## An Empirical Method for Prediction of Hypersonic Rarefied Flow-Field Structure

He Tao, Wang Jiangfeng \*

College of Aerospace Engineering, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, P. R. China

(Received 30 March 2015; revised 2 May 2015; accepted 3 June 2015)

Abstract: Numerical simulations are presented about the effects of gas rarefaction on hypersonic flow field. Due to the extremely difficult experiment, limited wind-tunnel conditions and high cost, most problems in rarefied flow regime are investigated through numerical methods, in which the direct simulation Monte-Carlo (DSMC) method is widely adopted. And the unstructured DSMC method is employed here. Flows around a vertical plate at a given velocity 7 500 m/s are simulated. For gas rarefaction is judged by the free-stream Knudsen number (Kn), two vital factors are considered; molecular number density and the plate's length. Cases in which Kn varies from 0.035 to 13, 36 are simulated. Flow characters in the whole rarefied regime are described, and flow-field structure affected by Kn is analyzed. Then, the dimensionless position  $D^*$  of a certain velocity in the stagnation line is chosen as the marker of flow field to measure its variation. Through flow-field tracing and least-square numerical method analyzing, it is proved that hypersonic rarefied flow field expands outward linearly with the increase of  $\sqrt{Kn}$ . An empirical method is proposed, which can be used for the prediction of the hypersonic flow-field structure at a given inflow velocity, especially the shock wave position.

**Key words:** hypersonic rarefied flow; Kn; direct simulation Monte-Carlo (DSMC) mothod; linear expansion; flowfield prediction

**CLC number:** V211. 25

Document code: A

Article ID: 1005-1120(2017)05-0543-10

#### 0 Introduction

With the rapid development of hypersonic vehicle technology, more and more researches are focused on the rarefied flow regime, in which continuous medium hypothesis is no longer valid and a micro molecule model needs to be constructed. The studies should be carried on through the methods of the rarefied gas dynamics<sup>[1]</sup>.

According to the gas rarefaction which is judged by the free-stream Knudsen number (Kn), the rarefied flows are divided by Tsien<sup>[2]</sup> into three regimes: The slip flow regime(0.01< Kn < 0.1), the transitional flow regime (0.1 < Kn < 10), and the free-molecular flow regime (Kn>10). And Kn is the ratio of the mean free path λ and the characteristic length L. In rarefied regimes, there always exist some conspicuous hypersonic phenomena such as low free-stream density, high velocity and complex environment encompassing the vehicle. So it's very difficult and high-cost to carry on a wind-tunnel experiment which has extremely approximate conditions to the real flight atmosphere and few experimental data are seen in references. Due to the limited experiment conditions, Bird[3] from Australia proposed a numerical method in 1976, called the direct simulation Monte-Carlo (DSMC) method, which is proved to be a very useful approach to simulate the rarefied gas flows and considered as the representative achievement in the late 20th century[4].

In the present researches about the effects of the Knudsen numbers on rarefied flows, much at-

How to cite this article: He Tao, Wang Jiangfeng. An empirical method for prediction of hypersonic rarefied flow-field structure[J]. Trans. Nanjing Univ. Aero. Astro., 2017,34(5):543-552.

http://dx.doi.org/10.16356/j.1005-1120.2017.05.543

<sup>\*</sup> Corresponding author, E-mail address: wangjf@nuaa.edu.cn.

tention is mainly paid to the aerodynamic properties of hypersonic aircrafts<sup>[5-11]</sup>. Leith Potter et al. ever gave a computational method for the prediction of aerodynamic forces and moments of axisymmetric hypersonic bodies in the transitional flow region according to data from numerical simulation and experiment[11]; Moss presented variations of drag and heating coefficients as a function of rarefaction when simulating ballute's aerodynamics[8]; Ozawa et al. found a bridging function to represent the aerodynamic characteristics of Mars explorer by carrying out a series of numerical simulations from the free-molecular flow to the continuum flow[10]. However, in these researches the structure features of flow field affected by gas rarefaction get little attention, neither do we have any engineering method to predict them.

