Molecular Simulation of Rarefied Supersonic Free Jets by DSMC Method*

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The direct simulation Monte Carlo method is applied to the study of supersonic jets through a thin orifice. The influence of roughness of the cell network and the number of molecules in a cell on the simulation results is examined. The structure of the jets can be characterized using the rarefaction parameter introduced by Muntz et al. (AIAA J., 1970). The temperature nonequilibrium between the directions parallel and normal to the jet axis is reproduced.

Key Words: Rarefied Gas Flow, Molecular Flow, Free Jet, DSMC, Shock Wave

1. Introduction

Rarefied supersonic free jets through an orifice or a nozzle need to be studied in detail because these are applicable to the discharge of gas into a vacuum chamber or rocket propulsion in space. We have applied the direct simulation Monte Carlo (DSMC) method(1) to the structural analysis of free jets and shown that a Mach disk and a barrel shock in a free jet can be reproduced by the molecular simulation(2). The calculations in which jet structures vary with stagnation pressures agree well with the experiments using a mass-sampling technique. After publishing our first paper(3) on this study, we received many questions about the calculation. One purpose of the present paper is to answer the questions especially regarding the cell network and the number of molecules in a cell and another is to characterize the structure of jets using the rarefaction parameter introduced by Muntz et al(4), in 1970. This paper also refers to nonequilibrium phenomena in jet flow fields, such as the temperature discrepancies between the directions normal and parallel to the jet axis.

2. DSMC Calculation

The jet flow field is assumed to be axisymmetric so that molecules move in an imaginary two-dimensional plane (x-y or x-r plane). Although each molecule departs from the x-y plane, due to its velocity component w in the z direction, in the axially symmetric flow field with the axis in the x direction, the location of the molecule is rotated about the x axis and the molecule returns again to the x-y plane. The v and w velocity components are also rotated around the axis. Calculations are made for various conditions (Table 1); 1/\(Kn\)=20 to 25 000, where \(Kn\)

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<tr>
<th>1/(Kn)</th>
<th>(p_1/p_0)</th>
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<td>25000</td>
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is the Knudsen number based on the mean free path \( \lambda \) of an upstream stagnation and the orifice diameter \( d \), and \( p_0/p_1 = 20, 50, \) and \( 100 \), where \( p_0 \) is the stagnation pressure and \( p_1 \) is the background pressure. The VHS molecular model\(^{(1)}\) for a monatomic gas of argon is used. The temperature index of viscosity coefficient \( \omega \) at room temperature is adopted. The temperature of a free jet drops suddenly as the jet expands, but for a gas of a single species a constant value of the index is available in the simulation. The null-collision scheme\(^{(4)}\) is used for intermolecular collisions. It is similar to the no-time-counter scheme\(^{(1)}\) by Bird, both schemes belonging to the maximum collision number method, but it uses an instantaneous value \( N \) for the number of molecules in a cell in the calculation of the maximum collision number \( N(N-1)(\sigma c_r)_{\text{max}} \Delta t/2 V \), where \( (\sigma c_r)_{\text{max}} \) is the maximum of the product of the total collision cross section \( \sigma \) and the relative speed \( c_r \), \( \Delta t \) is the time step over which the molecular motion and the intermolecular collisions are uncoupled, and \( V \) is the volume of a cell. This is in contrast with Bird’s scheme in which the time average \( \bar{N} \) instead of \( (N-1) \) is used, such as \( N\bar{N}(\sigma c_r)_{\text{max}} \Delta t/2 V \). It would be preferable to use \( N(N-1) \), as indicated later. A subcell method (a double cell structure) is used for a cell network near the centerline of a jet in which the number of molecules per cell is significantly small. Alternatively, cells with a large volume are applied here. When the subcell method is used in the present calculation, each cell (each large cell) located along the centerline contains four subcells, the 1st ~ 4th subcells from the centerline, and the 5th and 6th subcells from the centerline make another large cell. One molecule of collision pairs is selected at random from a large cell. The second molecule is selected from the subcell in which the first molecule is located, if the subcell has at least two molecules. Otherwise the second molecule is selected from the adjacent subcell belonging to the same large cell.

