Comparisons of the Maxwell and CLL Gas/Surface Interaction Models Using DSMC

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Abstract

Two contrasting models of gas-surface interactions are studied using the Direct Simulation Monte Carlo (DSMC) method. The DSMC calculations examine differences in predictions of aerodynamic forces and heat transfer between the Maxwell and Cercignani–Lampis–Lord (CLL) models for flat plate configurations at freestream conditions corresponding to a 140 km orbit around Venus. The size of the flat plate is that of one of the solar panels on the Magellan spacecraft, and the freestream conditions are one of those experienced during aerobraking maneuvers.

Results are presented for both a single flat plate and a two-plate configuration as a function of angle of attack and gas-surface accommodation coefficients. The two plate system is not representative of the Magellan geometry, but is studied to explore possible experiments that might be used to differentiate between the two gas surface interaction models.

Nomenclature

A	area of plate
Ar	argon
C_D	drag coefficient, $\frac{2D}{\rho_\infty V_\infty^2 A}$
C_H	heat-transfer coefficient, $\frac{2q}{\rho_\infty V_\infty^3}$
C_L	lift coefficient, $\frac{2L}{\rho_\infty V_\infty^2 A}$
CLL	Cercignani–Lampis–Lord model
CO	carbon monoxide
CO_2	carbon dioxide
D	drag
E	energy per molecule
L	lift
N_2	molecular nitrogen
p	normal momentum
q	heat flux
V_∞	freestream velocity
x,y	coordinates in plane of the plane
z	coordinate normal to flat plane
α	thermal energy accommodation coefficient
ϵ	fraction of diffuse scattering in Maxwell model
ρ_∞	freestream density
σ	momentum accommodation coefficient
θ_i	angle of attack
θ_r	angle of reflection
Θ_r	mean angle of reflection in CLL model
τ	tangential momentum

Subscripts

i	incident
n	normal
r	reflected
t	tangential
w	wall
∞	freestream

Introduction

In hypersonic flight at very high altitudes, gas-surface interactions are one of the dominant physical processes that govern aerodynamic forces and heat transfer. Our present understanding of these interactions is severely limited, especially for the highly energetic gas-surface collisions that occur during orbital or high-altitude aerobraking and entry conditions. Therefore, the prediction of aerothermodynamic performance is less accurate than desired for these conditions (Ref. 1).

The Direct Simulation Monte Carlo (DSMC) method of Bird (Ref. 2) is commonly used to simulate rarefied flow problems, and the accuracy of the method depends directly on the accuracy of the gas-surface interaction model. The most widely used model is the Maxwell model, which is based on classical thermodynamics, in which it is assumed that molecules will either reflect diffusely with complete energy accommodation, or will reflect specularly with no change in energy. An accommodation coefficient, ϵ, is defined which specifies the percentage of molecules that will be scattered diffusely, with $\epsilon = 0$ giving complete specular reflection, and $\epsilon = 1$ giving complete diffuse reflection.

While the Maxwell model is useful for describing the overall thermodynamic behavior of gas-surface interactions, it does not accurately describe the detailed molecular behavior frequently observed in fundamental gas-surface scattering experiments. For moderate to high energy scattering from engineering surfaces, the flux distribution of scattered molecules frequently has a lobular shape that is centered about an angle, Θ_r, which tends to approach the specular angle for very high energies and/or low angles of attack (Ref. 1). The Cercignani–Lampis–Lord model (CLL) (Ref. 3) is one of several models developed to handle such behavior. In the CLL model, the transformations of the normal and tangential components of velocity are assumed to be mutually independent. Analysis of the flux distribution of scattered molecules shows it to be centered around an average scattering angle, $\langle\Theta_r\rangle$, which is a function of normal and tangential accommodation coefficients, α_n and σ_t.

$$\langle\Theta_r\rangle = f(\alpha_n, \sigma_t)$$

The mean energy of the reflected molecules is also a function of the normal and tangential accommodation coefficients.

$$\langle E_r\rangle = F(\alpha_n, \sigma_t)$$

The purpose of this paper is to examine the differences in aerothermodynamic quantities (forces and heat transfer) predicted with these two gas-surface interaction models. The Maxwell and CLL models are incorporated into a DSMC code, and calculations are performed for hypersonic rarefied flow about flat plates. The conditions selected are the same as those used in a study by Rault (Ref. 4) of the Magellan spacecraft orbiting Venus. Calculations are performed for a single flat plate having dimensions the same as one of the solar panels of the Magellan spacecraft. Calculations are also performed for a two-plate configuration to explore possible experiments that might be used to differentiate between the two gas-surface interaction models.

