

出國報告（出國類別：參加研討會）

出席 2012 年國際傳輸現象會議
心得報告

服務機關：國防大學理工學院機電能源及航太工程學系

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目次

封面.....	I
目次.....	II
摘要.....	III
目的.....	4
過程.....	4
心得及建議.....	5
附件.....	6

摘要

國際傳輸現象會議 (International Symposium on Transport Phenomena) 是國際工程學界有關傳輸現象學術與應用的重要會議，由太平洋熱流工程中心 (The Pacific Center of Thermal-Fluids Engineering) 發起，自 1985 年起已舉辦 23 屆，參與活動的學者包含美、歐、亞、澳等各國學者，研究範圍包含宏觀到微觀、實驗理論與計算的質量動量與能量傳輸等，在學術上具重要地位。議程內容計有 5 場邀請專家發表主題講演，19 項議題場次有 186 篇論文以口頭報告或海報張貼方式發表。本人所提有關極音速稀薄氣體熱動力模擬之論文於 11 月 20 日下午進行海報展示與討論。與在場的日本學者 Prof. Mochizuki, 英國學者 Dr. Ligrani 和大會主席 Prof. Mallinson 等有相當熱烈的問答與激盪交流，獲益良多。此次會議除了發表自己的研究成果外，藉由參與各項議程活動了解本學術領域的現況與發展趨勢，聽取與會學者們提出的報告和相互的討論，確有吸收新知開闊視野之實效，有助於個人未來於本學術領域研究工作之精進。

目的

1. 發表研究成果。
2. 與國際學者進行學術交流。

過程

1. 第 23 屆國際傳輸現象會議 (The 23th International Symposium on Transport Phenomena, ISTP-23) 於 2012 年 11 月 19 日至 23 日在紐西蘭首都奧克蘭市 (Auckland) 的奧克蘭大學舉行。國際傳輸現象會議是國際工程學界有關傳輸現象學術與應用的重要會議，由太平洋熱流工程中心 (The Pacific Center of Thermal-Fluids Engineering) 發起，自 1985 年起至本次已舉辦 23 屆，參與活動的學者包含美、歐、亞、澳等各國學者，研究範圍包含宏觀到微觀、實驗理論與計算的質量動量與能量傳輸等，在相關學術界具重要地位。議程計有 5 場邀請專家發表主題講演，186 篇論文以口頭報告或海報張貼方式發表。略分為 19 個不同科技議題 (Technical Session)：Combustion, Multiphase, Air-Conditioning, Bioengineering, Experimental and Computational Fluid Dynamics, Clean Green Energy, Environment, Industrial, Droplet and Films, Form and Gels, Heat Exchanger, Turbomachinery, Turbulence, Electronic Cooling, Micro and Nano Scale Transport, Renewable Energy, Fuel Cells, Heat Transfer in Electronic Equipment, Natural and Mixed Convection 等。
2. 19 日下午報到並參加歡迎茶會。20 日上午開幕典禮及奧克蘭大學領導能源研究的 Prof. Archer 給的大會演講，題目是紐西蘭的潔淨能源，內容是為了在 2025 年達成百分之九十電力由再生能源供應的目標，如何更有效的開發地熱風力和天然氣等。Prof. Archer 與我同是美國史丹福大學校友特於演講後 Tea Break 時間上前致意。
3. 本人所提之論文為”極音速稀薄氣體流過淺槽的直接模擬蒙地卡羅法研究”(Study of Hypersonic Rarefied Gas Flow over Shallow Cavity by DSMC Method) 於 11 月 20 日下午 13 點 50 分至 15 點 30 分進行海報展示與討論。本論文研究重點在於針對高空高速飛行載具，進行氣體分子直接模擬蒙地卡羅法 (Direct Simulation Monte Carlo, DSMC) 分析時，探討固體壁面邊界條件設定可能遭遇的困難和尋求解決之道。與在場的日本學者 Prof. Mochizuki, 英國學者 Dr. Ligrani 和大會主席 Prof. Mallinson 等多位大師級學者及專家們有相當熱烈的問答與激盪交流，獲益良多。
4. Prof. Mochizuki 是舊識，特別詳細了解本人近年發展處理絕熱壁氣固作用模式 (Gas-Surface Interaction Model) 的新成果。Dr. Ligrani 則很欣賞本人所提出之等向

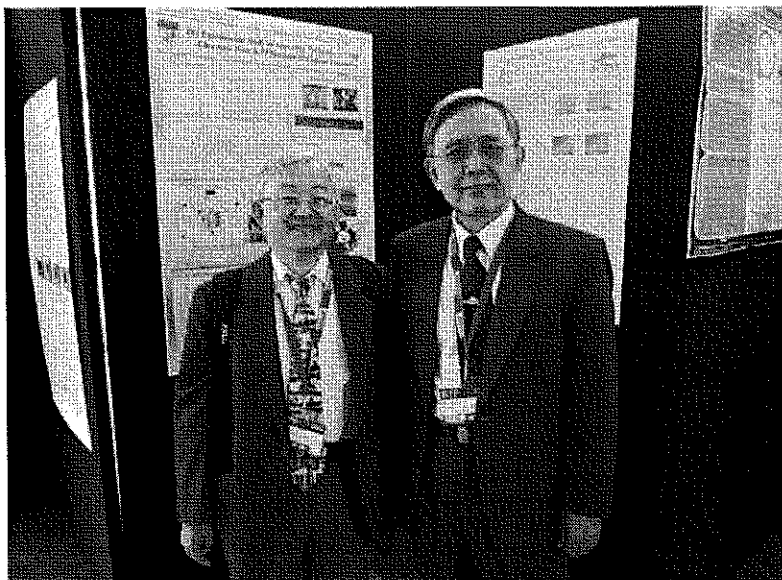
性散射 (Isotropic Scattering) 模型作為絕熱壁邊界條件的簡明有效。 Prof. Mallinson 對稀薄氣體流過真實固體表面各種可能的質量動量與能量傳輸現象的複雜性表示理解，並期許本人再接再厲。華梵大學李弘毅陸軍官校許綜升等幾位國內學者亦參與討論，海報展示的結果中，有關氣固作用模式各種動量與能量調適係數的效應，引起最多興趣與問答。

5. 21 日下午回報 Dr. Ligrani 的指教，特別去聽他有關渦輪葉片流場表面熱傳增進技術研究的主題講演。另外也聽取與本人研究主題較為相關的微奈米傳輸議題 (Micro and Nano Scale Transport) 幾場論文發表，如日本 Prof. Murakami 的液固介面奈米結構型態影響能量傳輸的分子動力學研究報告，以及韓國學者 Dr. Kim 的表面粗糙和親水性對沸騰熱傳影響的奈米尺度研究等。
6. 22 日議程與本人研究主題較無相關，由 Prof. Mallinson 和華裔的 Dr. Liu 陪同參觀奧克蘭大學主校區美麗校園中的工學院和建築學院。
7. 23 日上午參觀奧克蘭大學塔瑪基創新研究校區 Tamaki Innovation Campus。主要特色在帆船遊艇的研發設計。有船體和船帆流體力學結構材料和穩定操控相關的實驗與模擬設備，如風洞和高速電腦等一應俱全。本人對船帆空氣動力的模擬分析很感興趣，與在場學者同好們就模擬軟體的適用限制，以及如何與實驗相輔相成，有相當熱烈的討論。