The simulated domain is divided into two regions, upstream and downstream of the thin orifice. The typical size of the upstream region is \( 0.75d \times 0.75d \) and that of the downstream region is \( 15d \times 2.5d \) for the conditions \( 1/\text{Kn}=2500 \) and \( p_0/p_1=50 \) (Fig. 1). The diffusely reflecting surface of the orifice is assumed. Velocities of each molecule entering through the upstream boundary are generated using the Maxwell distribution with some flow velocity normal to the boundary. On the other hand, those of molecules entering through the downstream boundary (boundary normal or parallel to the axis in the downstream region) are generated by the Maxwellian at the background pressure without flow velocity. The number of simulated molecules, dealt with simultaneously in a computer, ranges from \( 1 \times 10^6 \) to \( 5 \times 10^8 \) and the maximum number of cells is about \( 1.4 \times 10^6 \). The upstream cell network is constructed by square cells but in the downstream, the dimensions of a cell along the axis vary exponentially with its position up to the location of the Mach disk since the minimum density appears immediately before this location.

3. Results and Discussion

3.1 Cell network

The simulated region of physical space is divided into a network of cells in the DSMC calculation and the molecular motion and the intermolecular collisions are uncoupled over a small time interval. The number of cells and the number of molecules would become prohibitively large near the continuum regime because the cell dimensions would be smaller than the local mean free path. However, we use large cell dimensions independent of the local mean free path in order to simulate the entire jet structure in this study. In this paragraph, we consider the influence of roughness of the cell network on the results of the calculation. The boundary condition of the downstream region is improved\(^{(19)}\) in the calculation for this discussion to eliminate influences other than the cell dimensions and the number of molecules to the extent possible. Figures 2 and 3 indicate the density profile \( \rho/\rho_0 \) of a jet flow field for \( 1/\text{Kn}=2500 \) and \( p_0/p_1=50 \) that is calculated with the dimensions of the cell located near the orifice being about 14 times the local.
mean free path (the number of molecules is $5.1 \times 10^8$, the number of cells is $1.4 \times 10^9$), where $\rho_0$ is the density at the upstream stagnation. On the other hand, Fig. 4 is obtained with cell dimensions two times larger than that shown in Fig. 3. Since the number of molecules per cell is almost the same in both calculations, the total number of molecules in Fig. 4 becomes about one-eighth of that in Fig. 3. Figure 5 shows the zone where the difference (absolute value) between these two results reaches more than 0.4 percent of the stagnation density. The difference appears only near the outlet of the orifice and in the area between the barrel shock and the jet boundary, where a sudden increase in density is observed as shown in Figs. 2 to 4. Figure 6 indicates the zone where the absolute value of the difference divided by the local density shown in Fig. 3 (fine network of cells) is larger than 10 percent. The reason why the values near the locations of the Mach disk and the barrel shock become large is that these locations shown in Figs. 3 and 4 do not match precisely. Since the density changes greatly there, the value as shown in Fig. 6 becomes large even if the shift of the locations of the Mach disk and the barrel shock is small. Besides, although the difference in the area between the barrel shock and the jet boundary is also appreciable, the value is less than 10 percent in an extensive flow field of the jet. As can be seen, the difference occurs in the region where the density reaches a maximum, such as the location between the barrel shock and the jet boundary and the location directly behind the intersection of the Mach disk and the barrel shock, where the maximum density decreases as the dimensions of cells increase. Nevertheless, the density profiles in both calculations are almost the same throughout the flow field. We can say that the jet flow field is somewhat modified by a finer network of cells but the result with a coarse network of cells would still be acceptable. The velocity profiles and the temperature profiles also show almost the same tendencies as the density profiles, although these data are not shown in this paper.
3.2 Number of molecules per cell