In this paper, an unstructured DSMC technique is employed to study the effects of Kn on rarefied flow-field structure. The flow around a two-dimensional vertical plate is computed at a velocity 7 500 m/s, with two vital factors considered: Molecular number density and plate's length. Many cases are simulated with Kn varying from 0.035 to 13.36, which covers the whole rarefied regime. With the analysis of the simulation results, the flow-field characters at different Kn ranges are described and an empirical method is proposed for the prediction of the hypersonic flow-field structure at a given inflow velocity, especially the shock wave position.

## 1 DSMC Method

In DSMC methodology, the gas is composed of thousands of simulated molecules, each of which represents large quantities of real molecules. The position coordinates and velocity components of simulated molecules are stored in the computer. In a time step, one molecule moves at a constant velocity until it makes a collision with another or a wall boundary. Then the molecular information is updated, preparing for

the next time step. When the flow field comes to a stable state after enough cycles, macroscopic properties such as density and temperature can be obtained through accumulation of each simulated molecule's information.

In this paper, all calculations are performed using a DSMC code developed by Dr. WANG X D from Nanjing University of Aeronautics & Astronautics(NUAA). The code is proved to be stable, highly-efficient and robust with abundant validations<sup>[12-15]</sup>. Unstructured mesh nique[12,16] is introduced in the DSMC method. In the continuous flow, based on the computational fluid dynamics methods(CFD), for example, the finite-volume method<sup>[17]</sup>, grids are mainly used for spatial discretization and required to have regular shapes with no discontinuities in the lines or surfaces. However, grids in DSMC method play a different role with the former, and are employed to store molecular information, search and locate molecular position, identify and select possible collision partners and attain flow-field statistical information. Compared with Cartesian grids<sup>[5,7]</sup>, unstructured mesh technique has the advantages such as surface-highly-fitting and easily-generated. But molecule searching is difficult in unstructured grid system. To improve the efficiency, a search technique<sup>[12]</sup> which combines volume (area) coordinate search method and alternative digital tree(ADT) search algorithm is adopted in the program.

In addition, several important models and techniques in the DSMC method are employed as follows: (1) For gas-surface interaction, Maxwell diffuse reflection model is used, assuming that molecular velocity components reflected by the wall satisfy Maxwell distribution; (2) surface temperature is supposed to be constant; (3) for molecular mutual collision, the variable hard sphere(VHS) model is employed, in which collision cross section varies with molecular relative velocity; (4) for possible collision partners selection, the no-time-counter(NTC) scheme<sup>[18]</sup> is a-

dopted, which decreases the requirement of algorithm to the mesh scale; (5) for the energy exchange between kinetic and internal modes, the Larsen-Borgnakke statistical model<sup>[19]</sup> is introduced; (6) for a fast and load-balancing computation, a MPI-parallel algorithm of the unstructured DSMC method<sup>[15]</sup> is used with an adaptive domain decomposition technique introduced. All the simulations in this paper are run on a 16-node PC-cluster system using Linux OS; (7) perfect-gas model is introduced and chemical reactions are neglected temporarily.

# 2 Numerical Simulation of Vertical Plate Flow

In this section, to investigate the effects of gas rarefaction on flow-field structure, the flows around a 2-D vertical plate are simulated at a velocity 7 500 m/s using the unstructured DSMC method as presented in the previous section. In the process, molecular number density and characteristic length are considered, which affect the gas rarefaction. Kn in the simulation cases varies from 0.035 to 13.36.

