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摘要

自 2007 年起開始 2 年舉辦 1 次的「亞洲計算熱傳與流力研討會」至今爲第三屆。該研討會宗旨在提供亞洲地區的學術或工程研究人員，交流各自領域中計算熱傳與流體力學方面的研究結果，舉凡理論、分析及應用等各方面均爲該研討會討論的議題。議程豐富以 8 個主題略分爲 19 個不同科技議題共 24 場次，每個場次約有 4~6 篇論文由報告人分享其研究成果。除邀請 10 位知名專家學者專題演講外，來自 11 個國家共有 123 篇論文以 20 分鐘口頭報告方式發表。本人所提之論文於 9 月 23 日下午進行報告與討論。與在場的大阪府立大學副教授 Dr. Masayuki Kaneda 和英國科技設備委員會(STFC)學者 Dr. Emerson 教授等有相當熱烈的問答交流與激盪，獲益甚多。本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瞭解計算熱流領域的現況與發展趨勢。並聽取與會學者們提出的論點以及相互研討，吸收新知開闊視野，對個人及研究團隊未來於熱傳和流力領域之研究與教學均有助益。

一、目的

1. 發表研究成果。
2. 與國際學者進行學術交流。

二、過程

1. 第三屆亞洲熱傳與流體力學研討會於 2011 年 9 月 22 日至 26 日在日本京都府的京都大學百週年時計台紀念館舉行。該研討會是以提供亞洲地區的學術或工程研究人員進行各自領域中計算熱傳與流體力學方面的研究結果交流爲宗旨。舉凡理論、分析及應用等各方面學術交流，均爲該研討會邀請對象。本次研討會由日本熱傳學會(The Heat Transfer Society of Japan, HTSJ)主辦，國際熱質傳中心(International Centre for Heat and Mass Transfer, ICHMT)及京都大學能源科學計畫協辦。
2. 該研討會議程豐富計有 8 個主題 10 場次邀請專家發表與討論，約有 123 篇論文以 口頭報告方式發表。略分爲 19 個不同科技議題(Technical Session)：Environmental and Radiative Heat Transfer, Optimization and Control Methods, Micro/Nano and Rarefied Flows, Turbulent Heat Transfer, Multiphase Flows, Lattice Boltzmann Simulations, Flows with Phase Changes, Molecular Dynamics Simulations, Turbulent Flows, Numerical Schemes, Simulations of Complex Phenomena, Natural and Mixed Convection, Interface and Boundary Capturing Schemes, Conductive and Conjugate Heat Transfer, Engineering Applications, Flows with Chemical Reactions, Acoustics and Others, Bio Fluid Dynamics,及 Heat Exchangers 等重要領域。
3. 本人所提報之論文於 9 月 23 日下午 14 點 30 分至 14 點 50 分由博士班研究生林宗漢進行口頭報告與討論。與在場的日本學者 Dr. Masayuki Kaneda 副教授和英國科技設備委員會(STFC)專家 Dr. Emerson 教授等有相當熱烈的問答交流與激盪，獲益甚多。

三、心得及建議

1. 本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瞭解計算熱流領域的現況與發展趨勢，和本研究團隊同屬微奈米稀薄流及分子動力模擬領域的共有十餘篇論文發表。藉此機會聽取與會學者們提出的論點以及相互的研討，吸收新知開闊視野，對個人及研究團隊之研究與教學均有助益。
2. 研討會期間，也曾與英國受邀學者，科技設備委員會的 Emerson 教授以及多位日本本地與韓國學者進行學術討論；此外在研討會期間與來自國內清大林昭安、李雄略、交大陳俊勳、中央曾重仁、華梵李弘毅、逢甲宋齊有、虎尾科大蔡永利、鄭仁杰、台南大學顏維謀及成大張克勤、黃正弘等多位教授們晤談甚歡，對亞洲各國學界在計算熱流的研究現況與發展遠景，有新的認識和樂觀的看法。國內熱流相關的理論與應用研究在學界同仁們辛勤耕耘之下，在此國際學術會議上獲得相當程度的肯定，但仍須繼續投注更多資源與心力積極增加參與度以提升國際學術地位。