The number of molecules per cell should be decreased in order that the total number of molecules does not exceed the permitted amount in the available computer system. Especially in the study of steady flow, the process of an unsteady state before the steady state is obtained can be calculated rapidly with a small number of molecules. The minimum number of molecules per cell on time average occurs at the location directly before the Mach disk in the jet axis, and is about one per cell (not per subcell) in a typical calculation. There is the question of whether a possible collision pair can be found in the cell that has only one molecule on time average. The answer is that since the cell with one molecule on time average has occasionally no molecule at all as a statistical fluctuation, it must also have two or more molecules occasionally in order to keep one molecule on time average.

The statistics proves that the average number of molecules, which seems insufficient, leads correctly to the theoretical collision rate. The theoretical number of collisions $\nu$ per unit time in a cell is

$$\nu = \frac{N(N-1)/2V}{\sigma_{TC}}$$

(1)

where $\sigma_{TC}$ is the average of the product of the total collision cross section and the relative velocity. Suppose that the cell has $M$ molecules on average (time average or ensemble average). To determine the probability that at any instant the number of molecules in the cell is a particular number $N$, we consider the situation that $KM$ molecules are distributed among $K$ boxes. The probability $P_N$ that $N$ molecules are located in a particular box is

$$P_N = \frac{K^M C_N(1/K)^N((K-1)/K)^{KM-N}}$$

(2)

The probability $Q_N$ that intermolecular collisions occur in the cell containing $N$ molecules can be evaluated by the number of collisions per unit time for the box now considered $\nu_N$, and that for all boxes $\nu_{KM}$ using the following equations.

$$\nu_N = \frac{N(N-1)/2V}{\sigma_{TC}}$$

(3)

$$\nu_{KM} = \frac{KM(KM-1)/2KV}{\sigma_{TC}}$$

(4)

$$Q_N = \frac{K\nu_N}{\nu_{KM}} P_N$$

$$= \frac{(N(N-1)/KM(KM-1))K^2P_N}{(N(N-1)/M^2)P_N}$$

(5)

where $V$ and $KV$ are the volume of one box and that of all boxes, respectively, and $\sigma_{TC}$ is assumed to be the same value in Eqs. (3) and (4). Table 2 shows the probability $P_N$ calculated by Eq. (2) and the collision probability $Q_N$ calculated by Eq. (5) for $K = 10000$. If the sum of $Q_N$ over all $N$ is unity, which is easy to prove, the average number of molecules per cell $M$ can give a correct collision rate. Table 2 also shows that the correct collision rate is obtained even in the case of $M = 0.1$. In this development, Eq. (3) does not use the average value $M$, but use instead the individual value $N$ as the number of molecules in a box. Although Bird uses the average number of molecules $M(=\bar{N})$ in the no-time-counter method instead of $N-1$, the instantaneous value should be used as described previously. Note that in the above derivation, the number of molecules per box is small due to an increase in the number of boxes and a decrease in the volume of a box, but in an actual molecular simulation the number of molecules per cell becomes small even with a fixed cell volume, because the number density $n$ decreases. In this case, since the apparent total collision cross section $\sigma_{R}(\propto 1/n)$ becomes large even if the volume in Eq. (3) changes to $KV$, Eq. (5) can be obtained.

