



The angular distribution at the outlet of a capillary in a wide range of rarefaction



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ABSTRACT

The angular distribution at the outlet of a capillary is an important topic in rarefied gas dynamics. Here the procedure to calculate the near field angular distribution based on velocity distribution function or DSMC (Direct Simulation Monte Carlo) method was proposed. Then, the angular distribution at the outlet of cylindrical capillary was evaluated with different rarefaction parameter δ using DSMC method with open source solver dsmcFoam. The results showed that the normalized flux intensity at small polar angle decreased with δ when δ was smaller than 10, and the distribution did not approximate the cosine distribution when δ at the inlet was large enough. Besides, capillary with conical end was also evaluated. The results showed that the conical end could decrease the divergence of the beam even δ at the inlet increased to 50 when the outlet was set as vacuum. Last, the influence of CL (Cercignani Lampis) accommodation coefficients and VSS (Variable Soft Sphere) parameters on the angular distribution was studied.

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1. Introduction

The study of the flow through a capillary or tube is a popular problem in rarefied gas dynamics, and a detailed summary of the research state on the topic was described in the review [1]. Within the studies of the flow through a capillary in rarefied regime, the angular distribution at the outlet is an important topic, especially in the design and calibration of an atomic hydrogen source which is based on hot capillary [2,3], and it will also be important in the design of the outgassing exit of an object in outer space.

The analytic form of the far field angular distribution at the exit of a cylindrical capillary in the free molecular regime has been derived with the simplification of intermolecular collisions, and the deductions were based on diffuse reflection model and the approximation that the number density on the wall along the capillary axis was linear [4,5]. Besides the analytic deduction, test particle Monte Carlo method was also used to calculate the angular distribution at the outlet of capillary [2,6,7]. In Refs. [2,6], the angular distribution at the outlet of a cylindrical capillary based on diffuse reflection was calculated. In Ref. [7], the angular distribution at the outlet of a cylindrical capillary with conical end was studied,

the distribution was based on CL reflection, and the influence of CL accommodation coefficients on the distribution was also evaluated.

However, only the angular distribution at the capillary outlet in the free molecular regime has been studied, and the intermolecular collisions are ignored. Here we will focus on the angular distribution at the outlet of a capillary in a wide range of rarefaction, and the distribution is based on the CL reflection model and VSS collision model. First, the procedure to calculate the near field angular distribution based on the velocity distribution function and DSMC method is proposed. Then, the angular distributions at the outlet of cylindrical capillary and capillary with conical end are calculated using DSMC method based on the open source solver dsmcFoam [8–10]. Finally, the influences of the CL accommodation coefficients and the VSS parameters on the angular distribution are evaluated.

2. The theory

2.1. The angular distribution at the capillary outlet in a wide range of rarefaction

2.1.1. Analytic solution when the velocity distribution is available

When the velocity distribution function $f(t, \mathbf{r}, \mathbf{v})$ is already available, it is viable to get the near field angular distribution at the outlet of the capillary. First, get the velocity distribution function $f_0(t, \Delta t, \mathbf{r}, \mathbf{v})$ of the molecules that can reach the outlet, or find the

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constraint equation $r(t, \Delta t, \mathbf{r}, \mathbf{v})$ that can assure that the molecules satisfying the constraint equation can reach the outlet within time interval Δt . Δt is set as a fraction of Δt_c (the mean free time between collisions), so that the collisions between molecules can be ignored within time interval Δt .

Then, integrate the velocity distribution function over the whole fluid region, and we can get the near field velocity distribution at the outlet,

$$f_c(t, \mathbf{v}) = \lim_{\Delta t \rightarrow 0} \int f_o(t, \Delta t, \mathbf{r}, \mathbf{v}) d\mathbf{r}, \quad (1)$$

or

$$f_c(t, \mathbf{v}) = \lim_{\Delta t \rightarrow 0} \int_{r(t, \Delta t, \mathbf{r}, \mathbf{v})} f(t, \mathbf{r}, \mathbf{v}) d\mathbf{r}. \quad (2)$$

With coordinate system conversion, the velocity distribution $f_c(t, \mathbf{v})$ can also be expressed as $f_s(t, v, \varphi, \theta)$, where v is the magnitude of the velocity, φ is the polar angle of the velocity, and θ is the azimuth angle of the velocity.