四、附件

參加該研討會照片及投稿論文資料。

報告會場與 Emerson 教授合影

與參加本會議的國內學者合影

Paper ID: #001

A Numerical Study on Rarefied Gas Natural Convection in 3-D Enclosure by DSMC Method

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Abstract

In this research, we investigate the Rayleigh-Bénard (RB) problem of rarefied gas flows in horizontal rectangular micro-enclosures by using Direct Simulation Monte Carlo (DSMC) method. Major concerns are the effects of rarefaction and side wall boundary conditions. In DSMC simulations of Rayleigh-Bénard convection, specular reflection conditions are usually specified for lateral side boundaries. However, the real enclosure is bounded by solid walls. The present work is thus also aimed to apply an improved gas-surface collision rule for modeling adiabatic wall condition. This gas-surface interaction model keeps the particle velocity magnitude invariant and the velocity direction of the reflected particle is set based on isotropic scattering uniform distribution in the half space. This boundary treatment is physically more reasonable for description of reflected molecules at adiabatic solid surface. From effective DSMC calculation and numerical visualization, insight into the influences of rarefaction and side wall boundary conditions on this classical problem can be obtained.

1. Introduction

Natural convection phenomena happens in our daily life. For example, climate and ocean current, are resulted from natural convection. Rayleigh-Bénard (RB) convection, a classical problem in fluid dynamics, is one kind of natural convection, too. The fluid is between two horizontal plates and heated from the bottom. The fluid transforms from pure conduction state to convection state as the temperature gradient reaches its critical value. Rayleigh [1] used Boussinesq approximation to analyze Bénard's [2] experiments. In the experiments, a thin layer of fluid was heated uniformly from a metal plate below it. Then the fluid transformed to convection state. So it is called Rayleigh-Bénard convection problem. There are a lot of researches adapted continuum model to investigate RB convection. In Koschmieder's book [3], Jeffreys was the first one to study RB problem with two rigid boundaries on both top and bottom walls.

This thermal driven flow was discussed widely in one centenary. Studying RB convection had many important results [4]~[8], in large scale regime. However, using molecular model to study RB problem began in 1980's. Molecular dynamics (MD) simulation [9,10] and direct simulation Monte Carlo (DSMC) [11,12] are commonly used methods in numerical simulation studying fluid behavior. In these two simulation tools, MD simulation is often used for dense fluids or liquids, such as water. The computational time in MD simulation is proportional to square of the number of molecules in the fluid system. Time consumption limits the number of molecules in MD simulation. On the other hand, DSMC method is commonly used for studying dilute gas. In DSMC, tremendous amount of real molecules are represented by small amount of simulation particles. Therefore, the number of particles in DSMC is much less than that in MD simulation. Bird [13] proposed DSMC method for studying shock. Then DSMC was applied for investigating dilute gas [14]. In 1990, Garcia [11] used DSMC to study RB convection. It seems to be the first DSMC computation in RB problem .

After Garcia's investigation, Cerciginani and Stefenov [12] studied Bénard instability using the same method, however the definition of Rayleigh number (Ra) were different from each other. Several classical problems, critical Ra , flow patterns and flow instability, are commonly studied. The influence of temperature difference or aspect ratio is often discussed in studying RB convection. Watanabe et al [15] studied critical Ra in two-dimensional RB computation. Their results were in good agreement with which in traditional hydrodynamics. However, Garcia et al [16] had different expression on the results of Watanabe [15]. Garcia pointed out that the boundary condition influence flow in Watanabe's studying. Watanabe and Kaburaki [17] studied RB convection with large aspect ratio in three-dimensional regime. They discussed the flow pattern transformation and got obvious contributions in this three-dimensional simulation. Stefanov et al. [18~20] explored the effects of Knudsen number (Kn) and Froude number (Fr) in two- and three-dimensional RB problem. They discussed this problem systematically and predicted periodic and chaotic attractors.