Accommodation Coefficients and Gas-Surface Interaction Models

A variety of definitions for accommodation coefficients exists in the literature. The traditional definition of "thermal accommodation" is usually expressed as:

$$\alpha = \frac{E_i - E_r}{E_i - E_w}$$

where E_i is the incident energy per molecule, E_r is the reflected energy, and E_w is the energy per molecule corresponding to fully diffuse scattering with full accommodation to the wall temperature. This definition is frequently extended to other flux quantities to yield normal and tangential momentum accommodation, σ_n and σ_t,

$$\sigma_n = \frac{p_i - p_r}{p_i - p_w} \qquad \sigma_t = \frac{\tau_i - \tau_r}{\tau_i}$$

and a general definition of accommodation coefficient is given in Ref. 5. These various definitions have been defined partly for convenience in relating experimentally observed behavior to various empirical gas-surface models.

In the Maxwell model, the fraction of diffusely-scattered molecules, ϵ, is equivalent to the thermal accommodation coefficient defined above. Traditionally, the model is considered to have only this single adjustable parameter, and the momentum accommodation coefficients also follow once ϵ is specified, i.e. σ_n and σ_t are also determined by ϵ. However, σ_n and σ_t are sometimes viewed as being independent of the energy accommodation. In the traditional implementation of the Maxwell model in DSMC calculations, it has usually assumed that the energy and momentum accommodation are not independent, and that assumption is used in the present implementation.

The CLL model is derived assuming that there is no coupling between the normal and tangential momentum components, and treats the normal component of translational energy, α_n, and the tangential component of momentum, σ_t, as two independent, disposable parameters. However, in the implementation of the CLL model in DSMC, Bird (Ref. 2) has shown that it is equivalent to specify the normal and tangential components of translational energy since α_t can be considered equivalent to $\sigma_t(2 - \sigma_t)$. In presenting the results with the CLL model, we will use the quantities α_n and σ_t as the two disposable parameters.

In addition, the present simulations will also consider the accommodation of internal energy, α_i, the implementation of which is described below.

DSMC Method

The DSMC method is widely used for simulating rarefied flows and is described in detail in Ref. 2. The method consists of tracking the motion of representative molecules as they move in physical space while undergoing collisions with other molecules and with physical boundaries within or surrounding the computational volume. The volume is discretized into cells within which samples of density, momentum, and energy are stored for computing macroscopic properties of the flow. Surfaces within the computational volume are also discretized, and samples of momentum and energy transfer to elements of the surface are stored for computing macroscopic properties of the flow. Surfaces within the computational volume are also discretized, and samples of momentum and energy transfer to elements of the surface are stored for computing forces and heat transfer. In the present study, gas collisions are treated with the variable hard sphere (VHS) model with internal energy exchange allowed only for rotational degrees of freedom.

The DSMC computer code used in the present study is a three dimensional code described in Ref. 2 which uses uniform Cartesian cells. The code contains the Maxwell gas-surface interaction model and was modified to include the CLL model as an option. In the implementation of the Maxwell model, accommodation of internal energy is set equal to the parameter ϵ. Those molecules which scatter diffusely have their internal energies adjusted by sampling from an equilibrium distribution corresponding to the surface temperature, while molecules which scatter specularly retain their incident internal energy.

In the CLL model, accommodation of the internal energy is allowed to be independent of the translational accommodation. For all calculations presented here, however, the internal energy accommodation is kept equal to one or both of the translational accommodation coefficients, α_n or σ_t. For each molecule scattered by the surface in the CLL implementation, an energy state is sampled from an equilibrium distribution corresponding to the surface temperature, the reflected internal energy is given by:

$$E_r^i = \alpha_i E_i^i + (1 - \alpha_i) E_w^i$$

where E^i denotes the internal energy of the molecule.

Problem Conditions

The hypersonic flow over a flat plate lends itself well to experimentation because its simple geometry makes it an ideal situation in which to compare theory and experiment (Ref. 6–7). Because of earlier scientific discussions (Ref. 8) to use the Magellan spacecraft as a test for gas-surface interactions, a flat plate with the dimensions of a solar panel from the Magellan spacecraft was used for the DSMC calculations. The panel was placed in an environment consistent with Venus' atmosphere at an altitude of 140 km. Freestream conditions and panel dimensions taken from Ref. 4 are:

Density	$9.5 \text{ X } 10^{16}$ molecules/m^3
Temperature	225 K
Molar Composition	75.7% CO_2, 9.6% CO, 8.9% Ar, 5.8% N_2
Free Stream Velocity	8600 m/s
Free Stream Speed Ratio (s)	28.5
Surface Temperature	300 K
Panel length in X direction	2.53 m
Panel length in Y direction	2.5 m