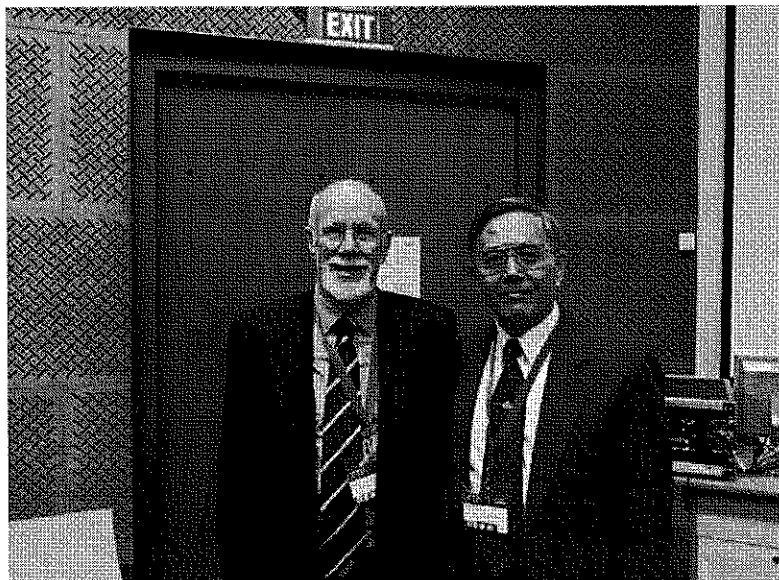
心得及建議

1. 此次會議除了發表自己的研究成果外，藉由參與各項議程活動了解本學術領域的現況與發展趨勢，聽取與會學者們提出的報告和相互的討論，確有吸收新知開闊視野之實效，有助於個人未來於本學術領域研究工作之精進。
2. 研討會期間也曾和幾位紐西蘭本地和日韓美英等國學者，以及來自國內成功大學的張錦裕教授，清華大學洪哲文教授，潘欽教授及中興大學林呈教授等多位學者專家們晤談甚歡。高雄應科大艾和昌教授給一場專題講演，他帶領的團隊另組成一個場次有關潔淨綠能的研討。成大黃正弘國際長和華梵大學李弘毅教授的團隊組成一個場次的有關電子裝備熱傳的研討表現突出。國內傳輸現象相關的研究在學界同仁們努力耕耘下，在此國際學術會議上獲得高度的肯定。
3. 奧克蘭大學工學院主辦本次會議，特別安排參觀該校最具特色的研究單位 Tamaki Innovation Campus。重點在先進複合材料、相變化研究群和帆船遊艇研發設計團隊。奧克蘭市又稱帆船之都，曾舉辦世界杯大賽，它們在船舶科技尤其是帆船工藝投注的心力和展現的實力，令人印象深刻，值得學習。
4. 本次會議所需費用較高，未能帶研究生一起參加，讓研究生在國際性的學術活動中得到啟發與學習的機會。國科會對國內研究生參加國際學術會議雖有補助，但仍顯不足。建議國科會或國防大學增加相關預算經費，多予國內或本校研究生參加國際學術會議足夠的鼓勵與獎助。

附件：參加該研討會照片海報及論文資料。



與參加本會議的學者在論文海報前合影



與大會主席 Prof. Gordon Mallinson 合影

極音速稀薄氣體流經淺槽之DSMC方法研究

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摘 要

極超音速稀薄氣體流動的研究在航太工程上有其實際的應用，尤其是在發展高空攔截器方面。光學視窗是攔截器上的重要元件之一，其設計是為有效的蒐尋目標物。視窗在整個載具的飛行包絡線中需保持其光學穿透性，然而飛行體在高空、高馬赫數的飛行條件下，其周圍的流場受到熱氣動力效應的影響，使得位於光窗後的尋標器性能受到干擾而降低，而不精準的偵蒐能力將導致飛行任務失效。由此可知，提供準確的流場資訊是必需的。

有賴於科技進展及運算能力的提升，極音速流場所造成光學視窗的熱響應可藉由數值計算獲得，在本研究中，以二維矩形淺槽做為簡化後的光窗模型。由於傳統解 Navier-Stokes 方程式的計算方法不適用於研究這樣一個高空且高速的稀薄氣體流場，因此採用 DSMC 方法作為研究本議題的工具。本研究採用改良的 DSMC 方法技術，並在固體邊界上採用合適的氣固交互作用模式進行研究。利用極音速氣體經過錐形體後的流場資訊做為研究條件，探討各種高度、飛行速度條件下，光學視窗的熱氣動力特性。

Study of Hypersonic Rarefied Gas Flow over Shallow Cavity by DSMC Method



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Abstract

In this study, rarefied gas flow over the optical window of a high-speed interceptor was simplified and investigated numerically as a two-dimensional rectangular cavity flow. Improved DSMC techniques and suitable gas-surface interaction models for solid boundary conditions were employed. Proper initial conditions were specified in which hypersonic flow went through a forebody with a wedge shape. Shallow cavity flow fields with varying altitudes and flight speeds are then examined. The length-to-depth ratio of the shallow cavity is fixed. The major concerns are the effects of gas-surface interaction models on simulations of the gas dynamic characteristics of this window system in various flight conditions.

Gas Surface Interaction

$$U_n^* = -|V_{mp}| \left[R_n^2 + (1 - \alpha_n) \cdot \left(\frac{U_n}{V_{mp}} \right)^2 + 2 \cdot R_n \cdot (1 - \alpha_n)^{1/2} \cdot \left(\frac{U_n}{V_{mp}} \right) \cos(2\pi R_{f2}) \right]^{1/2}$$

$$R_n = (-\alpha_n \ln R_{f1})^{1/2}$$

$$U_{n1}^* = |V_{mp}| \cdot [U_n^* \cos(\theta) - U_{t2}^* \sin(\theta)]$$

$$U_{t2}^* = |V_{mp}| \cdot [U_n^* \sin(\theta) + U_{t1}^* \cos(\theta)]$$

$$U_{n1}^*|_0 = R_n \cdot \cos(2\pi R_{f4}) + (1 - \alpha_t)^{1/2} \cdot \frac{(U_{n1}^2 + U_{t2}^2)^{1/2}}{V_{mp}}$$

$$U_{t2}^*|_0 = R_n \cdot \sin(2\pi R_{f4})$$

$$R_t = (-\alpha_t \ln R_{f3})^{1/2}, \quad \alpha_t = \sigma_t(2 - \sigma_t)$$

$$\theta = \arctan\left(\frac{U_{t2}}{U_{n1}}\right)$$

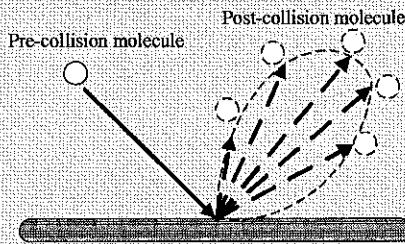


Figure 1. CLL Model

$$U_n^* = -|C| \cdot R_{f1}^{1/2}$$

$$U_{n1}^* = |C| \cdot (1 - R_{f1})^{1/2} \cdot \sin(2\pi R_{f2})$$

$$U_{t2}^* = |C| \cdot (1 - R_{f1})^{1/2} \cdot \cos(2\pi R_{f2})$$

$$|C| = (U_n^2 + U_{n1}^2 + U_{t2}^2)^{1/2}$$

$$|C| = |C^*|$$

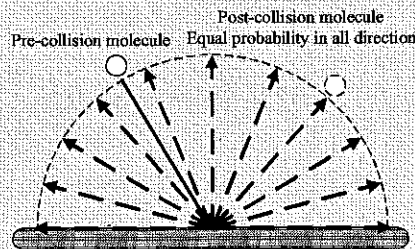


Figure 2. Adiabatic IS Model

Table 1. Simulation conditions get from hypersonic flow went through a wedged forebody