In this study, a side-walls treatment different from previous study is applied to modify adiabatic rigid wall in three-dimensional RB problem. Rarefied gas is studied in a rectangular enclosure. This treatment is much closer to real adiabatic wall than periodic one. The effects of Kn and temperature ratio are studied.

2. Numerical method

2.1. Rayleigh-Bénard convection in rarefied gas

A number of researchers studied the classical flow instability problem [21~23]. The flow is driven by temperature difference. Ra, a dimensionless parameter, is often considered. In hydrodynamics, Ra represents the product of Gr and Pr. In which, Gr is used for describing the ratio of buoyancy and viscous force. Pr is represented the relation between thermal and kinematical diffusivity. Ra can be shown as follows:

$$Ra = Gr \cdot Pr = \frac{g \Delta T L^3}{\upsilon \alpha} \tag{1}$$

In equation (1), g, L, υ, and α represent gravity, distance between top and bottom boundary, momentum diffusivity coefficient, and thermal diffusivity coefficient, respectively. Besides, ΔT is the temperature difference between top and bottom walls. As the ΔT reaches a critical value, then fluid transforms from conduction state to the convection one. Under this condition, one gets a critical value Ra_c.

Rarefaction of gas is represented by the non-dimension parameter shown as equation (2):

$$Kn \equiv \lambda / L_c \tag{2}$$

In which, $\lambda = 1/\sqrt{2}\pi d^2 n_0$ is the mean free path of molecules. L_C is the characteristic length. The symbol d and n_0 represent radius of molecule and number density, respectively. The larger of Kn, the more significant of Rarefaction effect. According to Bird [24] and Kamiadakis and Beskok [25], fluid flow can be divided into several regimes. Continuum flow ($Kn < 10^{-2}$), slip flow ($10^{-2} < Kn < 10^{-1}$), transition flow ($10^{-1} < Kn < 10$), and free molecule flow ($Kn > 10$). In general, Hydrodynamics studies fluid as continuum, however, this model is not able to describe flow phenomena precisely as the rarefaction effect geting significant. In this study, we adopt molecular model to avoid the break down in continuum one.

Because adopting molecular model, the definition of Rayleigh number (Ra) is different from which in macroscopic. In this investigation, Ra is defined as which in Stefanov et al. [20] proposed.

$$Ra = \frac{2048}{75\pi} \cdot \frac{(1-r_T)}{(1+r_T)^2 \cdot Fr \cdot Kn^2} \tag{3}$$

In equation (3), r_T is temperature ratio between top and bottom walls (T_C / T_H) ; Fr is Froude number, representing the ratio of kinematical and potential energy. Equation (4) shows the definition.

$$Fr = \frac{{V_{th}}^2}{g \cdot L_C} \tag{4}$$

2.2. Adiabatic boundary condition

Garcia et al [16] indicated the neglect boundary effect in Watanabe [15] will influence computation result obviously. Most of researchers adopted Maxwell's [26] gas-surface interaction rule. Even in MD simulation [27], for studying similar RB problem, also used the same rule to simplify model. Maxwell proposed two typical gas-surface interaction. One is specular reflection, another is diffuse reflection. In specular reflection, the tangential velocity keeps unchanged as the gas molecule reflected from surface. However, the normal velocity is as large as pre-collision one in magnitude but opposite in direction when molecule is reflected. For diffuse reflection, reflected molecule's velocity is only depended on surface's temperature. Besides, the direction of reflected molecule is equal probability in all directions. Cercignani and Lampis [28] were the precursors who investigated gas-surface interaction with molecular model. Lord [29,30] applied Cercignani and Lampis' model on DSMC simulation. Follower called this model as CLL model [24].

For simulation RB convection with DSMC method, the boundary condition is commonly treated as diffuse reflection (isothermal) on top and bottom boundaries. Specular reflection (adiabatic) is set in the lateral walls. Table 1 shows the boundary conditions adopted in previous studies. In Table 1, researchers used DSMC to study similar RB problem.