Results

Single Flat Plate

DSMC calculations were first performed with gas collisions disallowed and checked against free-molecule analytical predictions for both Maxwell and CLL models. Analytical solutions for the Maxwell model are taken from Ref. 2, while analytical solutions for the CLL model are taken from Ref. 5. The collisionless DSMC calculations agree with the analytical solutions within the limits of statistical error in the DSMC sample. In addition, for $\epsilon = 1$ in the Maxwell model and $\alpha_n = \sigma_n = 1$ in the CLL model, the two models produce precisely the same results.

DSMC simulations were then performed with collisions allowed. Once again, for $\epsilon = 1$ in the Maxwell model and $\alpha_n = \sigma_t = 1$ in the CLL model, the two models produce precisely the same results. Including gas-gas collisions, however, decreases both the drag and heat transfer slightly while increasing the lift significantly. The two models were then compared at an angle of attack of 45 degrees with varying accommodation coefficients (See Fig 6). For the CLL model α_n was kept equal to σ_t. The CLL and Maxwell models predict the same lift, drag and heat transfer when the accommodation coefficients are equal to zero or one. For accommodation coefficients not equal to zero or one, the CLL model produces larger lift, drag, and heat transfer than the Maxwell model. The differences are greatest for lift and drag when $\epsilon = 0.8$ and $\alpha_n = \sigma_t = 0.8$, where the CLL model gives a drag coefficient of 1.58 and a lift coefficient of 0.46 compared to values of 1.40 and 0.35 for the respective coefficients with the Maxwell model. The heat transfer coefficient, on the other hand, has its greatest difference when $\epsilon = 0.5$ and $\alpha_n = \sigma_t = 0.5$. Here, simulations with the CLL model produce a heat transfer coefficient of 0.44 compared to 0.35 predicted with the Maxwell model.

The effects of changing the tangential and normal accommodation coefficients independently in the CLL model are shown in Fig. 7. For the solid curves, the tangential accommodation coefficient is held constant (along with internal energy) at 0.5, while the normal accommodation coefficient is varied from 0.0 to 1.0. For the dashed curves, the normal accommodation coefficient is held constant(along with internal energy) at 0.5, while the tangential accommodation coefficient is varied from 0.0 to 1.0. Variations in α_n or σ_t seem to have approximately the same effect on both lift and heat transfer, i.e., as the normal and tangential coefficients vary from 0.0 to 1.0, the heat increases and the lift decreases. Varying α_n, however, has the opposite effect on drag than that caused by varying σ_t. When α_n is increased from 0.0 to 1.0 the drag coefficient decreased at approximately the same rate as the coefficient of lift. When σ_t is increased from 0.0 to 1.0, however, the drag coefficient increases at approximately the same rate as the lift coefficient decreases. Therefore, changing α_n has little effect on the lift-to-drag ratio; it remains nearly constant at a value of 0.6. Changing

σ_t, however, has a profound effect on the lift-to-drag ratio. As σ_t increases from 0.0 to 1.0, the lift-to-drag ratio decreases from 1.0 to 0.3.

The simulations were repeated with each coefficient held constant at 0.8 (along with internal energy) while the other coefficient was varied from 0.0 to 1.0. These simulations produced results similar to those simulations where the constant coefficient and internal energy were held constant to 0.5. When σ_t is held constant at 0.8, and α_n varies from 0.0 to 1.0, the lift-to-drag ratio remains constant at approximately 0.48. When σ_t is increased from 0.0 to 1.0, the lift-to-drag ratio decreases from 1.0 to .18.

One way to visualize the manner in which the two models produce these differing behaviors is to examine the density contours around the plate. When $\epsilon = 0.5$, the Maxwell model predicts that most molecules will be distributed more-or-less symmetrically along the windward side of the plate with only a slight bias in density toward the specular direction. When $\alpha_n = \sigma_t = 0.5$, however, the CLL model predicts that the distribution of molecules is strongly biased towards the specular direction. This behavior is caused by differences in the velocity distributions of the scattered molecules. With the Maxwell model, scattered molecules consist of a combination of specularly reflected molecules which have a Maxwellian velocity distribution characteristic of the surface temperature. For a "cold" plate, the same velocity magnitude as the incoming molecules and diffusely reflected molecules which have the diffusely reflected molecules remain in the vicinity of the surface longer and result in a density buildup near the plate. On the other hand, the CLL model provides a much more complex description of the velocity distribution of scattered molecules in which the overall mean velocity, temperature, and mean scattering angle are complex functions of the incoming velocity, the surface temperature, and the normal and tangential accommodation coefficients. For accommodation coefficients less than one but greater than zero, the CLL model gives a somewhat higher average velocity of scattered molecules and a more continuous distribution of molecules scattered near the specular angle. The result is that the molecules do not remain near the surface as long as with the Maxwell model, and lower densities occur near the plate. This behavior leads to speculation about possible differences one might encounter if other surfaces were present near the plate and is the motivation for the two plate calculations presented in the next section.

