The Positional and Angular Distribution of Molecules Flowing through Cylindrical Tube in Free Molecular Flow

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Abstract
To investigate the distribution of gas molecules passing through cylindrical tube in free molecular flow, the molecules are divided into "directly passing" ones which pass through from inlet to outlet directly and "reflective" ones which are reflected from inner wall to outlet and inlet, and mathematical models for the two kinds are established. The relative molecular incident rates (equal to the reflectivity) along tube wall are obtained by means of discretization and series accumulation, and they are illustrated as a series of straight lines. The molecular positional distribution is described by the local relative molecular areal density at different position of orifices and is researched in detail with analytical derivation, numerical integration and graphics. The "positional beaming effect" at outlet is demonstrated. The molecular directional distribution graphs at different positions are drawn as the curved surfaces within a unit sphere which corresponds to the cosine distribution style. The graphs at each point show the characteristics of sub-zone, discontinuation and axis asymmetry. It is also proved that the distributions at every point of outlet and inlet are complementary with each other both positionally and angularly.

1. Introduction
It is a traditional problem of gas kinetics that gas molecules flow in a cylinder tube in the free molecular flow. The “beaming effect”, as one of the typical problem of molecular gas dynamics, has been studied for a long time. It means that when the gas molecules flow in a cylinder tube in the free molecular flow, the angular distribution of escaping molecules at orifices deviates from the cosine law, which is originally obeyed by the molecules during the incidence and reflection.[1-8] Recent research also discovered that the positional distribution of escaping molecules is not uniformly distributed, although incident density distribution is even.[9-10] The “beaming effect” has a significant effect on some of ultra high vacuum systems in molecular flow, such as the cryopump and molecular beam epitaxy [11].

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Most former scholars studied the “beaming effect” by Monte Carlo simulation method and got the approximate statistical results about whole orifice[1-10]. In this paper, both the "positional beaming effect" and "angular beaming effect" at different position on orifices are quantitatively researched in detail with analytical derivation and numerical integration.

2. Hypothesis and Models

2.1 Basic Hypothesis

- The flow is free molecular flow, i.e. the collisions between gas molecules are neglected.
- The flow is steady, i.e. the molecular incident rate keeps constant.
- At inlet, molecules enter the tube evenly in position, and coincide with the cosine law in angle.
- The molecular incident rate equals to the molecular reflectance rate at any point on the inner wall of tube.
- After colliding with the inner wall of tube, molecules still follow the cosine law when reflecting.
- The molecules having left the tube are not taken account of again, i.e. the backflow from outlet is neglected.

2.2 Classification of Two Kinds of Molecules

Molecules entering into the tube from inlet can be divided into two parts: one is those which do not collide with tube wall, and pass through outlet directly; the other is those which collide with tube wall. Similarly, molecules leaving the tube can also be divided into two parts: one is the "directly passing" molecules which pass through the tube directly, and their passing model is shown in Fig. 1; the other is the "reflective" molecules which collide with tube wall at least one time before leaving tube through outlet or inlet, and their passing model is shown in Fig. 2. The molecules arriving at the outlet include both "directly passing" and "reflective" ones. The molecules returning to the inlet are all the "reflective" ones.

2.3 The Model for Directly Passing Molecules

In Fig.1, gas molecules pass through the tube from inlet area element $dS$ directly to outlet area element $dA$. $L$ is the tube length and $R$ is the tube radius. $r_i$ is the radius vector from the centre of inlet to $dS$. $r_o$ is the radius vector from the centre of outlet to $dA$. $\beta$ is the angle between outgoing direction and normal line of $dA$, and it is defined as "polar distance angle". Fig.1 (b) is the view opposite z axis direction. $\theta_i$ is the angle between vector $r_i$ and vector $r_o$. $\phi$ is the angle between $AB$ and x axis, and it is defined as "azimuth angle". $d$ is the diameter of the tube, $d = 2R$. $\rho_i$ is the radius vector from $dS$ to $dA$. $\rho_i^2 = L^2 + r_i^2 + r_o^2 - 2 \cdot r_i \cdot r_o \cdot \cos \theta_i$.