Tzeng et al [31] proposed one adiabatic gas-surface interaction to investigate instability phenomena in two-dimensional RB convection. In their reflection rule, the normal reflect velocity is unchanged in magnitude and direction opposite with pre-collision one. Then tangential velocity is depended on conservation of energy. They applied this reflection rule on the lateral walls. This study improves the reflection rule stated above. This improved reflection rule is based on energy conservation. Besides, the reflected velocity is equal probability in all directions. The purpose is to assimilate a uniform roughness surface. This treatment is much closer to real adiabatic rigid wall than specualr reflection.

2.3. Mathematical formation

DSMC method used statistical mechanism to solve Boltzmann equation. In this method, gas velocity distribution function is the most important for flow macroscopic properties. For equilibrium state, it can be shown as equation (5), so called Maxwellian distribution function.

$$f_0 = \left(\frac{\beta^3}{\pi^{\frac{3}{2}}}\right)\exp(-\beta^2 V^2)$$
$$\beta = \frac{1}{\sqrt{2RT}} = \sqrt{\frac{m}{2kT}} \tag{5}$$

All flow properties, momentum, energy, density, pressure, are related to integral of distribution function. So does the flux between gas and surface.

There are several gas-surface models proposed by previous researchers. However, it adopted diffuse or specular reflection to study rarefied gas in rectangular enclosure convection problem, generally[15,17-20]. It seems necessary to explain the specular and diffuse reflection first. Consider one particle interacts with solid wall. The velocity components along with directions of tangential keep invariable after scattering from solid wall. While normal component of velocity is reversed. It results that particle leaves surface with the same angle of incident and no kinematical energy exchanged. The following equation (6) shows relation of specular reflection.

$$\begin{aligned} V_n' &= -V_n \\ V_{t1}' &= V_{t1} \\ V_{t2}' &= V_{t2} \end{aligned} \tag{6}$$

In equation (6), V' and V are both after collision and pre-collision velocity. The subscript n and t represent the normal and tangential direction of surface. For diffuse reflection interfacial, the reflected velocity is showed as below:

$$\begin{aligned} V_n' &= -\left|V_{mp}\right| \cdot R_{f1}^{1/2} \\ V_{t1}' &= \left|V_{mp}\right| \cdot (1-R_{f1})^{1/2} \cdot \sin(2\pi R_{f2}) \\ V_{t2}' &= \left|V_{mp}\right| \cdot (1-R_{f1})^{1/2} \cdot \cos(2\pi R_{f2}) \end{aligned} \tag{7}$$

V_{mp}, as listed above, is most probability thermal velocity, which depended on interfacial temperature. R_f is a random number and its range is between 0 to 1.

In this literature, we proposed a novel interaction rule to model the adiabatic solid wall with uniform roughness. A real wall shows friction on flow and adiabatic condition leads to no heat flux. The velocity of scattered particle can be prescribed as below:

$$\begin{aligned} V_n' &= -\left|V\right| \cdot R_{f1}^{1/2} \\ V_{t1}' &= \left|V\right| \cdot (1-R_{f1})^{1/2} \cdot \sin(2\pi R_{f2}) \\ V_{t2}' &= \left|V\right| \cdot (1-R_{f1})^{1/2} \cdot \cos(2\pi R_{f2}) \end{aligned} \tag{8}$$

Equation (8) shows the mathematical form for the adiabatic rigid boundary, proposed in this research and applied on lateral walls in three-dimensional RB problem. Physically, it describes the particles through half-sphere with equal probability. The radius of sphere is V. To integrate the probability which particles across surface of the half-sphere is equal to 1. Then transfer coordinate from sphere to Cartesian.