Two Plate System

The DSMC code was altered to incorporate a second identical flat plate. The second plate is displaced 2.5 meters in the x and z directions from the original plate, placing it 2.5 meters in front of and above the original plate. This geometry gives an angular displacement of the center of each plate that is 45 degrees from the normal to the other plate and was selected because it was believed that it might maximize the interaction between the plates. Density contours illustrate the new geometry and the differences between the Maxwell and CLL model results.

DSMC calculations were performed at a constant angle of attack of 45 degrees while the accommodation coefficients for both the Maxwell and CLL models were once again varied from 0.0 to 1.0. Lift, drag, and heat transfer coefficients for the combined two-plate system are shown in Fig. 10. The CLL and Maxwell models again give identical results when the accommodation coefficients are equal to 0.0 or 1.0, just as for a single plate. Other features of the comparison are similar to those with the single plate; the CLL model predicts higher values for lift, drag, and heat transfer when the accommodation coefficients are not equal to zero or one, and the maximum differences between the two models occur in lift and drag when the accommodation coefficients are equal to 0.8 and in the heat transfer when the accommodation coefficients are equal to 0.5.

Because the coefficients are based on the reference area for a single plate one might expect all coefficients for the two-plate system to be twice as large as for the single plate. The heat transfer coefficient is indeed approximately twice as large. The lift coefficient, however, is only slightly larger that the single plate results, while the drag coefficient is only slightly larger at $\epsilon = \alpha_n = \sigma_t = 0.0$, but increases to almost twice the single plate value at $\epsilon = \alpha_n = \sigma_t = 1.0$. This behavior is caused by the interference between the two plates caused by molecules that are reflected from the windward side

of the rear plate hitting the leeward side of the front plate. The forces caused by these secondary reflections essentially cancel out the lift of one plate. In other words, the forces in the lift direction due to these secondary reflections are negative and are only a weak function of accommodation coefficient. A similar phenomena occurs for the drag force except that the cancelling force is more strongly dependent on the accommodation coefficients. Therefore, the drag increases significantly as the accommodation coefficients are increased rather than remaining relatively constant as it does for a single plate.

In the Maxwell DSMC calculations, ϵ was held constant at 0.5, while in the CLL DSMC simulations α_n and σ_t were held constant to 0.5. The behavior of the drag coefficient is somewhat similar to that for the single plate simulations, although the rate of increase with angle of attack is lower at smaller angles. The lift coefficient, however, shows a maximum at an angle of attack of 60 degrees rather than at 45 degrees as with the single plate, and a second local maxima occurs at 30 degrees with the Maxwell model. The presence of the second plate also causes the heat transfer coefficient to reach a maximum at an angle of attack other than 90 degrees as it does with the single plate. Furthermore, the CLL model and Maxwell models give different predictions for this angle, a fact that will be discussed in more detail.

To further examine the detailed behavior of the two-plate system, surface forces and heat transfer were extracted separately for each side of the plate. These sides are numbered as follows: Side 1 is the leeward side of the front plate, Side 2 is the windward side of the front plate, Side 3 is the leeward side of the back plate, Side 4 is the windward side of the back plate. For the present DSMC simulations, there were insufficient molecules striking the leeward side of the back plate (Side 3) to gather meaningful statistics on the surface forces and heat transfer. Sides 2 and 4 dominate the contributions to the total forces and heat transfer and show essentially the same qualitative behavior as that for the complete system. Side 1 shows some interesting qualitative variations with angle of attack but no distinct differences between the Maxwell and CLL model results.

