Numerical Simulation of Rarefied Plume Flow
Exhausting from a Small Nozzle

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Abstract. This paper describes the numerical studies of a rarefied plume flow expanding through a nozzle into a vacuum, especially focusing on investigating the nozzle performance, the angular distributions of molecular flux in the nozzle plume and the influence of the backflow contamination for the variation of nozzle geometries and gas/surface interaction models. The direct simulation Monte Carlo (DSMC) method is employed for determining inside the nozzle and in the nozzle plume. The simulation results indicate that the half-angle of the diverging section in the highest thrust coefficient is $25^\circ - 30^\circ$ and this value varies with the expansion ratio of the nozzle. The descent of the half-angle brings about the increase of the molecules that are scattered in the backflow region.

INTRODUCTION

Satellites and spacecrafts are usually equipped with small thrusters for the attitude control and the trajectory of the vehicles. Exhaust gas from the thruster expands into the space vacuum and generates a huge plume, which causes the contamination of sensitive instruments in the vicinity of the thrusters. Hence, it is very important to understand accurately the flow structure inside the nozzle and in the nozzle plume. The above-mentioned nozzle scale is quite small and the thrust is very low. Under these conditions, several phenomena including rarefaction effect, viscous losses, nonequilibrium and backflow contamination influence the nozzle performance. The rarefied plume flow exhausting from such a nozzle experiences transition and free-molecular flow regimes. Consequently, the conventional continuum gas dynamics that are based on the concept of a local equilibrium may not be adequate, and an approach based on molecular gas dynamics is required for the analysis of the low-density nozzle flow.

Such a nozzle flow has been examined previously in experimentally [1] and numerically [2,3] investigations. Additionally, recently, there has been an increased interest in using "micro" and "nano" satellites in space science missions, and a number of micro-nozzle has been developed [4] and their performance has been experimentally and numerically [5] studied. The direct simulation Monte Carlo (DSMC) method of Bird [6] is widely used in molecular gas dynamics to analyze low-density gas flows, and the proper technique for calculating the nozzle plume flow. In the present paper, the DSMC method is employed in the analysis of the rarefied plume flow expanding through a nozzle into a vacuum, and the main focus of the present study is to examine the nozzle performance, the angular distributions of molecular flux in the nozzle flow and the influence of the backflow contamination for the variation of the nozzle geometries and gas/surface interaction model.

NUMERICAL METHOD

The DSMC method, first introduced by Bird, is a popular simulation technique for rarefied gas flows. In the DSMC method, a real gas is simulated by a large number of statistically representative particles. The positions, velocities and internal energies of these simulated particles are stored and modified in time in the process of particles motion and interaction with a wall. The core of the DSMC algorithm consists of four primary processes: move the particles, index and cross-reference the particles, simulate collisions, and sample
the flow field. In the present study, this DSMC method is employed in the analysis of the rarefied plume flow expanding through a nozzle into a vacuum.