#### 2.1 Effects of molecular number density

Computational geometry model is a plate with the length L=4 m and the thickness h=0.05 m. Four cases are simulated with different molecular number density (N), the values of which are taken from the earth altitudes 100, 105, 110 and 115 km, that is, N = 1.19E + 19, 5. 02E+18, 2. 14E+18 and 9. 68E+17 m<sup>-3</sup> (the parameters in this paper are obtained from U.S. 1976 Standard Atmosphere Model<sup>[20]</sup>). And the corresponding free-stream Kn (based on the length L of the plate) are 0.035, 0.084, 0.197 and 0. 436, respectively. In these cases, flow conditions as follows are kept the same. The freestream velocity is 7 500 m/s in the direction vertical to the plate; The free-stream temperature and the wall temperature are respectively 240 K and 500 K; The gas components are assumed to be nitrogen molecules and oxygen molecules with the initial mole fractions 0.75 and 0.25.

The unstructured meshes around the plate are shown in Fig. 1. Mesh cells are constrained to be less than one-third of the local mean free path<sup>[19]</sup>. Computational domains all have the same boundary(-10 m,10 m)×(-10 m,10 m). Cell numbers are about 560 000, 220 000, 140 000 and 30 000 in the cases from left to right. Simulated molecule numbers are about 23 800 000, 10 000 000, 4 280 000 and 1 940 000.

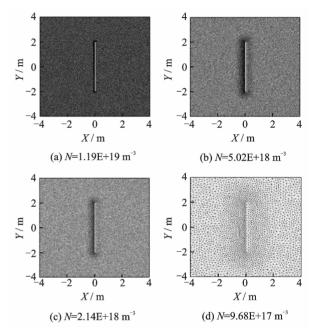


Fig. 1 Unstructured grids

In Fig. 2, the streamlines in flow field at different molecular number density N are illustrated. When N equals 1.  $19E+19~\rm m^{-3}$  at altitude  $100~\rm km$ , streamlines experience an apparent compression and distortion on both sides of the plate, indicating that there exists a strong bow shock in that region. And on the leeward side of the plate, a pair of symmetric separated vortexes emerges. Along with the decrease of molecular number density, the effect of compression and distortion gradually diminishes, the shock strength weakens and the vortex structure behind the plate disappears.

Fig. 3 presents velocity contours in flow field at different molecular number density N. When N equals 1.19E+19 m<sup>-3</sup> (Kn=0.035) at altitude

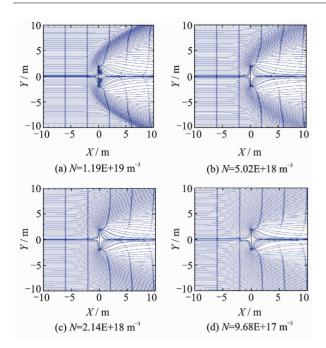


Fig. 2 Streamlines at different molecular number density

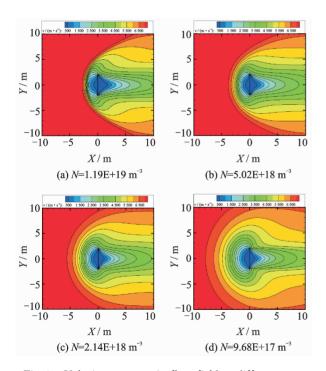


Fig. 3 Velocity contours in flow field at different molecular number density

100 km, the flow is in the slip regime and a strong detached bow shock is developed starting from the front of the plate and extending to both sides symmetrically. In the shock wave region, velocity contours are compressed sharply; as N decreases, Kn increases and the flow is close to

the transitional regime. It could be seen that the flow field expands outward gradually and the shock layer becomes thicker, the detached distance larger and the shock intensity weaker; When N reaches 9.68E+17 m<sup>-3</sup> (Kn = 0.436) at altitude 115 km, the shock wave disappears and the velocity in flow field diminishes slowly from the free-stream value to zero on the wall with no sharp changing. The inner flow-field structure shrinks close to the plate's two ends, while a large arc-expansion region is formed in the windward region of the plate. The reason for this phenomenon can be explained as follows: Flow field expands rapidly along with the increase of gas rarefaction. The shock wave disappears at some Knudsen numbers. For this reason, the inflow gas would not be compressed before arriving at the plate. When the free-stream molecules hit the surface, they get slowed down and accumulate constantly around the plate. Then a compression layer with high density would be formed on the windward surface of the plate from one end to the other. And a great density gradient is produced between the surface and the region away from the plate. So the flow field diffuses around with the center on the plate's windward surface and a large arc-expansion region is formed.