2.4. DSMC method

This study adopts DSMC method, which proposed by Bird [24], for investigating RB convection. DSMC is based on statistics mechanism. It uses statistics to find molecule velocity distribution function. That is equivalence to solve Boltzmann equation. In this method, amount of real molecules are represented by handful of simulation particles. There are several main processes in DSMC simulation. (1) Initialize conditions; (2) Move simulation particles; (3) Give index to identify particles; (4) Select collision pairs; (5) Sample the molecules properties; (6) Represent macroscopic properties by summing particles properties. The novel gas-surface interaction in this research is in process (2). Furthermore, in order to decrease computation time, this study adopts the modified no time counter (M-NTC) to select collision pairs. The M-NTC is proposed by Bird [32], in 2007.

Table 1 Boundary condition for Rarefied gas RB convection.

Author(year)	A	*Kn*	Boundary condition top & bottom	sides
Cercignani and Stefanov (1992) [12]	2, 3	0.01 0.02 0.05	Diff.	SP
Watanabe et al. (1994) [15]	2.016 2.83	0.016	Diff. Semi-Diff. Slip	SP
Watanabe and Kaburaki (1997) [17]	2:2:1~ 8:8:1	0.016	Diff.	SP
Stefanov et al. (2002)[18][19]	2	0.01~ 0.03	Diff.	SP
Stefanov et al. (2007) [20]	1.5:1.5:1 ~ 6:6:1	0.005 0.002 0.02	Diff.	SP
Tzeng et al. (2008) [31]	2.016 4	0.01~ 0.02	Diff.	SP Pt-SD
Present Work	2:2:1	0.01 0.02 0.04	Diff.	IS

*Diff.=diffuse, SP=specular, Pt-SD= partial specular and partial diffuse, IS= isotropic scattering

2.5. Simulation conditions

In this research, hard sphere model is adopted for the collisions between molecules. The temperature ratio between top and bottom wall is from 0.1 to 0.67. Kn number is between 0.01 and 0.04, Fr is fixed at 3. The computation domain $A = L_x/L_z : L_y/L_z : L_z/L_z$ is 2:2:1. Where L_x, L_y, and L_z are the box dimension in coordinate directions. Hereafter we fix A in our study. We should use $A = L_x/L_z = 2$ instead of the longer definition above. Air is considered as simulation molecule. The mass of air molecule is 4.8×10^{-26} kg. Diameter of molecule is 3.7×10^{-10} m. Initial pressure is 20 Pa. The top wall's temperature is fixed in 80 K. Under this situation, the number density is counted as 1.81×10^{22} m^{-3}, and the mean free path of molecule is 9.08×10^{-5} m. The grid is divided into 40x40x20 sampling cells. Each sampling cell is refined by 5x5x5 collision sub-cells. This is for the reason of making the sub-cell smaller than λ_0. The time interval is set as half mean collision time (τ_t), where $\tau_t = \lambda_0 / v_h$ is defined by mean free path and most probability thermal velocity. Mean collision time denotes an average time interval where is no collision occurrence. Besides, $v_h = (2k_B T / m)^{-1/2}$ is depended on bottom wall's temperature. Total simulation particles are 4×10^7. There are ten simulation particles in each sub-cell in computation domain.

3. Results and Discussion

3.1. Verification

Before investigating RB convection, we verified our programs first. In contrasting with Stefanov et al [20] the simulation results are showed in Figure 1. The simulation conditions are $Kn = 0.02$, $Fr = 3$, $r_T = 0.1$. The red line in Figure 1 represents the result of Finite difference (FD), which based on Navier-Stokes equation. And the circle symbol is the DSMC results of Stefanove, in 2007, The triangular symbol is present results. All the properties are in good agreement with previous study not only in quality but also in quantity.

3.2. Rarefaction

In the beginning, we investigate RB convection with different rarefaction conditions. Table 2 shows different simulation conditions with specular sidewalls boundaries. In this section, the lateral walls are set as specular reflection. Two different Kn numbers are studied with various r_T. Figure 2 shows the convection current as $Fr = 3.0$, $Kn = 0.01$, and different r_T. As $r_T = 0.67$, the convection phenomena is hard to find. However, under the condition $r_T = 0.2$, one can see a circular centerline in the slice of computation domain. The centerline denotes vertical velocity equal to zero. In this case, convection current flows down in the center of box, and rises up near sidewalls. As the $r_T = 0.1$, the convection pattern forms a pair of roll. The centerlines parallel to x axis.