Figure 1 shows the sorts of the nozzle geometries which is used in the present simulation, the axisymmetric conical type nozzle (left side) and the trumpet type nozzle (right side), where $D_1$ and $D_2$ indicate the diameters of the nozzle throat and the exit, respectively. $L$ is the nozzle length, the angle $\alpha$ is the half-angle of the diverging section and $R$ is the curvature of the trumpet type nozzle. In Table 1, the nozzle conditions in the present simulation are illustrated. The nozzle geometries of the cases 1 – 9 indicate the conical type, whereas that of the case 10 is trumpet type, where $R$ is set to 18 mm. The diameter of the nozzle throat $D_1$ is set to 0.3 mm for any cases. In the case of the conical type nozzle, two kinds of the expansion area ratios are considered, that is, 100:1 (cases 1 – 4) and 50:1 (cases 5 – 8). For each expansion ratio, the DSMC simulation of four sorts of half-angle ($\alpha = 15^\circ, 20^\circ, 25^\circ$ and $30^\circ$) is conducted. Moreover, the case 9 indicates the gas/surface interaction model of 80% diffuse - 20% specular reflection, it is compared with case 1, 100 % diffuse reflection model. The Reynolds number determined from the flow parameters in the nozzle throat and the throat width is 114, 226, 500 and 1140, corresponding to the Knudsen number at the nozzle exit $Kn = 0.01, 0.005, 0.002$ and 0.001. Wall conditions considered here are such that molecules impinging the nozzle wall suffer diffuse reflection (case 1 – 8, 10) and 80 % diffuse - 20 % specular reflection (case 9), and for the diffuse reflection, the temperature on the nozzle wall is assumed equal the reservoir temperature (300K). Nitrogen was adopted as test gases, and outflow conditions are imposed on ambient conditions. Collisions of molecules are simulated using the variable hard sphere (VHS) model [7]. The Borgnakke-Larsen statistical model [8] is employed for the calculation of the energy exchange between translational and rotational modes, together with temperature-dependent energy exchange probability of Boyd [9].

![Nozzle geometries](image)

**FIGURE 1.** Nozzle geometries

<table>
<thead>
<tr>
<th>Case</th>
<th>Expansion ratio</th>
<th>$\alpha$ [deg]</th>
<th>$L$ [mm]</th>
<th>$R$ [mm]</th>
<th>Ratio of diffuse ref.</th>
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<tr>
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</tr>
<tr>
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<td>7.5</td>
<td>-</td>
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<tr>
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<td>-</td>
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</tbody>
</table>
RESULTS AND DISCUSSION

Nozzle performance

First, we consider the nozzle performance for the variation of the nozzle geometries. Figure 2 shows Mach number profiles along the nozzle axis for the case 1, where \( x = -0.01 \) m indicates the nozzle throat and \( x = 0 \) m the nozzle exit. The theoretical Mach number at the nozzle exit is 6.94, however, Mach number in the simulation results is smaller than the theoretical value because of the viscous effects inside the nozzle. In the case of the Reynolds number \( Re = 114 \) and 228, Mach number is once decreased inside the nozzle.

Figure 3 shows the comparisons of thrust coefficient defined as the ratio of actual to ideal thrust force. The case 1, 2, 3 and 4 indicate the half-angle of diverging section \( \alpha = 15^\circ, 20^\circ, 25^\circ \) and \( 30^\circ \), respectively and the expansion area ratio is all 100:1 (see Table 1). For any cases, the simulation results present the descent of the thrust coefficient as the Reynolds number is decreased because the boundary layers inside the nozzle become thick as the effect of the rarefaction. In the cases of the lower Reynolds number (\( Re = 114 \) and 228), the thrust coefficient is increased as the half-angle \( \alpha \) becomes high, that is, the thrust coefficient is the largest at \( \alpha = 30^\circ \). On the other hand, for the higher Reynolds number (\( Re = 1140 \)), the maximum of the thrust coefficient is seen at \( \alpha = 25^\circ \). Therefore, more attention needs to be paid to determination of the half-angle according to the value of the Reynolds number at the nozzle throat.

In Fig. 4, the comparisons of the thrust coefficient for the various half-angles at expansion ratio 50:1 are illustrated. Unlike the case of expansion ratio 100:1, the maximum of the thrust coefficient is seen at \( \alpha = 25^\circ \) even if the Reynolds number is lower. Hence, the comparisons of two figures indicate that the half-angle at the maximum thrust coefficient varies with the expansion area ratio of the nozzle.

