref. 16 when the speed ratio was high. Therefore, α_2 is simplified as

$$\alpha_{\max} = \frac{(S^2 + \frac{5}{2})T - (S_r^2 T_r + \frac{1}{2} j T)}{(S^2 + \frac{5}{2})T - \frac{1}{2}(4 + j)T_w}, \quad j = 2 \quad (23)$$

and α_2 is no longer considered to be a free parameter. The equation for σ can be simplified after introducing the expressions for τ_i and

τ_r to read

$$\sigma = 1 - \sqrt{B} S_r \frac{\sin \theta_r}{\sin \theta_i} \quad (24)$$

This constitutes a nonlinear equation set for the Nocilla model parameters that must be solved iteratively. Iteration was normally stopped when 1% agreement between the assumed momentum accommodation coefficients from Eqs. (20–22) and those obtained, from the Nocilla model was obtained, but this degree of agreement was difficult to obtain at the largest incident angles. Further details concerning the determination of the parameters are given in Ref. 15.

Results

Examples of the application of the procedure described in the previous section are shown in Figs. 3 to 6. The conditions for the various cases are given in Table 1. Case D gives results previously published in Ref. 15 for comparison. The case-D results were computed using accommodation-coefficient correlation 1 from Ref. 4, which was given by Knechtel and Pitts²² as a fit to their 10-eV accommodation-coefficient measurements for the scattering of N_2^+ from aluminum. That correlation is given by the equations

$$\sigma' = 1.0 - 0.9 \exp(-2.8 \cos^2 \theta_i) \quad (25)$$

$$\sigma = 0.9 - 1.2 \exp(-1.47 \sin^4 \theta_i) \quad (26)$$

The momentum accommodation coefficient correlation given by Eqs. (20–22) will be called model I, and that from Eqs. (25) and

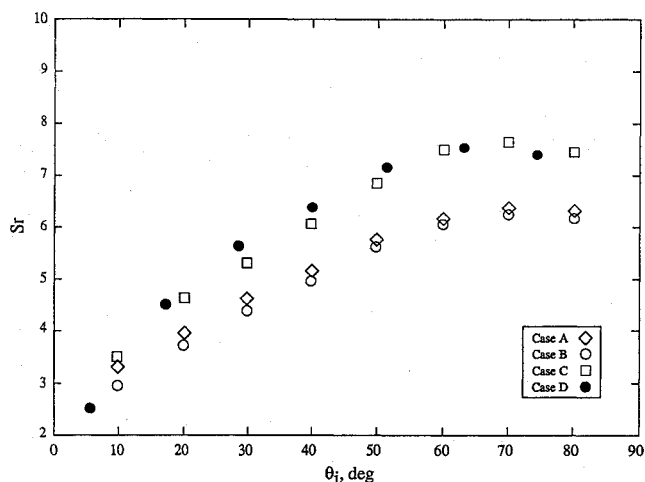


Fig. 3 Variation of the reflected speed ratio required for the Nocilla model to reproduce the momentum accommodation coefficients.

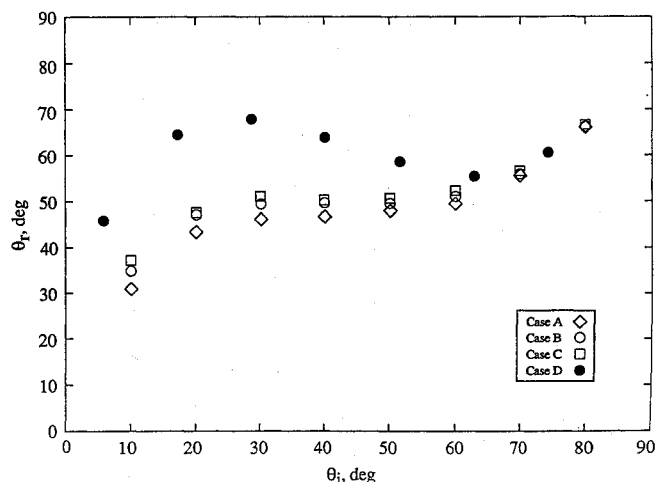


Fig. 4 Variation of the reflected angle required for the Nocilla model to reproduce the momentum accommodation coefficients.

Table 1 Conditions for computations

Case	Model ^a	Speed ratio	Air temp. K	Wall temp. K
A	I	8.0	1000	600
B	I	8.0	1000	300
C	I	10.0	1000	200
D	II	9.89	974	290

^aModel I given by Eqs. (20–22); model II given by Eqs. (25) and (26).