Then, Kn number is set as 0.04 with the same sidewalls boundary. Figure 3 shows the convection current and vertical velocity contour on the slice of middle z. The centerlines, under these conditions, form square. Convection current flows down to bottom wall inside of the centerline and rises up from outside.

3.3. Adiabatic rigid lateral walls

Now, the isotropic scattering (IS) boundary condition is applied on lateral walls. Simulation conditions list as Table 3. Similar to previous section, Fr number is fixed at 3 and two different Kn numbers are investigated with various temperature ratio. Under IS boundaries, the convection current seems less easier to form than specular sidewalls. With $Kn = 0.01$, convection pattern is formed as $r_T = 0.1$. However, in the other temperature ratio, $r_T = 0.5$ and $r_T = 0.67$, the convection current is not formed. When $r_T = 0.1$, the convection pattern is a pair of rolls. The centerlines are semi-paralleled to x axis. This result is similar to specular one in the middle of z direction. Nevertheless, the centerlines in IS condition are very different from specular one. Figure 4 and Figure 5 show the vertical velocity contour on middle z and velocity vector distribution for $Kn = 0.01$ with IS boundary.

Under the condition of $Kn = 0.04$, the simulation results are shown as Figure 6. In these convection patterns, square cells, one can find the direction of current rises up in the center but downwards near the lateral boundary. The convection patterns are similar to specular one, but flow direction are opposite with each other. In our study, we get similar convection patterns (roll and cell) that found in macroscopic RB convection.

Table 2 Simulation conditions with Specular sidewalls boundary.

No.	Kn	r_T	Convection mode
1	0.01	0.1	Rolls
2	0.01	0.2	Circular Cell
3	0.01	0.67	No
4	0.04	0.1	Square Cell
5	0.04	0.016	Square Cell
6	0.04	0.005	Square Cell

Table 3 Simulation conditions with Isotropic Scattering sidewalls boundary.

No.	Kn	r_T	Convection mode
1	0.01	0.1	Rolls
2	0.01	0.5	No
3	0.01	0.67	No
4	0.04	0.1	Square Cell
5	0.04	0.05	Square Cell
6	0.04	0.033	Square Cell

4. Conclusions

In the present study, 3-D natural convection of rarefied gas in rectangular enclosure has been investigated numerically. The effects of rarefaction, temperature ratio and side wall boundary condition on the flow pattern are examined. Form the preliminary results obtaind, the following conclusions can be drawn.

(1) RB convection forms square cell under the condition $Kn = 0.04$ both in IS and specular lateral walls. However as $Kn = 0.01$, in specular boundary, the

attractor of convection pattern are different. For r_T =0.1, convection pattern is a pair of rolls which parallel to x axis. For r_T =0.2, the pattern is circular cell. Both of them flow to bottom wall in the center and rise up near sidewalls. In IS condition, we only find a pair of rolls as $r_T = 0.1$. Besides, the computation results are different between IS and specular condition.

(2) The flow goes upward near the lateral boundary and downward in the center under the specular sidewalls boundary. However, in IS lateral boundary conditions, the direction of convection current tends to be upward in the center and downward near the sidewalls. This can be viewed as viscous phenomena between fluid and IS boundary. The viscous force drags fluid as it closes to IS boundary. In the center of computation domain, viscous effect is weaker than which in lateral. So the fluid is easier to rise up in the center under IS boundary.