H (km)	M _∞	T ₁ (K)	Theoretical			Simulation results		
			wave angle (degree)	M ₂	T ₂ (K)	wave angle (degree)	M ₂	T ₂
90	12	186.9	21.4	5.65	752.9	23.4	5.26	850.3
	10	186.9	21.9	5.28	596.1	23.9	5.03	646.4
	8	186.9	22.8	4.75	469.0	25.4	4.64	483.8
	6	186.9	24.6	3.99	366.3	27.3	3.83	387.3

Results

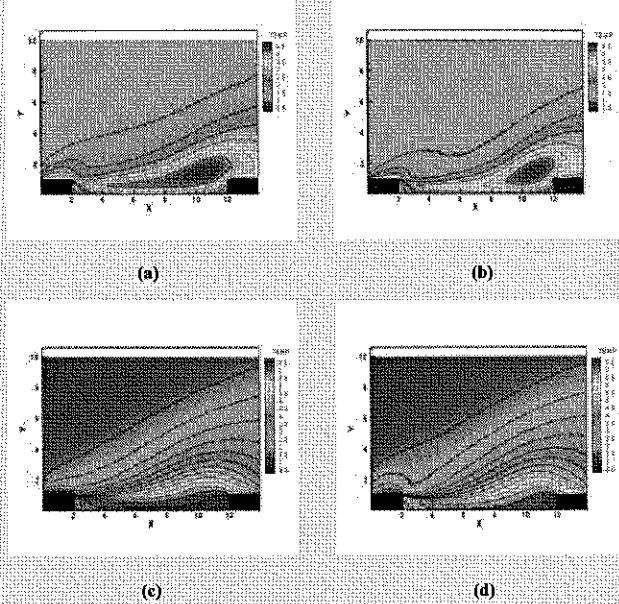


Figure 3. M_∞=12, Kn=0.95, normalized temperature contour in hypersonic shallow cavity flow. (a) CLL (α_n=0.75), (b) CLL (α_n=0.75), (c) Pt-SD, and (d) IS.

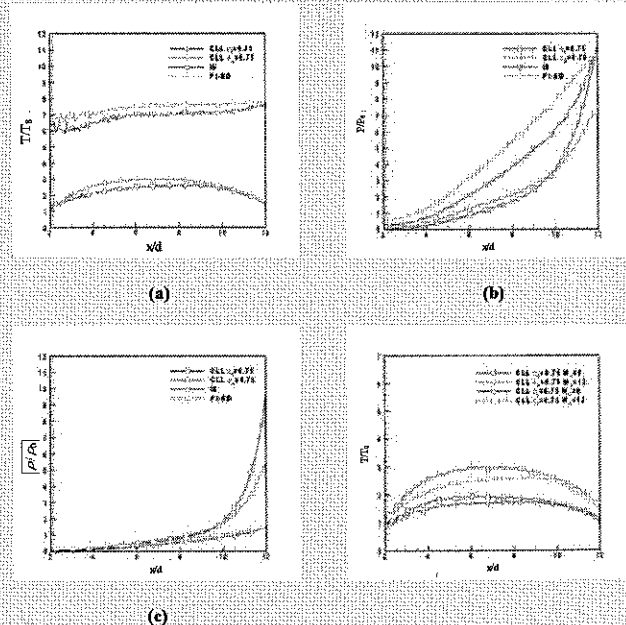


Figure 4. M_∞=12, Kn=0.95, comparisons of normalized flow properties distribution at bottom of cavity with different surface boundary models.

Figure 5. M_∞=8 and 12, Kn=0.95, normalized temperature distribution at bottom of cavity with CLL models.

Conclusions

- Gas surface interaction models influence overall flow field significantly in shallow cavity problem. Generally, they affect more on temperature and pressure, less on density.
- Adiabatic boundary conditions, such as IS and Pt-SD, result in more uniform and higher temperature distribution than that in CLL boundary.
- On CLL model, normal momentum accommodation coefficient (NMAC) influences temperature distribution more significantly than tangential momentum accommodation coefficient (TMAC).

Acknowledgments

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Study of Hypersonic Rarefied Gas Flow over Shallow Cavity by DSMC Method

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Abstract

In this study, rarefied gas flow over the optical window of a high-speed interceptor was simplified and investigated numerically as a two-dimensional rectangular cavity flow. With a high altitude rarefied flow field, the traditional computational method for solving the Navier-Stokes equation is inappropriate. The Direct Simulation Monte Carlo (DSMC) method is hence adopted to implement the investigation of the rarefied gases problem. Improved DSMC techniques and suitable gas-surface interaction models for solid boundary conditions were employed. Proper initial conditions were specified in which hypersonic flow went through a forebody with a wedge shape. Shallow cavity flow fields with varying altitudes and flight speeds are then examined. The length-to-depth ratio of the shallow cavity is fixed. The major concerns are the effects of gas-surface interaction models on simulations of the gas dynamic characteristics of this window system in various flight conditions.

Nomenclature

C	molecular velocity
d	depth of cavity
f_0	equilibrium velocity distribution function
H	altitude
k_B	Boltzmann constant
Kn	Knudsen number
l	length of cavity
M	Mach number
m	molecular mass
R	gas constant
R_f	random number between 0 to 1
T	Temperature
U	incident molecular velocity
U^*	reflection molecular velocity
V_{mp}	molecular most probable thermal velocity
α	accommodation coefficient
β	Reciprocal of the most probable molecular speed in an equilibrium gas
γ	specific heat ratio
δ	deflection wave angle
θ	wedge angle
λ	molecular mean free path
μ	viscosity coefficient

Subscripts

∞	freestream
n	normal direction
t	tangential direction
w	solid wall, surface
$0, 1, 2, 3$	particular value

Introduction

The investigation of hypersonic rarefied gas flow is realistically applicable in aerospace engineering, especially, in the development of high altitude interceptors. The optical viewing window is an important assembly designed for effective target seeking. The window must maintain its optical transparency throughout the operational flight envelope of the vehicle. However, under the conditions of high Mach number and high temperature, the performance of the seeker, which is behind the optical viewing window, is degraded by aerothermodynamic effects. Imprecise detection will result in a faulty mission. For this reason, it is necessary to provide accurate flow field information

In general, the atmosphere is considered as continuum and studied with the Navier-Stokes method. According to Diehl's report[1], however, the density of the atmosphere is less than at sea level as the altitude is over 60 km. The mean free path (λ) of molecules is raised to 3×10^{-4} m. Moreover, at altitudes higher than 100 km, the pressure decreases to 10^{-7} atm and λ of 4.7×10^{-1} m is reached. Under these rarefied conditions, viewing atmosphere as a continuum is not appropriate. The classical continuum model should be replaced by a molecular model. Direct simulation Monte Carlo (DSMC) is one of the most widely used molecular approaches in studying rarefied gas flow. Therefore, the DSMC method is adopted here to study hypersonic rarefied gas flow.