If the number of molecules per cell is zero or one ($N = 0$ or $N = 1$), no intermolecular collision occurs in the cell. The probability of such a situation $P_0 + P_1$ is 0.05% for $M = 10$ and is negligible, far from the significant figures in Table 2. However, the probability $P_0 + P_1$ is 73.6% for $M = 1$ and 99.9% for $M = 0.1$. In the case of $M = 0.1$, moreover, 90% ($= Q_2$) of intermolecular collisions occur in a cell that has only two molecules ($N = 2$). Suppose that the time step $\Delta t$ in the DSMC method is set equal to the mean free time $\tau$. The number of collisions during the time step $\Delta t$ is equal to half the number of molecules in a cell. If the calculation for $M = 0.1$ is repeated 10000 times, the
total number of molecules located in a particular cell is 1000 and therefore 500 collisions should be calculated. Since only about 90 molecules (10000 × 0.00452 × 2 = 90.4), or 45 collision pairs, are in the cell with two molecules at the same time, 90% of the 500 collisions, i.e., 450 collisions, should be calculated among the 45 pairs of molecules. That is, one pair of molecules must experience ten collisions on average. The collision of the same pair has no meaning after the first collision, which leads to the lower limit of the average number of molecules per cell. In the subcell method, even if a subcell has only one molecule, a collision partner is selected from an adjacent subcell, which prevents repetition of collisions with the same pair to some degree.

On the other hand, in the case of \( M = 1 \), a collision pair experiences one collision on average when \( N = 2 \). From this consideration, the present calculation adopts the minimum number of molecules in a cell with about one as the mean. The reliability of such a selection for the number of molecules can be confirmed by a comparison with the calculation for a smaller number of molecules. The density profile in the downstream flow field is calculated with the total number of molecules being \( 5.1 \times 10^6 \), which is about one-tenth of that shown in Fig. 3, and the minimum number of molecules is about 0.1. In Fig. 7, almost the same result as that in Fig. 3 is obtained except for the smaller area with the number of molecules per cell being less than 0.2, even if many cells near the jet axis have a very small number of molecules, less than one on time average, as in Fig. 8. The minimum number of molecules per cell being one is considered to be a sufficient condition in the present calculation for a free jet.

3.3 Classification of jet structures

Muntz et al.\(^{3} \) have categorized the characteristics of the rarefied jets into three regimes using the rarefaction parameter: \( \xi (=d(p/p_i)^{1/3}/T_a[dyne/cm/K]) \). The values of \( \xi \) in our calculation are shown in Table 1. The Mach disk, at which a sharp increase in density and temperature and a decrease in velocity can be seen, and the barrel shock are clearly observed for large values of \( \xi \) (the continuum regime). The location of the Mach disk agrees well with the empirical relation\(^{4} \) \( x/d = 0.67(p_i/p_o)^{1/2} \). The values of the flow properties almost agree with the numerical results\(^{7} \) obtained by the Euler equations. On the other hand, for small values of \( \xi \) (the scattering regime), the density decreases monotonically and no shock wave is observed. The decrease in axial-flow velocity and the increase in temperature begin at a

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**Table 2** Probability \( P_n \) and \( Q_n \)

| \( N \) | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| \( N=10 \) | \( N \) | 0.00 | 0.00 | 0.00 | 0.01 | 0.02 | 0.04 | 0.06 | 0.09 | 0.11 | 0.13 | 0.13 | 0.11 | 0.09 | 0.07 | 0.05 | 0.03 |
| \( \Sigma N \) | \( P_n \) | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| \( \Sigma Q_n \) | \( Q_n \) | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