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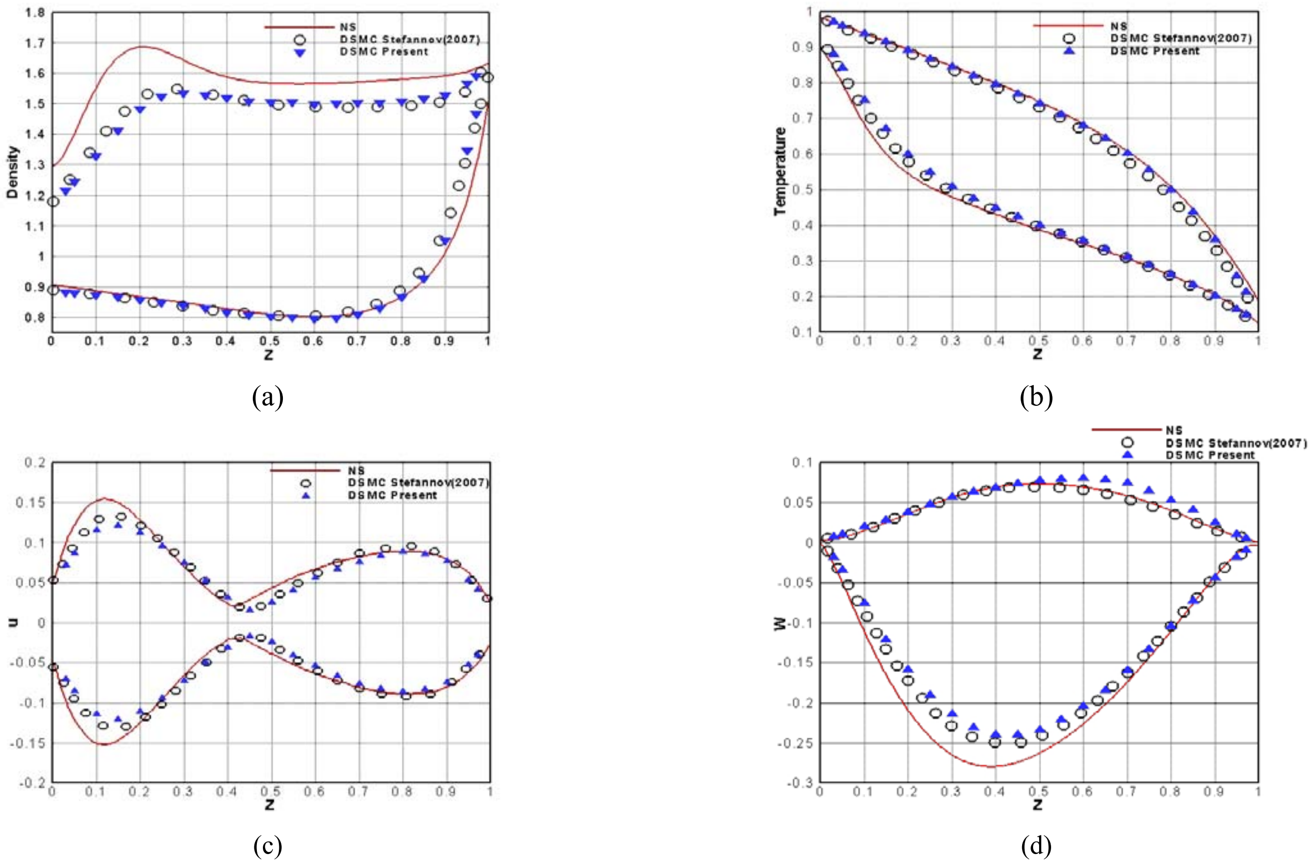
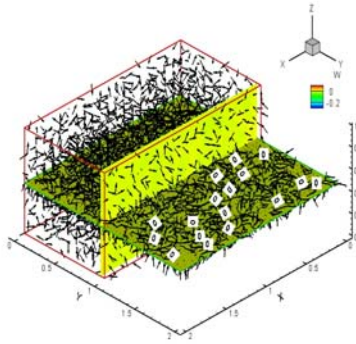
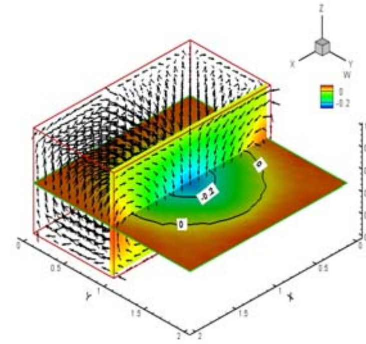


Figure 1 $Kn = 0.02$, $Fr = 3$, $r_T = 0.1$, and A=2. The properties distribution (maximum and minimum) along the z direction. (a)Density;(b)Temperature;(c)horizontal velocity; and (d)vertical velocity with Specular sidewalls boundary. Comparison of DSMC and continuum NS calculations.