Kogan[2] is one of the previous investigators of hypersonic rarefied gas flow. Bütetisch and Vennemann[3] studied hypersonic rarefied flow by means of the electron beam technique. It was not until Bergemann[4], who investigated near continuum hypersonic flow by gas kinetic simulation and considered wall-catalysis, that gas-surface interaction was reconsidered as a hypersonic rarefied flow. In 1998, Ivanov and Gimelshein[5] mentioned that the interaction of gas particles with the surface is one of the major difficulties in hypersonic rarefied gas dynamic problems. Gas-surface interaction models influence flow parameters substantially as the rarefaction of gas increases.

In this study, the flow field of a high-speed interceptor is divided into two parts. The first is a hypersonic wedge flow and the other is a shallow cavity flow. In a wedge flow, the simulation results are compared with theoretical compressible gas dynamics. Also, the flow parameters behind the oblique shock in wedge flow simulation results are set as the initial conditions for shallow cavity flow. Following Cercignani, Lampis, and Lord[6](CLL), isotropic scattering (IS), and partial specular partial diffuse (Pt-SD) gas

surface interaction models are studied in specifying boundary conditions for this rarefied gas flow problem.

Problem Description

In the forebody of a high speed interceptor, as in Figure 1, a hypersonic free stream passes through the wedged leading edge and forms a shock in the flow field. Behind the shock, the pressure, temperature, and density of flow rise immediately. In addition, the flow velocity is slowed and the flow changes direction to follow the wedged surface.

Because of high temperature and varying density near the surface, the performance of the interceptor's target seeking could be degraded. Obtaining more accurate flow field information would be useful for this engineering problem.

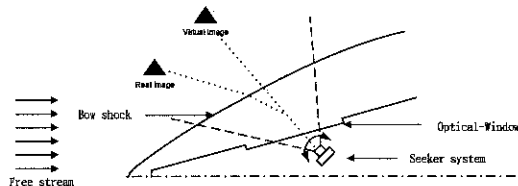


Figure 1 Schematic diagram of hypersonic flow over an optical window.

The hypersonic rarefied flow problem is interesting and attracts many researchers. In 1984, Moss and Bird [7] studied hypersonic reentry using DSMC at an altitude range of 92 to 150 km. Their results were in good agreement with continuum predictions at low altitude. However, rarefaction and slip effects rapidly departed from continuum predictions and DSMC results. In 1998, Riabov[8] studied hypersonic rarefied gas flow with several simple shapes using DSMC. Riabov's results showed that under low Reynolds number conditions, the influences of specific heat ratios (γ), viscosity parameters ($\mu \sim T^n$), and freestream Mach numbers (M_∞) are significant. Riabov[9] investigated hypersonic gas flow near two side-by-side plates and discussed the geometric factor and Knudsen number (Kn) effects on lift and drag. The Kn in Riabov's research ranged from 0.024 to 1.8. At the same time, Riabov[10] studied side-by-side cylinders under similar conditions.

In 2002, Santos and Lewis[11] used DSMC to study hypersonic flows passing through a wedge forebody with different freestream attack angles and wedge shapes at an altitude of 70 km. In 2003, Santos[12] studied the pressure and heat transfer coefficients under similar conditions and Santos[13] also investigated flat nose influence on heat transfer in a hypersonic wedge flow. In 2004, Santos[14] extended his research to gas surface interactions in a hypersonic wedge flow. In 2008, Padilla[15] studied gas surface interactions with hypersonic reentry problems. In 2010, Sampaio and Santos[16] studied reentry satellites at different altitudes and discussed pressure, heat transfer, and drag on the satellite.

In hypersonic cavity flow, Blair[17] investigated cavity flow with different length to depth ratios (l/d) and classified cavity flow by length to depth ratio to opened ($l/d < 10$) and closed ($10 < l/d < 13$) cavities. In Blair's research, he mentioned that as hypersonic flow passes through a closed cavity, there is an expansion wave in the leading side and a free shear layer impinging on the cavity's bottom wall. Moreover, Roshko[18] studied closed cavities and mentioned that a free shear layer will attach to cavity bottom then form two vortices on both sides. Heller et al[19]

studied cavity flow with a wind tunnel and discussed the pressure oscillations that occurred in different locations on the cavity bottom. East[20] did experiments similar to Heller's and found that oscillations in the cavity can be related to the acoustic depth mode. Tai and Lee[21] investigated cavity flow using cooling injections and solving Navier-Stokes equations. Lamp and Chokani[22] studied cavity flow numerically using the Navier-Stokes scheme. In Lamp's research, a small jet was used to force the shear layer with different amplitudes and frequencies.

In this study, hypersonic wedge flow has been investigated at altitudes ranging from 85 to 100 km and the deflection of oblique shock wave angles were compared with theoretical compressible gas flows. Different gas-surface interaction models for specifying solid boundary conditions were compared in this rarefied gas cavity flow. The initial conditions for cavity flow calculations were obtained from the simulation results of the wedge flow.

Numerical Method

As mentioned in the previous section, in this study, DSMC is chosen as the simulation method. Bird [23] proposed the DSMC method for studying shock. Then DSMC was applied to the investigation of dilute gas[24]. In 1994, Bird[25] wrote a book to introduce the DSMC method integrally. The DSMC method used a statistical method to solve the Boltzmann equation. In this method, the gas velocity distribution function is the most important for flow macroscopic properties. For the equilibrium state, it can be shown as in equation (1)—the so-called Maxwellian distribution function.

$$f_0 = \left(\frac{\beta^3}{\pi^2}\right) \exp(-\beta^2 C^2) \quad (1)$$

$$\beta = \frac{1}{\sqrt{2RT}} = \sqrt{\frac{m}{2k_B T}}$$

All flow properties—momentum, energy, density, and pressure—are related to the integral of the distribution function. Besides, the DSMC method simulates real gas flows with simulation particles, with each of the particles representing a great number of real gas molecules. Several physical procedures such as move, collision, indexing, and sampling gather flow properties from simulation particles. The gas-surface interaction is in the "move" procedure in DSMC. Heat flux and momentum flux between gas particles and body surface were simulated by proper gas surface interaction model.