#### 2. 2 Effects of the plate's length L

In this section, six plates are chosen as the computational geometries with different length: 10, 6, 3, 1.8, 1.1 and 0.8 m. The length-thickness ratios of the plates are all 80:1. For all cases, molecular number density N is 5.02E +18 m<sup>-3</sup>, which derives from the altitude 105 km. The other free-stream conditions are the same with Section 2.1. The corresponding Knudsen numbers (based on the length L of the plate) are 0.034, 0.056, 0.112, 0.187, 0.306 and 0.421. Grid cell numbers at different Kn are about 880 000, 490 000, 140 000, 80 000, 60 000 and 40 000, respectively. And the simulated molecules are about 26 800 000, 15 100 000, 4 280 000, 2 410 000, 1 810 000 and 1 070 000.

Fig. 4 shows velocity contours in four cases' flow field, the characteristic length L of which are 10, 3, 1.8 and 0.8 m. As we can see, when L equals 10 m (Kn=0.034), a strong bow shock wave is formed in front of the plate, which is similar to the case "N=1.19E+19 m<sup>-3</sup>" in Fig. 3. Along with the plate's length declining, the thickness of the shock wave increases and the intensity weakens. However, the whole flow-field region interfered by the plate is reduced. When L reaches 0.8 m (Kn=0.421), a large arc-expansion region emerges in front of the plate and the shock wave vanishes like the case "N=9.68E+17 m<sup>-3</sup>" in Fig. 3.

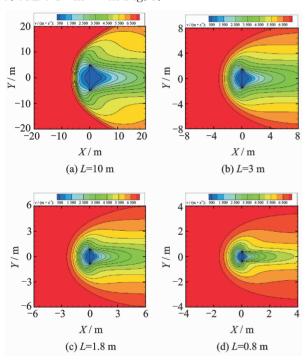


Fig. 4 Velocity contours at different characteristic length

Comparing Figs. 3, 4, it is indicated that the variation of flow-field characters induced by the falling down of molecular number density agrees well with that caused by the decreasing of characteristic length. The flow fields both expand around with Kn increasing.

Then, the distance of the  $93\%~V_{\rm inf}$  position in the frontal stagnation line to the plate is measured as the marker of flow field to evaluate its variation law precisely. And the distance is labelled as

D. Considering that the interfered area of flow field can be affected by the characteristic length L, a dimensionless distance  $D^*$  is employed through the conversion  $D^* = D/L$ . Fig. 5 illustrates the  $D^*$  values as a function of Kn. The little circles represent the simulation cases with the characteristic length L fixed in Section 2.1 (L =4 m), while the fold line shows the instances with the molecular number density N fixed in Section 2.2 ( $N=9.68E+17 \text{ m}^{-3}$ ). As seen from Fig. 5, the circles are almost distributed on the line. It is exactly indicated that the variation laws of the dimensionless flow-field structure caused by the two factors L and N fit perfectly with each other. And a conclusion can be drawn that the dimensionless flow-field structure is determined by the free-stream Kn at a given velocity, while the characteristic length of geometry or the molecular number density of inflow gas may be different.