Further calculations were then performed for other values of accommodation coefficients. An examination of these results showed that Side 4 was the only side which exhibited a distinct difference in qualitative behavior between the Maxwell and CLL models. In these calculations, the Maxwell model predicts that the heat transfer is maximized at an angle of attack which is independent of the accommodation coefficient, while the CLL model predicts that the angle of attack at which the heat transfer is maximized is a strong function of the accommodation coefficients. DSMC simulations were run for several other accommodation coefficients, and the results show that the angle of attack for maximum heat transfer for Side 4 always occurs at about 83 degrees with the Maxwell model while varying from about 55 degrees for $\alpha_n = \sigma_t = 0.1$ to about 83 degrees for $\alpha_n = \sigma_t = 1.0$ with the CLL model. The behavior with the CLL model is attributed to the lobular nature of the scattered molecules which are the backscattered from Side 1 (front plate) and return to Side 4 (back plate). Since the densities are relatively low for the current simulations, gas-gas collisions are not that important. Therefore, it is likely that a free molecular analysis could be performed using the CLL model to provide a full analytical description of this behavior.

Discussion

The relative insensitivity of the aerothermodynamic coefficients to the gas-surface interaction model for a single flat plate is not too surprising. Both the Maxwell and CLL models are constructed to give the same behavior in the limits where the gas and surface are in thermal equilibrium. In fact, under more continuum-like conditions, the two models give essential identical results (Ref. 2). For the Venus aerobraking conditions used here, the flow is highly rarefied, and gas-surface interactions dominate the aerothermodynamic behavior. Although there are many quantitative differences, they are generally small (order of 10–20%), and the qualitative behavior as a function of angle of attack and overall accommodation is essentially the same for the two models. The details of the flowfield, however, are quite different for the two models. The superposition of diffusely and

specularly scattered molecules given by the Maxwell model and the more continuous molecular flux distribution with its lobular shape given by the CLL model result in a radically different density field around the plate.

The differences in flowfield structure observed for the two models were explored for a two-plate system in the hopes of finding qualitative differences in some aerothermodynamic quantity. It was hypothesized that such differences might be exploited experimentally as a means of determining which model gives a better representation of the gas-surface behavior for high-velocity aerobraking and orbital flight conditions. Intuitively it was expected that by that by placing a second plate in the near vicinity of the first, there might be some sensitivity to the lobular nature of the scattering with the CLL model. In effect, the second plate might act as a "detector" for molecules scattered from the first plate. In fact, such a sensitivity was found, although the manner in which it was manifested was somewhat unexpected. The results show a qualitative difference in the angle of attack at which the maximum heat transfer occurs with the CLL model showing it to be strongly dependent on the accommodation coefficients while the Maxwell model gives results that are independent of accommodation coefficient. The surprising feature is that the qualitative difference appears to be the result of secondary backscatter from the rear side of the front plate to the front side of the rear plate. Thus it is a second-order effect, and even though the variations in heat transfer are quite large, the actual variations in heat transfer coefficient are quite small. This makes it more difficult to determine the location of the maxima and require very precise heat-transfer measurements in order to exploit this phenomena experimentally.

The calculations presented in this report have only covered a limited number of parametric variations. Further calculations in which the normal and tangential accommodation coefficients are varied over a wide range of combinations or where the internal energy accommodation is varied independently might provide more insight into the sensitivity of the aerothermodynamic quantities to gas-surface model. Other multiplate configurations and/or other geometries might also be worth investigating in order to identify conditions where experimental measurements might be more feasible. The significant differences observed in overall flowfield behavior between the Maxwell and CLL models even for these simple cases, however, suggest that it may be important to determine which gas-surface interaction model best represents the physical behavior expected for complex aerobraking configurations.

Closing Remarks

DSMC calculations have been made to examine differences in predictions of aerodynamic forces and heat transfer between the Maxwell and Cercignani–Lampis–Lord (CLL) gas-surface interaction models for flat plate configurations at freestream conditions corresponding to a 140 km orbit around Venus. The size of the flat plate is that of one of the solar panals on the Magellan spacecraft, and the freestream conditions are one of those experienced during aerobraking.

Results were calculated for both a single flat plane and a two-plate configuration as a function of angle of attack and gas-surface accommodation coefficients. The two-plate system is not representative of the Magellan geometry, but is studied to explore possible experiments that might be used to differentiate between the two gas-surface interaction models.

Although the Maxwell model and CLL model have fundamental differences, they give similar predictions of aerothermodynamic coefficients on a single flat plate. The two models, however, differ in their predictions of the flowfield around the plate. These differences lead to predictions for the angle of attack for maximum heat transfer in a two plate configuration that are distinctly different for the two gas-surface interaction models. The angle of attack at which maximum heat transfer occurs with the CLL model is a function of accommodation coefficient, while the angle of attack for maximum heat transfer for the Maxwell model is constant. Further investigation into this behavior could provide better understanding of the accommodation coefficients of materials and gases for orbital and aerobraking conditions.

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