Maxwell[26] proposed the models for gas surface interaction in 1879. In Maxwell's research, gas particles incident to the surface reflect from the surface in two ways. One is specular reflection and the other is diffuse reflection. In specular reflection, incident molecules preserve their tangential velocity unchanged. However, their normal velocity gets an equal magnitude with opposite direction. The reflection molecules' velocity can be written as equation (2).

$$\begin{aligned} U_n^* &= -U_n \\ U_{t1}^* &= U_{t1} \\ U_{t2}^* &= U_{t2} \end{aligned} \quad (2)$$

In equation (2), U and U^* are, respectively, the incident and reflection velocities. The subscripts n and t represent the normal and tangential directions of the surface. For diffuse reflection, the reflected velocity is shown as equation (3).

$$\begin{aligned}
U_n^* &= -|V_{mp}| \cdot (-\ln R_{f1})^{1/2} \\
U_{t1}^* &= |V_{mp}| \cdot (-\ln R_{f2})^{1/2} \cdot \sin(2\pi R_{f3}) \\
U_{t2}^* &= |V_{mp}| \cdot (-\ln R_{f2})^{1/2} \cdot \cos(2\pi R_{f3})
\end{aligned} \quad (3)$$

In Eq. (3), V_{mp} is the thermal velocity with the greatest probability, and which is dependent on surface temperature. R_f is a random number and its range is between 0 and 1. Maxwell also proposed that when gas molecules incident into a surface, a portion of the molecules are reflected diffusely and the others are specular. That can be written as α fraction reflected specularly and $(1-\alpha)$ fraction reflected diffusely. This concept has been widely adopted in the study of kinetic gas flow and implemented in the DSMC method for several decades. In 1971, Cercignani and Lampis [27] proposed a gas surface interaction (CL) model. In their research, predicted reflection molecule angles agreed well with electron beam experiments. Lord [6, 28] successfully integrated the CL model with the DSMC method and it is now referred to as the CLL model. The normal and tangential components of reflection velocity in the CLL model can be written as equations (4) and (5).

$$U_n^* = -|V_{mp}| \cdot \left(R_n^2 + (1-\alpha_n) \cdot \left(\frac{U_n}{V_{mp}} \right)^2 + 2 \cdot R_n \cdot (1-\alpha_n)^{1/2} \cdot \left(\frac{U_n}{V_{mp}} \right) \cos(2\pi R_{f2}) \right)^{1/2} \quad (4)$$

$$R_n = (-\alpha_n \ln R_{f1})^{1/2}$$

In equation (4), normal reflection velocity is dependent upon normal momentum accommodation α_n and pre-collision normal velocity U_n . As $\alpha_n = 1$, the normal reflection velocity is the same as the diffuse one.

$$\begin{aligned}
U_{t1}^* &= |V_{mp}| \cdot \left(U_{t1}^* \Big|_{ang} \cos(\text{angle}) - U_{t2}^* \Big|_{ang} \sin(\text{angle}) \right) \\
U_{t2}^* &= |V_{mp}| \cdot \left(U_{t1}^* \Big|_{ang} \sin(\text{angle}) + U_{t2}^* \Big|_{ang} \cos(\text{angle}) \right) \\
U_{t1}^* \Big|_{ang} &= R_t \cdot \cos(2\pi R_{f4}) + (1-\alpha_t)^{1/2} \cdot \frac{(U_{t1}^2 + U_{t2}^2)^{1/2}}{V_{mp}} \\
U_{t2}^* \Big|_{ang} &= R_t \cdot \sin(2\pi R_{f4}) \\
R_t &= (-\alpha_t \ln R_{f3})^{1/2}, \quad \alpha_t = \sigma_t (2 - \sigma_t) \\
\text{angle} &= \arctan \left(\frac{U_{t2}}{U_{t1}} \right)
\end{aligned} \quad (5)$$

Similarly, tangential reflection velocity along the interaction plane, $U_{t1}^* \Big|_{ang}$ and $U_{t2}^* \Big|_{ang}$ also depend on tangential momentum accommodation σ_t and pre-collision tangential velocity U_{t1} and U_{t2} . When $\sigma_t = 1$, tangential reflection velocity along the interaction plane is equal to that in the diffuse model. As shown in equation (5), the difference is that tangential reflection velocity U_{t1}^* and U_{t2}^* are related to the angle of interaction plane.

Tzeng et al [29] proposed a novel gas surface interaction model to modify the adiabatic solid boundary and investigate instability phenomena in a two-dimensional RB convection. In their reflection rule, the normal reflection velocity is unchanged in magnitude and direction, which is opposite to the pre-collision one. Then the

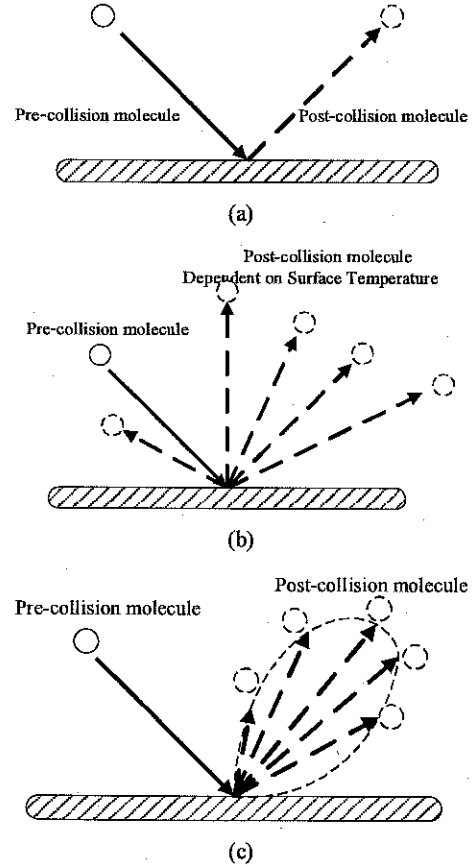
tangential velocity is dependent on the conservation of energy. This Pt-SD model is shown in equation (6).

$$\begin{aligned}
U_n^* &= -U_n \\
U_{t1}^* &= \left(|C|^2 - |U_n|^2 \right)^{1/2} \cdot \sin(2\pi R_f) \\
U_{t2}^* &= \left(|C|^2 - |U_n|^2 \right)^{1/2} \cdot \cos(2\pi R_f) \\
|C| &= \left(U_n^2 + U_{t1}^2 + U_{t2}^2 \right)^{1/2}
\end{aligned} \quad (6)$$

In equation (6), the normal velocity reverses but the two velocity components tangential to the wall, U_{t1}^* and U_{t2}^* , reflect randomly. Recently, Tzeng et al [30] proposed an improvement of the gas surface collision rule for adiabatic walls, the IS model. The reflection molecule's velocity can be written as equation (7).

$$\begin{aligned}
U_n^* &= -|C| \cdot R_{f1}^{1/2} \\
U_{t1}^* &= |C| \cdot (1-R_{f1})^{1/2} \cdot \sin(2\pi R_{f2}) \\
U_{t2}^* &= |C| \cdot (1-R_{f1})^{1/2} \cdot \cos(2\pi R_{f2}) \\
|C| &= \left(U_n^2 + U_{t1}^2 + U_{t2}^2 \right)^{1/2}
\end{aligned} \quad (7)$$

Figure 2 shows four different gas surface interaction models. In this research, several different gas surface interaction models were studied in cavity flows.



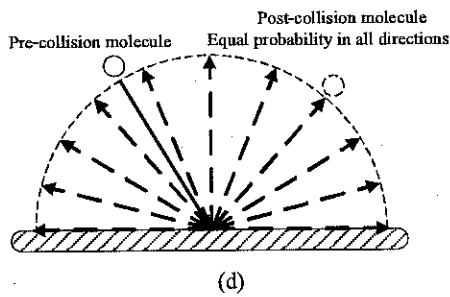


Figure 2. Gas-surface interaction models. (a) specular reflection, (b) diffuse reflection, (c) CLL model, and (d) isotropic scattering (IS).