(a)



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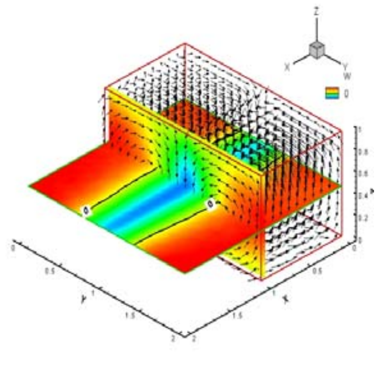
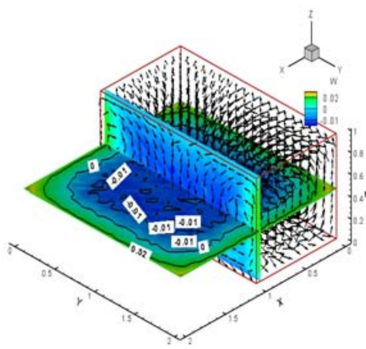
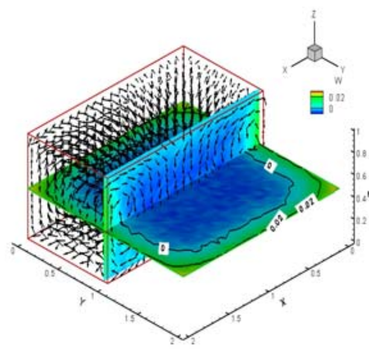


(c)

Figure 2 Under Specular sidewalls boundary, Kn =*0.01,* and Fr =*3,* vertical velocity contour and velocity vector distribution for different temperature ratio. (a) r_T = 0.67; (b) r_T = 0.2; (c) r_T = 0.1.



(a)



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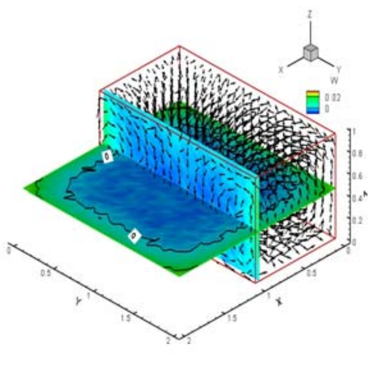


(c)

Figure 3 Under Specular sidewalls boundary, Kn =0.04, and Fr =3, vertical velocity contour and velocity vector distribution for different temperature ratio. (a) r_T =0.005;(b) r_T = 0.016;(c) r_T = 0.1.

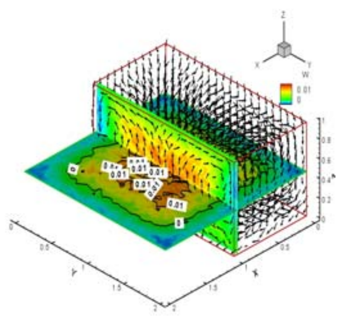
(a) (b)

Figure 4 Under IS sidewalls boundary, Kn =0.01, and Fr =3, r_T =0.1 vertical velocity contour and velocity vector distribution (a)Slice at middle z and x direction; (b) Near top, and sidewalls.

(a) (b)

Figure 5 Under IS sidewalls boundary, Kn =0.01, and Fr =3, vertical velocity contour and vector distribution for different temperature ratio. (a) r_T = 0.5; (b) r_T = 0.67.

(a) (b)



(c)

Figure 6 Under IS sidewalls boundary, Kn =0.04, and Fr =3, vertical velocity contour and velocity vector distribution for different temperature ratio. (a) r_T = 0.033; (b) r_T =0.05; (c) r_T = 0.1.