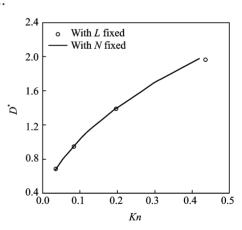


Fig. 5 Variation of flow field caused by different factors

## 2. 3 Analysis of the flow-field structure in the whole rarefied flow regime

For the numerical researches in Sections 2.1—2.2, the range of Kn is restricted from 0.034 to 0.436, which belongs to the slip flow regime and a fraction of the transitional flow regime. To investigate the variation of flow-field characters in the whole rarefied flow regime, some cases are added in the section. The computational geometry is still the plate in Section 2.1 with the length L=4 m and the thickness h=

0.05 m. The molecular number density (N) are respectively taken from the altitudes 120, 125, 130, 135, 140,145, 150,155 and 160 km<sup>[20]</sup>. The corresponding free-stream Kn are 0.83, 1.4, 2.19, 3.22, 4.53, 6.16, 8.14, 10.53 and 13.36. The other free-stream conditions are the same with Section 2.1.

For atmosphere in the altitudes beyond 120 km is highly rarefied, the calculation amount decreases a lot. So meshes in the cases can be generated with uniform scale for the surface grids and the far-field grids, which is the standard for the altitude 120 km. The number of real molecules represented by one simulated molecule is identical for all the cases, on the premise that every cell has enough molecules for simulation. Considering the expansion of flow field, the boundary of computational domain is extended to  $(-30 \text{ m}, 30 \text{ m}) \times (-30 \text{ m}, 30 \text{ m})$  for the cases in which Kn varies from 0.83 to 3.22, and  $(-40 \text{ m}, 40 \text{ m}) \times (-40 \text{ m}, 40 \text{ m})$  for the cases in which Kn varies from 4.53 to 13.36.

Fig. 6 shows the velocity contours of flow field in part of the cases: Kn = 1.4, 3.22, 6.16 and 10.53. Comparing with Fig. 3, we can see that the main topology structures of the flow field

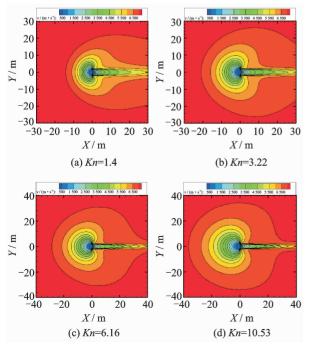


Fig. 6 Velocity contours in flow field at different Kn

in the transitional flow cases and the free-molecule flow cases are similar with the case Kn = 0.436. The variations are primarily presented that the arc-expansion region before the plate dilates toward surroundings almost proportionally and the whole flow-field interfering area is larger and larger.

Analyzing the cases in Sections 2. 1, 2, 3, flow properties along the stagnation line are illustrated in Figs. 7 (a—c) with Kn changing from 0.035 to 10.53, including velocity and density. Fig. 7 (a) shows that velocity in all cases falls down along the stagnation line before the plate. And the value decreases more gently with Kn being larger because of the flow field's expansion, which indicates that the shock layer becomes thick. When Kn increases to a certain value, the velocity changes at an approximately average gradient, showing that the shock wave is unapparent. In the leeward region, the velocity goes up again. In Figs. 7(b, c), it can be seen that density in front of the plate is raised at different Kn. An especially obvious phenomenon is that the increase of density is composed of two stages at Kn = 0.035, which are located in the shock wave region and the thermal boundary layer, respectively. The reason for the first rise stage is that the shock wave is so strong and thin that the gas flow is compressed sharply when acrossing that region. The result agrees well with Bird's numerical simulation to one-dimensional steady flow using DSMC method<sup>[18]</sup>. However, there is only one-rise stage in the stagnation line in the other cases, which is in the thermal boundary layer. The reason can be explained as follows: when Knrises, the intensity of shock wave fades and the thickness increases. The compression effects on gas molecules are too weak so that can be ignored. The thermal boundary layer extends out along with flow field's expansion and intersects with the shock wave region. As a result, two-rise stages are replaced by only one-rise stage.