Results and discussions

In this study, the collisions between molecules are simulated by using the variable hard sphere (VHS) molecular model. In addition, this study adopted the modified no time counter (MNTC) [31] and sampling technique. The geometry of the wedge body is shown in Figure 3.

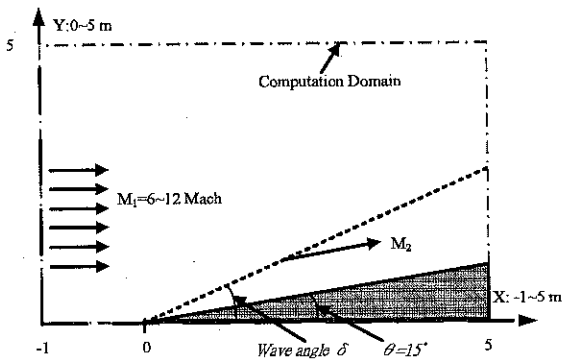


Figure 3 Geometry and computation domain of hypersonic wedge flow.

According to compressible gas dynamics, the wave angle can be related to the wedge angle by equation (8).

$$\tan \theta = 2 \cot \delta \left[\frac{M_1^2 \sin^2 \delta - 1}{M_1^2 (\gamma + \cos 2\delta) + 2} \right], \text{ when } \theta < \theta_{\max} \quad (8)$$

In equation (8), M_1 is the flow velocity in front of the oblique shock. The simulation conditions in the hypersonic wedge flow are shown as

Table 1. The Freestream Mach number (M_∞) is 12, and diffuse reflection (full accommodation) is used as the gas-surface interaction model in this wedge flow portion. Also, Freestream Mach numbers from 6 to 12 are also investigated at an altitude of 90 km.

H (km)	Temperature (K)	Speed of sound (m/s)	Number density	Mean free path λ (m)
85	188.84	2.75E+02	1.71E+20	9.88E-03
90	186.87	2.74E+02	7.12E+19	2.37E-02
95	188.42	2.75E+02	2.92E+19	5.79E-02
100	195.08	2.80E+02	1.19E+19	1.42E-01

Table 1 Wedge flow simulation conditions.

Table 2 shows the computation results with freestream Mach 12 at various altitudes. The simulation results show that wave angles rapidly depart from theoretical ones as the altitude increases. At

high altitude, the number density of gas molecules decreases and the molecular mean free path increases. Under this rarefied condition, the interaction between gas particles and the surface is much less than that at lower altitudes. Theoretical results were based on continuum assumptions. However, as the altitude increased, the state of the gas flow is far from the continuum. The rarefied effect strongly influences flow properties.

H (km)	M_1	T_1 (K)	Theoretical			Simulation results		
			δ (degree)	M_2	T_2 (K)	δ (degree)	M_2	T_2 (K)
85	12	188.8	21.4	5.65	760.8	22.2	5.26	849.2
90	12	186.9	21.4	5.65	752.9	23.4	5.26	850.3
95	12	188.4	21.4	5.65	759.1	25.5	5.31	842.0
100	12	195.1	21.4	5.65	786.0	29.2	5.33	868.4

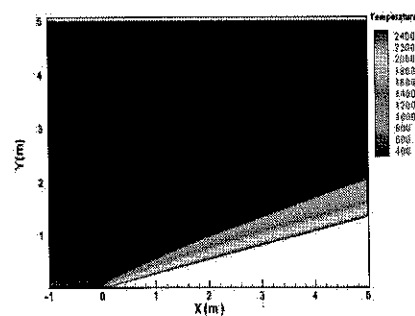
Table 2 Wedge flow simulation results at various altitudes.

In Table 3, different freestream Mach numbers are investigated at an altitude of 90 km. The shock wave angles in these computations are larger than the theoretical values. In addition, the temperatures behind the shock waves are also higher than the theoretical results.

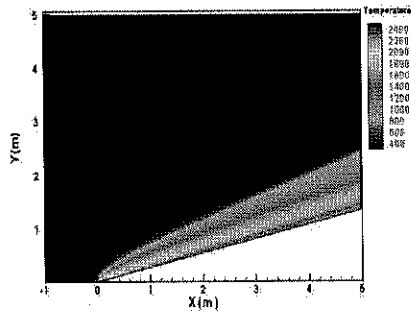
H (km)	M_1	T_1 (K)	Theoretical			Simulation results		
			δ (degree)	M_2	T_2 (K)	δ (degree)	M_2	T_2
12	186.9	21.4	5.65	752.9	23.4	5.26	850.3	
90	10	186.9	21.9	5.28	596.1	23.9	5.03	646.4
8	186.9	22.8	4.75	469.0	25.4	4.64	483.8	
6	186.9	24.6	3.99	366.3	27.3	3.83	387.3	

Table 3 Wedge flow simulation results with different freestream Mach numbers at an altitude of 90 km.

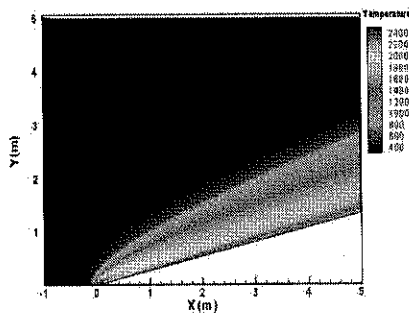
Figure 4 presents temperature contours at different altitudes. With the same freestream Mach number, the oblique shock wave angle increases as the altitude increases. At high altitudes, the molecule mean free path increases, which means that Kn increases with altitude and the rarefied effect is much more significant than at lower altitudes.



(a)



(b)



(c)

Figure 4 Hypersonic wedge flow temperature contours at different altitudes. (a) 85 km, (b) 95 km, and (c) 100 km.

In the cavity flow studies, simulation results from hypersonic wedge flow at 90 km are used to set the initial conditions. Figure 5 shows a shallow cavity diagram. The length to depth ratio (l/d) is fixed at 10 in this computation. The freestream Mach numbers are 8 and 12 in the wedge flow study. Three different gas surface interaction models are investigated. Figure 6 shows the normalized temperature contour in a hypersonic shallow cavity flow. The temperature distributions are obviously different with each gas surface interaction model. In isotropic scattering and Pt-SD boundary conditions, high temperatures are located near the cavity bottom. With the CLL model as the surface boundary condition, the high temperature region is close to the trailing edge of the cavity. This result indicates that the gas-surface interaction model obviously influences flow properties.

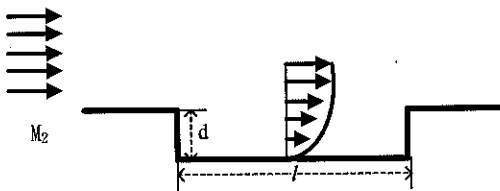
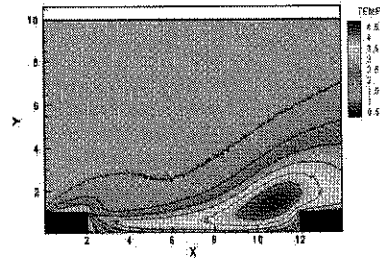
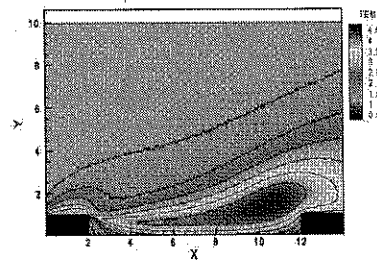


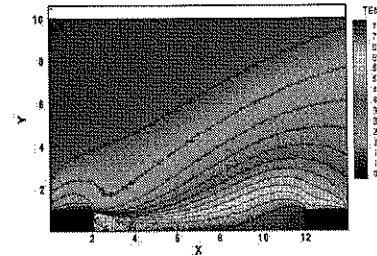
Figure 5 Schematic diagram of hypersonic shallow cavity flow.



