Numerical Simulation of Flows Field Characteristics of High Altitude Liquid Rocket Exhaust Plume

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Abstract. The simulation of flow field structures of high altitude liquid rocket exhaust plume is of great significance for infrared radiation calculation. Considering the flow field’s symmetry construction, half of the 2-D zone was chosen as the calculation zone. In order to reduce the amount of calculation, we had made an equivalent reduction of the calculation zone. By using the direct simulation Monte Carlo (DSMC) method, a solver was constructed to simulate the flow field structure of the 120km altitude liquid rocket exhaust plume. The simulation results show that the flow field of the high altitude liquid rocket exhaust plume has the following three characteristics: a. the whole flow field indeed contains continuous flow and rarefied flow; b. rarefied gas effect plays a significant role to form a recirculation zones that surpass the nozzle; c. Non-equilibrium effect is remarkable in shock wave region and the boundary layers.

1. Introduction

The rocket engine plume is the product of the interaction between the rocket engine jet and the atmospheric environment. Different working conditions or atmospheric environment for rocket engine will result in different flow field structures of the exhaust plume, which in turn will display diversified infrared radiation characteristics.

As we all know, there are two types of rocket engines: solid and liquid. The flow field characteristics in high altitude are different due to the different rocket engines. The liquid rocket exhaust plume in high altitude contains continuous gas flow and rarefied gas flow without particles. The solid rocket exhaust plume is characterized by a highly rarefied two-phase flow composed of alumina particles whose flow field simulation is more complicated. Therefore, this study only focuses on the simulation of flow field characteristics of high altitude liquid rocket exhaust plume, which is the basis of infrared radiation simulation of liquid rocket exhaust plume.

In the past decades, many studies had been carried out on flow field simulation of rocket exhaust plume, most of which, however, were focused on relatively low to medium altitudes used by computational fluid dynamics (CFD) method\textsuperscript{[1]}. The high altitude rocket exhaust plume, above 100 km, for which flow field structure may have different characteristics from that at the low or medium altitudes.
In recent years, some simulations have been done on the flow field of high altitude plumes. Candler et al.\cite{2}, Vitkin et al.\cite{3} carried out the solution of Navier-Stokes equations for the gas simulation, which is not accurate for rarefied gas flow of the plume. Burt and Boyd conducted their studies using a DSMC-based simulation (Direct Simulation Monte Carlo) which allows the treatment of rarefied aspects of the plume\cite{4}. However, DSMC method is too long for calculating continuous flow without necessary simplification. The domestic Cai Guojun and Xu Xiaoying team numerically simulated the high-altitude molecular flow field and independently developed the plume calculation software (PWS) using the DSMC method, but they did not take disequilibrium into account\cite{5,6}.

In order to make up for the limitations of domestic and foreign research, our study deals with simulation of flow field characteristics of high altitude plume in liquid rocket using a DSMC, with the aspects of rarefied and disequilibrium taken into account.

2. The direct simulation Monte Carlo solver

The direct simulation Monte Carlo (DSMC) method was first used by Bird (1994), which has gained acceptance as an accurate, robust and broadly applicable technique for modeling gas flows under disequilibrium conditions over several decades\cite{7}.

A solver is constructed to simulate the flow field structure of the high altitude plumes based on DSMC method as follow steps\cite{8}. Frist, the flow field area is divided into several computational grids. A limited number of simulated molecules are used in each computational grid to replace a large number of real gas molecules. Second, the molecular motion is decoupled from the collision. Molecular motion is solved according to Newton's law and updated the grid in which the molecules are located based on the latest position. Third, a hard sphere collision model is established to describe intermolecular collisions. During each time step, some fraction of the molecules in a grid collided with each other, and probabilistic techniques are used for calculations of individual collisions. All molecules are then moved through the grid according to assigned velocities. Finally, all the calculation grids are iterated several times, and the macroscopic physical parameter distribution of the flow field is statistically obtained.

As no assumptions are made about the shape of the gas velocity distribution, the DSMC method retains validity for all flow regimes between free molecular and continuum, so long as binary collisions are the dominant type of molecular interaction. The equilibrating effect of these collisions may be characterized by the Knudsen number (Kn), which is defined as the ratio of the gas mean free path to a macroscopic length scale based on boundary dimensions, flow structures or gradients in bulk gas properties\cite{9}.

3. Parameters of instance

The reference coordinate system is set first for the ease of analysis. We set the nozzle axis as the z-axis, the center of the nozzle as z=0, and the direction away from the nozzle as positive. The solid angle direction of the zenith angle is set to coincide with the positive direction of the z-axis.

The parameters of the flow field are set on the supposition that rockets fly at the altitude of 120 km as follows: considering the flow field’s symmetry construction, half of the 2-D zone is chosen as the calculation zone shown in Fig. 1. The size of the calculation zone is 150 m x 30 m, the radius of the throat and outlet of nozzle are 10 cm and 30 cm respectively. The boundary conditions definitions are shown in Table 1. Neglecting the unimportant species, the species calculated in this paper are shown in Table 2. Collision between gas phases is selected as a hard ball collision model.
Table 1. Boundary conditions definitions

| zone | Boundary type         | pressure (MPa) | Temperature (k) | Velocity (Ma) |
|------|-----------------------|----------------|-----------------|---------------|
| AB   | Pressure inlet        | 4.8            | 3550            | ——            |
| CD   | Pressure far field    | 0.1            | 500             | 0.2           |
| DE   | Pressure far field    | 0.1            | 500             | 0.2           |
| EF   | Pressure outlet       | 0.1            | 500             | ——            |

Table 2. Mole fractions of species in the combustion chamber and in the free stream

| Species | Combustion chamber | Free flow |
|---------|--------------------|-----------|
| H₂O     | 0.5                | 0         |
| CO₂     | 0.1                | 0         |
| N₂      | 0.4                | 0         |

In order to reduce the computational complexity, it is considered that the nozzles are evenly distributed, and the nozzle parameters are calculated by the FLUNT software to obtain an average gas velocity of 2776.364 m/s, a temperature of 1918.450 K, a pressure of 0.916 atm, and a density of 0.011 kg/m³. The time step is 1×10⁻⁷ s.