Last, integrate the velocity distribution function $f_s(t, v, \varphi, \theta)$ over v and θ , we can get the near field angular distribution at the outlet,

$$f_a(t, \varphi) = \int \int f_s(t, v, \varphi, \theta) d\theta dv. \quad (3)$$

When the flow through capillary is in a steady state, the velocity distribution does not vary with the time, then the angular distribution can be expressed as

$$R(v_{it}, v_{rt}) = \frac{1}{\sqrt{\pi\sigma_t(2-\sigma_t)}} \exp\left(\frac{-(v_{rt} - (1-\sigma_t)v_{it})^2}{\sigma_t(2-\sigma_t)}\right)$$

$$R(v_{in}, v_{rn}) = \frac{2v_{rn}}{\pi\alpha_n} \exp\left(\frac{-(v_{rn} - (1-\alpha_n)v_{in})^2}{\alpha_n}\right) \int_0^\pi \exp\left(\frac{2(1-\alpha_n)^{1/2}v_{rn}v_{in}}{\alpha_n} \cos\theta\right) d\theta, \quad (6)$$

$$f_a(\varphi) = \int \int f_s(v, \varphi, \theta) d\theta dv. \quad (4)$$

2.1.2. Numerical solution based on the direct simulation of the physics of the flow

The DSMC method is a solution of the Boltzmann equation based on the direct simulation of the physics of the flow [11]. In DSMC simulation, the molecular motion and intermolecular collision are uncoupled in a small time step Δt by the repetition of the following procedure:

1. Calculate the position of the molecules based on their velocities within time step Δt . If the trajectory intersects with the boundary, the gas-surface interaction is performed according to a given scattering law, and the movement of the molecules is calculated within the residual time after gas-surface interaction.
2. Generate new molecules at boundaries where there is an inward flux, and compute a representative number of collisions corresponding to Δt and the number of molecules in the cell. The velocities of the molecules after collision are replaced by the

post-collision values in accordance with a given law of the intermolecular interaction.

When the gas flow is stabilized at a specific time t in the simulation, we can get the velocity distribution function $f(t, \mathbf{r}, \mathbf{v})$ by analyzing the velocities of the molecules in every cell, and then the analytic solution can be used to calculate the angular distribution at the outlet. Alternatively, it is easier to get the angular distribution at the outlet by simply analyzing the velocities of the molecules that leave the outlet boundary within time step Δt (or within several Δt after the flow in the capillary is stabilized) in DSMC simulation.

2.2. The reflection on the wall and the intermolecular collisions

It can be seen from subsection 2.1 that the gas-surface interaction and the intermolecular interaction are the main processes that can alter the molecule's velocity. Here we will use the CL reflection model and the VSS collision model in the calculation.

2.2.1. The CL reflection

The reflection on the wall can be characterized by the scattering kernel $R(\mathbf{v}_i, \mathbf{v}_r)$, and the distribution after reflection is

$$f^+(\mathbf{v}_r) \mathbf{v}_r \cdot \mathbf{n} d\mathbf{c}_r = - \int_{\mathbf{c}_i \cdot \mathbf{n} < 0} R(\mathbf{v}_i, \mathbf{v}_r) \mathbf{v}_i \cdot \mathbf{n} f^-(\mathbf{v}_i) d\mathbf{v}_i \cdot d\mathbf{v}_r, \quad (5)$$

where $f^-(\mathbf{v}_i)$ and $f^+(\mathbf{v}_r)$ denote the distribution functions of the incident molecules and the reflected molecules, and \mathbf{n} is the unit normal vector of the wall surface. The scattering kernels of tangential and normal velocity for CL reflection [11,12] are

where σ_t is the accommodation coefficient due to the tangential moment, α_n is the accommodation coefficient due to the energy of the normal velocity, v_{it} and v_{in} are the tangential and normal components of the incident velocity, v_{rt} and v_{rn} are the tangential and normal velocity components after reflection.

The implementation of CL reflection model in DSMC simulation has been described by Ref. [13]. First, all the velocity components are normalized by $\beta = (2kT_w/m)^{1/2}$, where k is the Boltzmann constant, T_w is the temperature of the wall, and m is the molecule mass. Then, the velocity components after reflection can be expressed as

$$\begin{aligned} v_{rt1} &= \bar{v}_t + r_1 \cos \theta_1 \\ v_{rt2} &= r_1 \sin \theta_1 \\ v_{rn} &= \left(\bar{v}_n^2 + 2r_2 \bar{v}_n \cos \theta_2 + r_2^2 \right)^{1/2}, \end{aligned} \quad (7)$$

where v_{rt1} , v_{rt2} are the tangential velocity components after reflection, $\bar{v}_t = (1-\sigma_t)v_{it}$, $r_1 = \sqrt{-\sigma_t(2-\sigma_t)\ln \xi_1}$, $\theta_1 = 2\pi\xi_2$, $\bar{v}_n = \sqrt{(1-\alpha_n)v_{in}}$, $r_2 = \sqrt{-\alpha_n \ln \xi_3}$, $\theta_2 = 2\pi\xi_4$, and $\xi_1, \xi_2, \xi_3, \xi_4$ are random numbers evenly distributed over (0,1). The diffuse reflection model is a special case of CL reflection model with $\alpha_n = 1$ and

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