**Fig. 7** Contours of normalized density \( \rho/\rho_s \) for a small number of molecules \((1/Kn=2500, \rho_i/\rho_s=50)\)
shorter distance from the orifice than the distance at which the density starts to deviate from the isentropic value. Since the supersonic flow is not protected by shocks anymore, some molecules in the background gas invade deeply into the jet core and scatter the molecules of the expanding flow. Consequently, the supersonic flow region is reduced. Figure 9 for the continuum regime and Fig. 10 for the scattering regime indicate the ratio of the number of molecules coming from the upstream boundary to the total number of molecules in each cell of the flow field. As shown in Fig. 9, almost all of the molecules near the axis come from the upstream boundary in the continuum regime. However, the molecules coming from the downstream boundary increase in the scattering regime, as shown in Fig. 10. Figure 11 shows the density distributions along the axis for the three different flow regimes. The continuum flow fields can be seen for jets with $\xi > 5$ and the scattering flow fields are obtained for $\xi < 3$ in the present calculations. For
intermediate values of $\xi$ (the transition regime; $0.3 < \xi < 5$ in the present calculation), the shock waves broaden and the scattering by the background gas also occurs. For a constant pressure ratio $p_0/p_n$, the location showing an increase in density (apparent shock wave) shifts to the upstream region as $\xi$ decreases. The curves denoted by ‘Euler’ in the continuum regime are the results of the calculation\(^7\) by the finite difference method with Euler’s equation, in which an inviscid fluid is assumed, i.e. $1/Kn = \infty$. Although the Mach disk obtained by Euler’s equation has no thickness, its location agrees well with the results of the present DSMC calculation, that is, the empirical relation proposed by Ashkenas and Sherman\(^6\) is also consistent with our results. In the scattering regime, the density profile without a Mach disk was obtained for helium by Muntz\(^9\) and for nitrogen by Sharafutdinov\(^10\) when $\xi < 0.3$. Some experiments\(^9,10,11\) in the transition region have been performed, in which the increase in density can be observed when $0.3 < \xi < 5$. These results are consistent with the present calculations.

3.4 Nonequilibrium phenomena in a free jet

Figures 12 and 13 show the temperatures in the directions parallel and normal to the symmetric axis, normalized by the stagnation temperature $T_0$. The nonequilibrium of temperature appears throughout the flow field in the scattering regime (Fig.12). Figure 14 indicates the temperature profiles and the axial-flow velocity profile along the axis for $1/Kn = 50$ and $p_0/p_n = 50$, where the velocity is normalized by the most probable molecular speed $c_w$ at the stagnation. A macroscopic kinetic energy parallel to the axis (axial-flow velocity) changes at first into a microscopic energy of random velocity parallel to the axis (parallel temperature) and then into one normal to the axis (normal temperature). Figure 15 shows the distributions of the velocity components normal and parallel to the axis at $x/d = 4.5$ along the jet axis in the same condition as in Figs. 12 and 14, where the normal distribution represents the mean values of the velocity components for the $y$ and $z$ directions. The distribution of each velocity component corresponding to the above two temperatures is almost Maxwellian. On the other hand, near the continuum regime, both
temperatures are very similar except for an overshoot of the parallel temperature at the Mach disk (Fig. 13). The macroscopic kinetic energy changes into microscopic random energy at the location of the Mach disk, as shown in Fig. 16. Although the transformation of energy, owing to the sudden drop of the flow velocity, proceeds rapidly between the flow velocity parallel to the axis and the parallel temperature, since the increase in normal temperature needs the transformation of energy between the normal and parallel temperatures, it does not proceed so rapidly and an overshoot of the parallel temperature is induced. Bird also reproduced such an overshoot of the parallel temperature in one-dimensional shock wave analysis by the DSMC method.

4. Concluding Remarks

The DSMC method is used to simulate a free jet which expands to a finite background pressure and the following results are obtained.

1) The influence of the roughness of the cell network on the calculation is investigated. Although the locations of the shock waves shift slightly and the gradients of the flow quantities are somewhat reduced for a rough network of cells, the results of calculations would still be acceptable.

2) The minimum number of molecules in a cell is surveyed. In the present calculation for a free jet, it is sufficient that each cell has only one or more molecules on time average for reasonable results to be obtained.

3) The structure of the free jets can be characterized by the rarefaction parameter introduced by Muntz et al. into three regimes: the continuum, the transition and the scattering regimes.

4) The nonequilibrium translational temperatures between the directions normal and parallel to the jet axis are reproduced. In the scattering regime, the nonequilibrium appears throughout the flow field. In the continuum regime, on the other hand, the nonequilibrium is represented as an overshoot of the parallel temperature.

References