Although the mesh division as mentioned above is set in perfect condition, the calculation needs further simplifying, as the actual amount is still excessively large. The final calculation domain size is reduced by 5000 times for calculation. The grid is automatically generated by the program, 300 grids are arranged in the x direction, 100 grids are arranged in the y direction, and two sub-grids are arranged in the x and y directions in each grid. For the adaption of the DSMC’s grid scale requirements (approximately one-third of the mean free path), a uniform grid is used in x-direction, and an exponential function relationship grid is used in y-direction. The final calculated grid is shown in Fig. 2.
4. Results and Discussions
Substituting the calculated initial conditions into the above calculation steps, the flow field calculation results are as follows: Fig. 3 presents the average density profiles of mixed gas. Fig. 4 presents the density contour map of mixed gas. Fig. 5 presents the speed cloud map in the X direction.

As shown in Fig. 3 and Fig. 4, since the external environment is a vacuum, the gas rapidly expands after exiting the nozzle, and no low-altitude Mach disk is formed. Moreover, the gas density is larger near the outlet of the nozzle, and the farther the gas is diffused away from the nozzle, the density gradually decreases. As can be seen from Fig. 5, there is a region where the x velocity is negative above the nozzle, indicating the existence of a significant recirculation zone. That is one of the characteristics which could not be found at the low flow field. The calculation results are consistent with the conclusions given in literature[10].

It can be seen in conjunction with Fig. 3, Fig. 4 and Fig. 5 that there is a region where the density gradient changes more intensely in the region close to the recirculation zone, and the contour changes are unstable. The reason for this phenomenon is that the rarefied gas effect of these regions is significant, and the number of simulated molecules is small, resulting in a large statistical fluctuation. In the future, it is necessary to increase the mesh density in these regions, and to translate the calculated boundary from the CD to the AB position (as shown in Fig. 1), which will lead to more accurate calculation results.

![Figure 3. The average density profiles of mixed gas](image1)

![Figure 4. The density contour map of mixed gas](image2)
Figure 5. The speed cloud map in the X direction.

The temperature cloud diagram of the mixed gas is shown in Fig. 6, the translational temperature cloud diagram is shown in Fig. 7, and the rotation temperature cloud diagram is shown in Fig. 8. In rarefied gas, the translational temperature is a measure of the difference in molecular translational kinetic energy.

It can be seen from Fig. 7 that in the recirculation zone, the difference in the kinetic energy of the gas molecules in the grid is large, resulting in a high temperature distribution in the recirculation zone. The rotational temperature is proportional to the rotational energy and inversely proportional to the rotational freedom. It can be seen from Fig. 7 and Fig. 8 that the distribution trend of the translational temperature and the rotational temperature is basically the same, but the rotational temperature is higher than the translational temperature as a whole, which indicates that shock wave and the boundary layer have a non-equilibrium effect, and the rarefied gas effect is remarkable.

Figure 6. The temperature cloud diagram of the mixed gas

Figure 7. The translational temperature cloud diagram of the mixed gas
Figure 8. The rotation temperature cloud diagram of the mixed gas

The Knudsen number is usually used to divide the boundary between the rarefied flow and the continuous flow. The region where the Knudsen number surpassing 0.05 is generally considered to be a rarefied flow region. Therefore, we will enlarge the nozzle outlet, and the Knudsen number cloud map is shown in Figure 9. The red areas are rarefied flow, and the other color areas are continuous flow. The entire liquid rocket plume flow field is indeed a mixed flow field containing continuous flow and rarefied flow.

Figure 9. The Knudsen number cloud map near the nozzle outlet

5. Summary

The high altitude liquid rocket exhaust plume flow field contains continuous flow and rarefied flow, so the traditional CFD method is no longer applicable. The direct simulation DSMC method is needed. Existing studies are only limited on the calculation of the flow field characteristics of high altitude liquid rocket exhaust plume in partial rarefied flow, instead of the whole flow.

To remedy the limitation, this study simulates liquid rocket plume flow field at high altitude by DSMC through dynamic meshing and scaling reduction techniques. Significant rarefied gas effect in high altitude liquid rocket flow field and rapid gas-phase molecular expansion brings about recirculation zones that surpass the nozzle. The rotational temperature is higher than translational and rotational temperature, which indicates non-equilibrium effect is remarkable in shock wave region and the boundary layers. It is foreseeable that high altitude flow field characteristics of liquid rocket exhaust plume, which are different from low-altitude flow field, will cause huge changes in infrared radiation of high altitude liquid rocket exhaust plume.

Various rational approximation is employed in the above-mentioned algorithm indeed, such as the assumption that the parameters at the nozzle exit are evenly distributed and the adoption of shrink ratio thought to reduce the calculation amount on flow field. Further and deeper studies study will be carried out to obtain the infrared radiation data in the future on the basis of the accurate simulation of high altitude exhaust plume flow field as mentioned above. These data are worthwhile to provide relevant industrial sector for the detection and penetration of rockets.
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