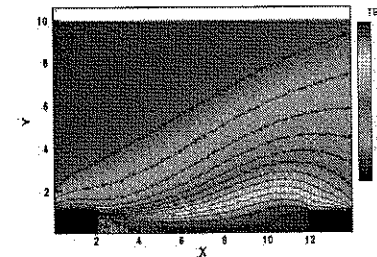
(a)



(b)



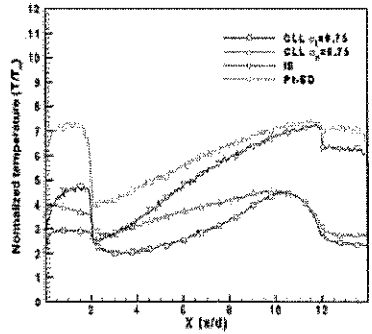
(c)



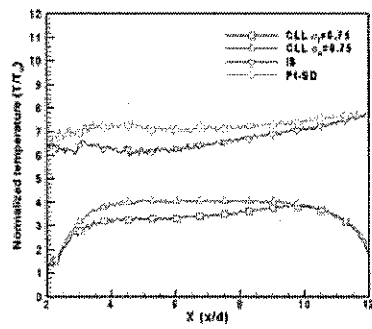
(d)

Figure 6 $M_\infty = 12$, normalized temperature contour in hypersonic shallow cavity flow. (a) CLL ($\sigma_n = 0.75$), (b) CLL ($\sigma_n = 0.75$), (c) IS, and (d) Pt-SD.

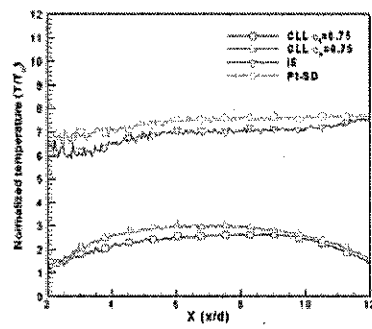
Figure 7 and Figure 8 show the temperature and pressure distribution, respectively, along the top, middle and bottom levels of a cavity with different surface boundary models. The results indicate that with Pt-SD and IS boundaries, the temperature and pressure of the flow are higher than within the CLL boundary. Also, there is a low pressure and low temperature region in the front side of the cavity. This is due to hypersonic flow passing through the cavity and expanding in the leading part of the cavity.



(a)

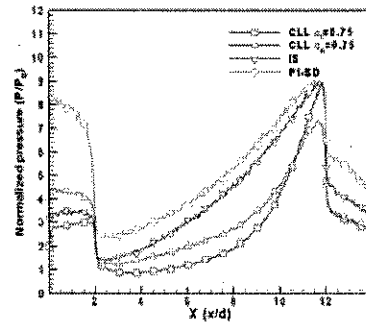


(b)

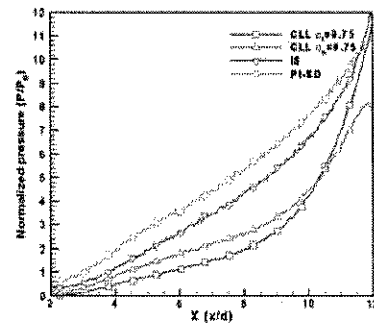


(c)

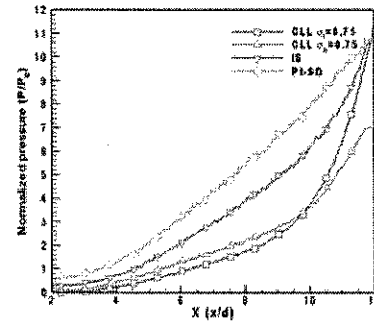
Figure 7 $M_\infty = 12$, comparisons of normalized temperature distribution at (a) top, (b) middle, and (c) bottom of cavity with different surface boundary models.



(a)



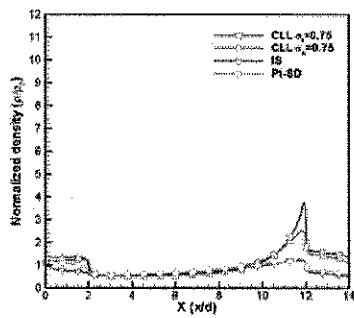
(b)



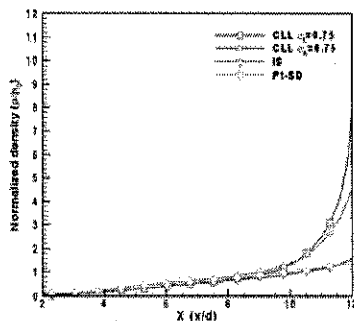
(c)

Figure 8 $M_\infty = 12$, comparisons of normalized pressure distribution at (a) top, (b) middle, and (c) bottom of cavity with different surface boundary models.

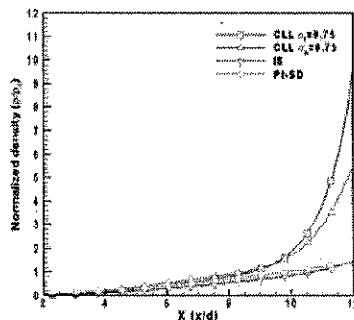
Figure 9 shows the density distribution with different boundary conditions. The density distributions are less influenced by various surface models. Figure 10 shows different freestream Mach numbers with various accommodation coefficients in the CLL model. The results indicate that normal momentum accommodation coefficients influence temperature distribution more significantly than tangential momentum accommodation coefficients.



(a)

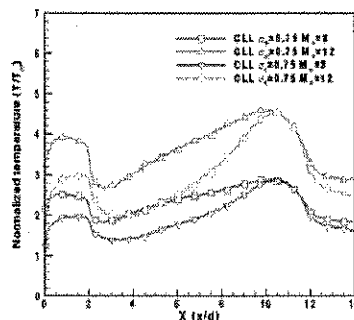


(b)

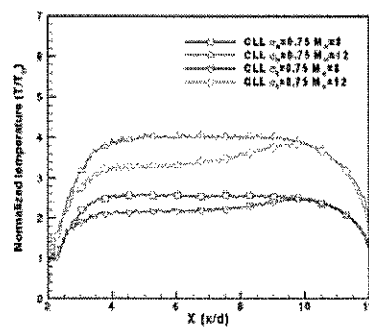


(c)

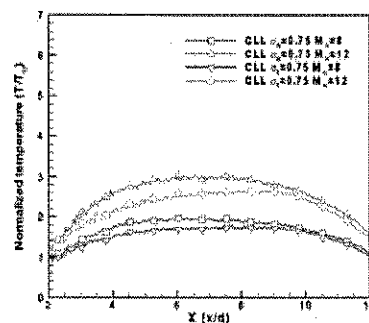
Figure 9 $M_\infty = 12$, comparisons of normalized density distribution at (a) top, (b) middle, and (c) bottom of cavity with different surface boundary models.