According to the researches in Sections 2.1—

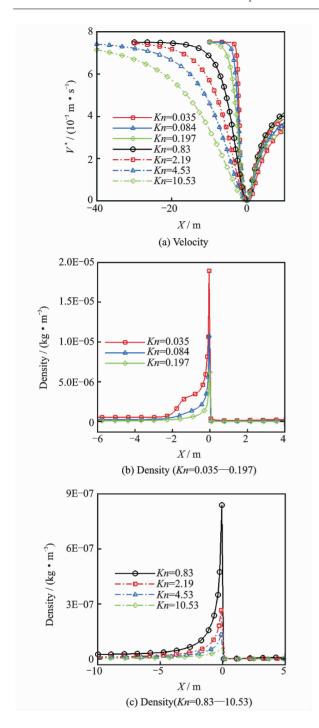


Fig. 7 Flow properties along the stagnation line

2. 3, the hypersonic flow-field characters around a vertical plate in the whole rarefied regime can be concluded as follows. In the slip flow regime with a small Knudsen number, there exist apparent hypersonic aerodynamic features in flow field, such as strong shock wave, thin shock layer and short detached distance. Flow properties have a sharp variation across the shock wave. In the flow close to the transitional regime, flow field

gradually expands outward and the shock layer becomes thicker with the intensity weakened. When the free-stream Knudsen number arrives at about 0.4, the shock wave is unobvious and has a tendency to disappear. At the same time, an arc-expansion region appears in front of the windward surface. When it comes to the transitional flow regime and the free-molecule flow regime, flow fields all have a similar topology structure and the main variations are shown that the arc-expansion structure in the windward region dilates toward surroundings almost proportionally and the whole flow-field interfering area is larger and larger.

## 3 Empirical Method

Through the investigation in the previous section, the variation of flow-field characters in the whole rarefied regime is presented qualitatively, that is, the flow field expands around with Kn increasing. To describe the variation law quantitatively and precisely, the approach in Section 2. 2 is employed again to measure the expansion scale of the flow field. The dimensionless position  $D^*$  of a certain velocity in the stagnation line is chosen as the marker of the flow field. And the cases in Sections 2. 1 and 2. 3 are further analyzed with Kn varying from 0.035 to 13.36.

In the section, two velocities  $70\%~V_{\rm inf}$  and  $50\%~V_{\rm inf}$  in the stagnation line are selected and the corresponding dimensionless positions are labelled as  $D_1^*$  and  $D_2^*$ , respectively. Fig. 8(a) shows the scattered data of  $D^*$  in every case. As seen in the picture, the variation curve of  $D^*$  as a function of Kn is close to a parabola with the symmetric axis on X-axis, no matter for the  $70\%~V_{\rm inf}$  position or the  $50\%~V_{\rm inf}$  position. It's indicated that the flow field expands outward parabolically at a gentle gradient with the Knudsen number rising.

According to the above analysis, a fitted line of  $D^*$  as a function of  $\sqrt{Kn}$  is plotted based on the least square method, as presented in Fig. 8(b). We can find that the calculation data are almost completely distributed on the fitted

line in the two positions. And it is proved that the variation of  $D^*$  versus  $\sqrt{Kn}$  satisfies the linear function  $D^* = a\sqrt{Kn} + b$  perfectly, where a and b are respectively the slop and intercept of the line. In this paper, for the  $70\%~V_{\rm inf}$  position, the coefficients are  $a_1 = 1.230~7$ ,  $b_1 = 0.338~4$ ; for the  $50\%~V_{\rm inf}$  position,  $a_2 = 0.750~8$ ,  $b_2 = 0.346~8$ .

As a conclusion, it is indicated that flow field expands linearly with  $\sqrt{Kn}$  increasing under perfect-gas flow conditions.