Next, the effect of wall interaction models inside the nozzle is investigated. The comparisons of the thrust coefficient between two different gas/surface interaction models are shown in Fig. 5. One model is 100% diffuse reflection (case 1) and the other one is 80% diffuse - 20% specular reflection (case 9). The axisymmetric conical type nozzle which is expansion ratio 100:1 and half-angle \( \alpha = 15^\circ \) is considered here as the nozzle geometry. The simulation results demonstrate that the thrust coefficient is increased by including the specular reflection as the gas/surface interaction model. Furthermore, in this figure, the comparisons between two different nozzle geometries are presented, the conical type (case 1) and the trumpet type (case 10). In the case of the trumpet type nozzle, the cross-section of the nozzle is rapidly increased near the nozzle exit, therefore, the density of the trumpet type at the nozzle exit is smaller than that of the conical type. Consequently, the thrust coefficient is decreased approximately 10% by changing the nozzle geometry from the conical type into the trumpet one.
Case 1 ($\alpha = 15^\circ$)  
Case 2 ($\alpha = 20^\circ$)  
Case 3 ($\alpha = 25^\circ$)  
Case 4 ($\alpha = 30^\circ$)  

Expansion ratio 100:1

Thrust coefficient

**FIGURE 3.** Comparisons of thrust coefficient for various half-angles of diverging section (expansion area ratio 100:1)

Case 5 ($\alpha = 15^\circ$)  
Case 6 ($\alpha = 20^\circ$)  
Case 7 ($\alpha = 25^\circ$)  
Case 8 ($\alpha = 30^\circ$)  

Expansion ratio 50:1

**FIGURE 4.** Comparisons of thrust coefficient for various half-angles of diverging section (expansion area ratio 50:1)

Case 9 (diffuse 80%)  
Case 10 (trumpet type)

**FIGURE 5.** Comparisons of thrust coefficient for various types of the nozzles

**Nozzle plume**

In Fig. 6, the sphere considered the center of the nozzle exit plane as the center of the sphere is illustrated. The angular distributions of molecular flux is defined as the distributions of molecular flux effusing from the nozzle into the spherical unit solid angle $d\omega$. In the present simulation, since the axisymmetric nozzle is employed, the following equation is satisfied,

$$
\int_{4\pi} f(\theta) d\omega = 2\pi \int_0^\pi f(\theta) \sin \theta d\theta = 1
$$

(1)
where \( f(\theta) \) is called the angular distributions of the molecular flux [10]. Figure 6 also shows a plane of \( \phi = 0 \) (a \( xy \)-plane). The molecular flux effusing into the region of \( \theta > \pi / 2 \) is treated as the backflow. In the case of the free molecular flow, these angular distributions are dependent on only the geometry of the nozzle because the nozzle plume is collisionless flow. However, if there are intermolecular collisions in the nozzle plume, the angular distributions may vary with not only the geometry of the nozzle but also the Knudsen number and the Reynolds number of the nozzle throat. Therefore, the detail investigation of the angular distributions for the nozzle plume is required.

**FIGURE 6.** molecular flux effusing from the nozzle into the spherical unit solid angle

**FIGURE 7.** Comparison the nozzle plume between translational temperature (upper) and rotational one (lower) for \( Re = 228 \)

**FIGURE 8.** Comparison the nozzle plume between translational temperature (upper) and rotational one (lower) for \( Re = 1140 \)
FIGURE 9. Comparisons of angular distributions of molecular flux for various Reynolds numbers (expansion area ratio 50:1).

FIGURE 10. Comparisons of angular distributions of molecular flux for various half-angles of diverging section (expansion area ratio 50:1).

FIGURE 11. Comparisons of angular distributions of molecular flux for various types of the nozzle.

Figures 7 and 8 show the DSMC simulation results of the translational and rotational temperature for case 5 ($Re = 228$ and 1140, respectively). It is apparent that the boundary layers become thin inside the nozzle as the Reynolds number is increased. The number of simulated molecules that are scattered in the higher angle $\theta$ is extremely low, therefore, the rotational temperature in this region is higher than the translational one due to the decrease of the translational and rotational energy exchange.