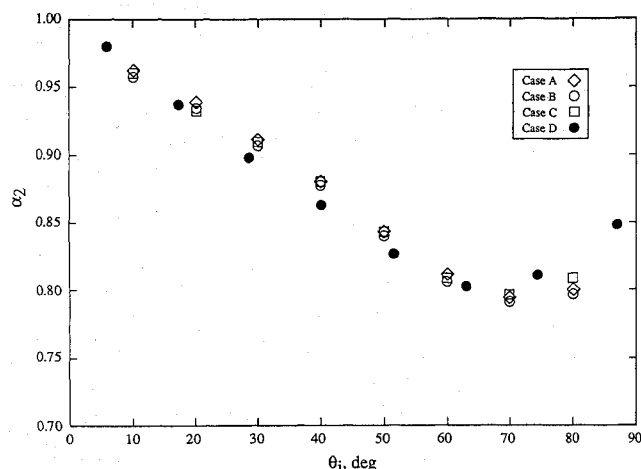


Fig. 5 Variation of the thermal accommodation coefficient required for the Nocilla model to reproduce the momentum accommodation coefficients.

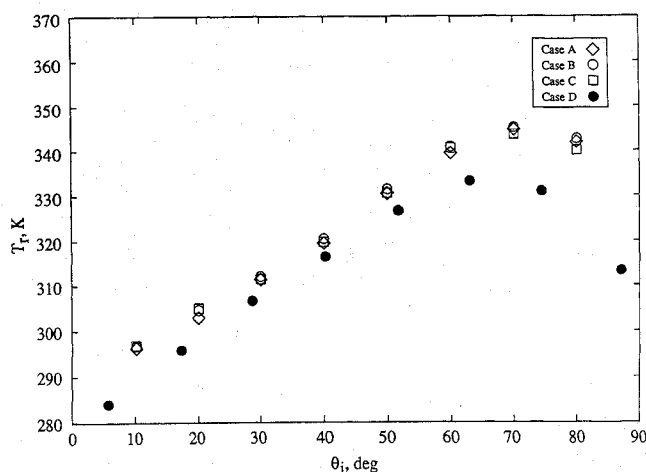


Fig. 6 Variation of the reflected temperature required for the Nocilla model to reproduce the momentum accommodation coefficients.

(26) model II. These models are compared in Fig. 2. The correlations in model I, were developed by the authors as a representation of the entire body of applicable measurements.⁴

Both models predict that the reflected speed ratio is greater than 1.0 for all θ_i and that it increases in magnitude with increasing angle from the surface normal with a maximum value at $\theta_i = 60$ to 70 deg, which depends upon the speed ratio. The predicted value is insensitive to the accommodation-coefficient model that is used. These predictions are in agreement with the limited measurements of S_r , which indicate that S_r increases in magnitude with increasing θ_i and frequently has a magnitude greater than one.³

The angle of the reflected lobe, θ_r , is found to be a nonlinear function of the incident angle θ_i . In this case the predicted reflected angle displays great sensitivity to the accommodation coefficient correlation (Fig. 2). Model I predicted an almost monotonic increase of θ_r with θ_i , whereas model II predicted a local maximum at about 30 deg. The angle θ_r does not appear to be very dependent upon the incident speed ratio. While there is a dearth of measurements of θ_r in this energy range, the measurements that do exist indicate that θ_r

increases with θ_i (Ref. 3); frequently, theoretical work has assumed that $\theta_r = \theta_i$ (Ref. 17). The prediction of a nonlinear relation has not previously been noted, although it can be obtained from the equations in Ref. 16.

Both of the models predict similar variations of the thermal accommodation coefficient α_2 with θ_i , as shown in Fig. 5. This variation decreases from approximately 1.0 at normal incidence to about 0.79 at 70 deg and then increases. The predicted value of the thermal accommodation coefficient is similar to that computed by Varakin and Farafonov²³ using high-energy measurements of momentum accommodation-coefficients, but did not agree with other estimates (see Ref. 15). Likewise, the two models predict a similar angular variation and magnitude for the temperature of the reflected velocity distribution. These results are unexpected, since they show essentially no variation of T_r with speed ratio or wall temperature but only with the accommodation-coefficient correlation. The value of T_r is independent of the wall temperature despite the fact that the thermal accommodation coefficient is always close to one. Since S_r increases greatly with increasing θ_r , whereas T_r is relatively constant, the mean reflected speed must increase, and the lobe of the reflected pattern is predicted to become more narrow as θ_i increases. However, there are essentially no data with which to compare these predictions.³

Concluding Remarks

The reflected velocity distribution function can now be obtained by curve-fitting the computed values of the Nocilla model parameters S_r , θ_r , α_2 , and T_r . This model of the reflected velocity distribution function will provide the wall boundary condition that is required for DSMC computations of the aerodynamic performance for bodies that are in the transition or free-molecule flow regimes. The present results apply to bodies moving at large speed ratios. The procedure described is dependent upon having measurements of the momentum accommodation coefficients for the applicable gas, surface, energy, and wall temperature conditions of interest.

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