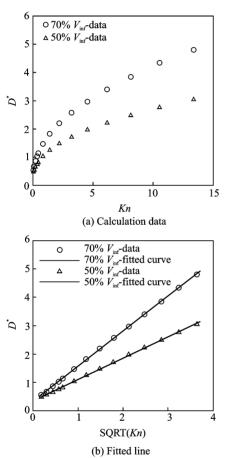


Fig. 8 Effect of varying Kn on  $D^*$  of flow field in rarefied regime

According to the variation law, an empirical method is proposed for flow-field structure prediction at different Knudsen numbers in a given velocity. It is implemented as follows. First, two flows at different Knudsen numbers in a given velocity are chosen as the fundamental cases and then simulated using the DSMC method. After that, marked positions are selected. According to the empirical formula  $D^* = a\sqrt{Kn} + b$ , the two

coefficients a and b can be calculated. Then,  $D^*$  positions in another free-stream Kn condition can be obtained. Changing the marked position and repeating the process, velocity distribution along the stagnation line at another Kn are plotted, instead of numerical simulation which costs a long time and computational resource. Thus, primary flow field at different Knudsen numbers in a given velocity is predicted.

To establish the prediction method, thirteen cases covering the whole rarefied regime are simulated. As shown of the numerical results in Fig. 8(b), all the marked points are distributed on the fitted curve. Analyzing from another aspect, if two of the thirteen cases are chosen as the basic cases, the others all can be considered as the verification cases to the prediction method in this paper.

In the meanwhile, it is indicated that the empirical method can be used for the prediction of shock wave position. When Kn is close to zero, the free stream would become a continuum flow and  $D^*$  tends to a constant number b according to the empirical formula  $D^* = a\sqrt{Kn} + b$ . In continuum regime, shock wave can be thought as a thin face, through which a supersonic flow turns to the subsonic. If  $D^*$  is located at an appropriate position ( $Ma^* = 1 - Ma_{inf}$ ), the coefficient b can be considered as the predicted shock position.

However, in this paper, the simulation geometry is limited to a two-dimensional vertical plate with no other geometries considered. Chemical reactions are ignored. Based on the variable control principle, the free-stream conditions except molecular number density are kept the same, such as the velocity state, the gas components and inflow temperature. And the effects of these conditions on the flow-field variation law versus Kn are not considered in this paper. Therefore, the empirical method need to be validated further more in the future's work about the application, the suitability, the influence factors, and so on.

### 4 Conclusions

The effects on the flow-field structure of the gas rarefaction judged by the free-stream Knudsen number are studied based on the DSMC method. A 2-D vertical plate is chosen as the investigated object. The flow around the plate is simulated with two vital factors considered: Molecular number density and characteristic length. And the velocity is kept a constant with 7 500 m/s. The Knudsen numbers in all computational cases vary from 0.035 to 13.36, which covers the whole rarefied regime. At last, an empirical method is proposed for the prediction and analysis of the rarefied flow field. Significant findings of the researches are presented as follows.

- (1) The variation of the dimensionless flow-field structure caused by the factors molecular number density and characteristic length agrees well with each other. And Kn is the decisive factor to the variable flow field at a given velocity.
- (2) In the slip flow regime, there exists strong shock wave in flow field. With Kn rising, flow field expands outward and the shock wave gradually disappears. In the transitional flow regime and the free-molecule flow regime, flow fields all have a similar topology structure.
- (3) A linear expansion happens in rarefied flow field with the increase of  $\sqrt{Kn}$ . An empirical formula is proposed for prediction of hypersonic flow-field structure, that is,  $D^* = a\sqrt{Kn} + b$ , in which  $D^*$  is the dimensionless position of a certain velocity in the stagnation line.

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Mr. He Tao received his B. S. and M. S. degrees in Bachelor of Engineering from Nanjing University of Aeronautics and Astronautics in 2013 and 2016, respectively. His research is focused on rarefied flow through DSMC numerical technique.

Prof. Wang Jiangfeng is a professor and doctoral supervisor in College of Aerospace Engineering, Nanjing University of Aeronautics and Astronautics (NUAA). He received his Ph. D. degree in CFD from NUAA in 2000, and the second Ph. D. degree in University of Paris VI, Paris, France, in 2002. His research is focused on hypersonic vehicle design, numerical simulation of hypersonic high temperature gas effect and combustion flow, and parallel computing technology.

(Executive Editor: Xu Chengting)