In Fig. 9, the angular distributions of the molecular flux $f(\theta)$ is compared for various Reynolds numbers. Due to the increase of the intermolecular collisions, the angular distributions in the region where the angle $\theta$ is small ($\theta < 30^\circ$) are increased, and for the larger angle ($\theta > 30^\circ$) the angular distributions are decreased, as a result, the profile of the angular distributions is peaked.

Figure 10 shows the comparisons of the angular distributions of the molecular flux for various half-angle of. The angular distributions of small angles ($\theta < 40^\circ$) is almost identical for any cases, however, the discrepancy between these cases is seen as the angle $\theta$ becomes large. Hence, it is apparent that the influence of the backflow is increased as the half-angle of the nozzle is small.
The comparison of the angular distributions between two gas/surface interaction models is presented in Fig. 11. The angular distribution of case 5 is nearly identical to that of case 1 at $\theta < 55^\circ$, whereas, a little discrepancy between two models is seen at $\theta > 55^\circ$. Figure 11 also illustrated the comparison between the conical and the trumpet type nozzle. The simulation results indicates that, as well as the case 5, the angular distributions of the trumpet type is smaller than that of the conical type at $\theta > 55^\circ$. Consequently, by changing the nozzle geometry into the trumpet type, the influence of the backflow may be reduced.

**Backflow contamination**

Finally, the influence of the backflow contamination is investigated in more detail. As shown in Fig. 6, the molecular flux scattering into the region of $\theta > \pi/2$ is considered as the backflow. Therefore, the ratio of the molecular flux effusing into the backflow region to the total molecular flux, backflow ratio is given by

$$P_{bf} = \frac{2\pi \int_{\pi/2}^{\pi} f(\theta) \sin \theta d\theta}{\pi}$$  \hspace{1cm} (2)

Figure 12 presents the comparisons of the backflow ratio between various half-angles of the diverging section. The smaller half-angle of the nozzle leads to the decrease of the thrust coefficient and Mach number at the nozzle exit. Therefore, the expansion angle at the edge of the nozzle exit is increased, and as a consequence, this causes the increase of the backflow ratio. For the cases 1, 2 and 3, the backflow ratio descends as intermolecular collisions are increased, whereas for case 4, the backflow ratio once is decreased and after that, it is slightly increased at $Re > 224$. Due to specify whether the minimum value of the backflow ratio exists for the half-angle except $\alpha = 30^\circ$, the calculation in the wider range of the Reynolds number is required.

In Fig. 13, the comparisons of the backflow ratio for expansion area ratio 50:1 are shown. As well as the expansion ratio 100:1, the smaller half-angle of the nozzle gives rise to the ascent of the backflow ratio except $Re = 1140$. In the cases of $\alpha = 25^\circ$ and $30^\circ$, the backflow ratio is slightly increased at $Re > 570$. The comparisons of two figures demonstrate that the descent of the expansion ratio brings about the increase of the backflow ratio.

The comparisons of backflow ratio for various types of nozzles are illustrated in Fig. 14. It is apparent that the backflow ratio is decreased by including the specular reflection as the gas/surface interaction model. Moreover, for the trumpet type nozzle, the simulation results indicate the descent of the backflow ratio.
CONCLUSIONS

The DSMC simulation of a rarefied plume flow expanding through a nozzle into a vacuum is conducted, especially focusing on the nozzle performance, the angular distributions of the molecular flux in the nozzle plume and the influence of the backflow contamination. As the Reynolds number is small, the thrust coefficient is decreased because the boundary layers become thick as the effect of the rarefaction. Consequently, this causes the descent of Mach number at the nozzle exit, therefore the angular distributions are gentle and the backflow ratio is increased. Concerning the half-angle of the diverging section, the smaller half-angle leads to the ascent of the backflow ratio. By including specular reflection as the nozzle wall conditions, the thrust coefficient is increased, and the backflow is reduced. Furthermore, the trumpet type nozzle causes the descent of the thrust coefficient, whereas the influence of the backflow is reduced.

REFERENCES