(a)



(b)



(c)

Figure 10 $M_\infty = 8$ and 12 , comparisons of normalized temperature distribution at (a) top, (b) middle, and (c) bottom of cavity with CLL models.

Conclusions

In this study, hypersonic rarefied gas passing through a wedge body simulated by DSMC is compared with theoretical results. The simulation results are used to set initial flow conditions on shallow cavity problems. The effects of gas surface interaction models are investigated in a hypersonic cavity flow and some conclusions are obtained:

1. In a hypersonic wedge flow, the deflected shock angles are greater than the theoretical ones, especially, at high altitude. This can be attributed to rarefaction effect.
2. Gas-surface interaction models influence overall flow fields significantly in shallow cavity problems.
3. Adiabatic boundary conditions, such as IS and Pt-SD, result in more uniform and higher temperature distribution than that in CLL boundary conditions.
4. Gas-surface interaction has a minor influence on density distribution in cavity flow studies. This is due to gas-surface interaction having a dominant effect on molecular velocity distribution function that affects momentum and heat flux more and influences mass flux less.

Acknowledgments

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References

- [1] Diehl, W.S., *National Oceanic and Atmospheric Administration*. US Air Force(GPO, Washington, DC).1976.
- [2] Kogan, M., On Hypersonic Rarefied Gas Flows. *Prikl. Matem. i Mekhan.* **26**, 1962.
- [3] Bütetfisch, K. and Vennemann, D., The Electron-Beam Technique in Hypersonic Rarefied Gas Dynamics. *Progress in Aerospace Sciences.* **15**, 1974, 217-255.
- [4] Bergemann, F., Gaskinetic Simulation of Near-Continuum Hypersonic Flow with Consideration of Wall-Catalysis. *Cologne, Germany.* 1994.
- [5] Ivanov, M. and Gimelshein, S., Computational Hypersonic Rarefied Flows. *Annual Review of Fluid Mechanics.* **30**, 1998, 469-505.
- [6] Lord, R.G., Some Extensions to the Cercignani-Lampis Gas-Surface Scattering Kernel. *Physics of Fluids A: Fluid Dynamics.* **3**, 1991, 706-710.
- [7] Moss, J. and Bird, G., Direct Simulation of Transitional Flow for Hypersonic Reentry Conditions. in *American Institute of Aeronautics and Astronautics, Aerospace Sciences Meeting.* 1984. 22nd, Reno, NV; United States.
- [8] Riabov, V.V., Comparative Similarity Analysis of Hypersonic Rarefied Gas Flows near Simple-Shape Bodies. *Journal of Spacecraft and Rockets.* **35**, 1998, 424-433.
- [9] Riabov, V.V., Aerodynamics of Two Side-by-Side Plates in Hypersonic Rarefied-Gas Flows. *Journal of Spacecraft and Rockets.* **39**, 2002, 910-916.
- [10] Riabov, V.V., Interference between Two Side-by-Side Cylinders in Hypersonic Rarefied-Gas Flows. *AIAA Paper.* **3297**, 2002, 1-9.
- [11] Santos, W.F.N. and Lewis, M.J., Angle of Attack Effect on Rarefied Hypersonic Flow over Power Law Shaped Leading Edges. in *23rd International Symposium on Rarefied Gas Dynamics.* 2002.
- [12] Santos, W.F.N., Compressibility Effects on Flowfield Structure of Truncated Wedges in Low-Density Hypersonic Flow. in *17th International Congress of Mechanical Engineering.* 2003.
- [13] Santos, W.F.N., Aerothermodynamic Characteristics of Flat-Nose Power-Law Bodies in Low-Density Hypersonic Flow. in *22nd Applied Aerodynamics Conference and Exhibit.* 2004.
- [14] Santos, W.F.N., The Effect of Incomplete Surface Accommodation on Heat Transfer and Drag of Truncated Wedge in Rarefied Regime. in *3rd Brazilian Congress of Mechanical.* 2004.
- [15] Padilla, J.F., *Assessment of Gas-Surface Interaction Models for Computation of Rarefied Hypersonic Flows*, Ph.D Thesis, University of Michigan, 2008.
- [16] Sampaio, P.A.C. and Santos, W.F.N., Computational Analysis of the Aerodynamic Heating and Drag of a Reentry Brazilian Satellite. in *6th National Congress of Mechanical Engineering.* 2010.
- [17] Blair, A.B., Cavity Door Effects on Aerodynamic Loads of Stores Separating from Cavities. *Journal of Aircraft.* **26**, 1989, 615-620.
- [18] Roshko, A., Some Measurements of Flow in a Rectangular Cutout. 1955, DTIC Document.
- [19] Heller, H.H., Holmes, D.G., and Covert, E.E., Flow-Induced Pressure Oscillations in Shallow Cavities. *Journal of Sound and Vibration.* **18**, 1971, 545-553.
- [20] East, L.F., Aerodynamically Induced Resonance in Rectangular Cavities. *Journal of Sound and Vibration.* **3**, 1966, 277-287.
- [21] Tai, C.H. and Lee, Y.K., Nonreactive Viscous Solver for Hypersonic Flows over Recessed Cone with Injection. *Journal of Spacecraft and Rockets.* **32**, 1995, 24-31.
- [22] Lamp, A.M. and Chokani, N., Computation of Cavity Flows with Suppression Using Jet Blowing. *Journal of Aircraft.* **34**, 1997, 545-551.
- [23] Bird, G.A., Approach to Translational Equilibrium in a Rigid Sphere Gas. *Physics of Fluids.* **6**, 1963, 1518-1519.
- [24] Bird, G., Direct Simulation and the Boltzmann Equation. *Physics of Fluids.* **13**, 1970, 2676-2681.
- [25] Bird, G.A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford University Press.1994.
- [26] Maxwell, J.C., On Stresses in Rarefied Gases Arising from Inequalities of Temperature. *Philosophical Transactions of the Royal Society of London.* **170**, 1879, 231-256.
- [27] Cercignani, C. and Lampis, M., Kinetic Models for Gas-Surface Interactions. *Transport Theory and Statistical Physics.* **1**, 1971, 101-114.
- [28] Lord, R.G., Some Further Extensions of the Cercignani-Lampis Gas-Surface Interaction Model. *Physics of Fluids.* **7**, 1995, 1159-1161.
- [29] Tzeng, P.Y., Soong, C. Y., Liu, M. H., Yen, T. H., Atomistic Simulation of Rarefied Gas Natural Convection in a Finite Enclosure Using a Novel Wall-Fluid Molecular Collision Rule for Adiabatic Solid Walls. *International Journal of Heat and Mass Transfer.* **51**, 2008, 445-456.
- [30] Tzeng, P.Y., Chou, I.W., Liu, C.H., and Li, W.K., Improvement of the Gas-Surface Collision Rule for Adiabatic Walls in DSMC Modeling of Rarefied Gas Convection in a Micro Enclosure. *Journal of Aeronautics, Astronautics and Aviation, Series A.* **43**, 2011, 147-158.
- [31] Bird, G.A., Sophisticated DSMC, in *DSMC07 meeting*, Santa Fe, 2007.