![Fig. 1 Model for directly passing molecules from inlet to outlet](image-url)
According to the cosine law, the number of molecules flying directly from inlet area element $dS$ to outlet area element $dA$ is given by

$$dN_{dS-dA}(r_s) = \gamma \cdot dS \cdot \frac{1}{\pi} \cdot \cos^2 \beta \cdot \frac{1}{\rho_1^2} \cdot dA$$

(1)

Where $\gamma$ is the molecular incidence rate at inlet. $dS = r_i \cdot dr_i \cdot d\theta_i$ is substituted into Eq (1). Eq. (1) can be written as

$$dN_{dS-dA}(r_s) = \gamma \cdot \frac{L^2}{\pi} r_i \cdot dr_i \cdot d\theta_i \cdot dA$$

(1a)

By the integral to $dr_i$ and $d\theta_i$, the number of molecules from whole inlet cross section directly to $dA$ can be acquired

$$dN_{dS-dA}(r_s) = \frac{\gamma \cdot L^2}{\pi} \int_0^1 r_i \int_0^{2\pi} \frac{r_i}{\rho_1} d\theta_i$$

(2)

According to geometrical similarity, in all latter calculations, it is assumed that the diameter of the tube $d = 1$, that is $R = 0.5$, and the tube length is defined as times of diameter.

2.4 The Model for Reflective Molecules

In Fig.2, gas molecules reflect on tube wall and fly from wall area element $dW$ to outlet area element $dA$. $z$ is the axial distance from inlet to $dW$. Fig. 2 (b) is the view opposite $z$ axis direction. $\theta_2$ is the angle between $\overline{AO}$ and $\overline{BO}$. Both $\beta$ and $\phi$ are the same with Fig. 1, i.e. the "polar distance angle" and "azimuth angle" respectively. $\rho_2$ is the radius vector from $dW$ to $dA$. $R$ is the radius of the tube. $\rho_2^2 = (L-z)^2 + R^2 + r_o^2 - 2 \cdot R \cdot r_o \cdot \cos \theta_2$ for outlet, or $\rho_2^2 = z^2 + R^2 + r_o^2 - 2 \cdot R \cdot r_o \cdot \cos \theta_2$ for inlet. $\psi$ is the angle between $\rho_2$ and the normal line of $dW$. $\cos \alpha_2 = (R-r_o \cdot \cos \theta_2)/\rho_2$. $\beta_2$ is the angle between $\rho_2$ and the normal line of $dA$. $\cos \beta_2 = (L-z)/\rho_2$ for outlet, or $\cos \beta_2 = z/\rho_2$ for inlet.

![Diagram](image_url)

According to the cosine law, the number of molecules reflecting from the area element $dW$ to the area element $dA$ at outlet is given by

$$dN_{dW-dA}(z, r_o) = \frac{\gamma'(z)}{\pi} \cdot \cos \alpha_2 \cdot \cos \beta_2 \cdot \frac{1}{\rho_2^2} \cdot dW \cdot dA$$

(3)

As $dW = R \cdot d\theta_2 \cdot dz$, the total number of molecules reflecting from whole tube wall to the area element $dA$ at outlet is
3. Relative Incident Rate Distribution along Inner Tube Wall

3.1 Conception

Prior to calculating the distribution of "reflective" molecules, the reflectivity $\gamma'(z)$ distribution along tube wall should be acquired. Given hypothesis 3, reflectivity at any point on the inner wall of tube is equal to its incident rate. Under steady flow, if the incident rate at inlet $J$ is constant, the reflectivity $\gamma'(z)$ is stable along the tube, and its value is determined by the distance from reflecting location to inlet. $\gamma'(z)$ is proportional to inlet incident rate $\dot{J}$ and is expressed by

$$\gamma'(z) = h(z) \cdot \gamma$$  \hspace{1cm} (5)

where $z$ is the distance from reflecting location to inlet and is set as times of diameter, $h(z)$ is relative incident rate along tube wall. The target of this section is to obtain $h(z)$.

3.2 Formula

In the research of transmission probability, former scholars had deduced relative incident rate[12-14]. Relative incident rate can be written by

$$h(x) = \int_0^L w_{rr}(\xi - x) \cdot h(\xi) \cdot d\xi + \frac{R}{2} w_{sr}(x)$$  \hspace{1cm} (6)

where $w_{rr}(\xi - x)$ is the probability that a molecule, which is in accordance with the cosine law, leaves an element ring located at a distance $\xi$ from inlet, strikes directly another element ring located at a distance $x$ from inlet. $w_{sr}(x)$ is the probability averaged over the inlet cross section that a molecule leaving the inlet section strikes directly a element ring at a distance $x$ from inlet. The former polynomial is the contribution by the whole tube wall reflection. The latter polynomial is the contribution by inlet incidence. The superposition is the reflectivity of the reflecting point.

Since Eq. (5) is difficult to be solved analytically. Here we execute approximate calculation by numerical computation. The method is to divide the tube into numerous element rings, as shown in Fig. 3. The element ring length $b = L/n$, thus reflectivity of one element ring $i$ is the contribution by both all other elements and inlet.

![Fig. 3 The tube is divided into numerous element rings](image)

The relative incident rate can be transformed into

$$h(l_i) = \sum_{j=1}^{n} h(l_j) \cdot g_{ij} + g_{ii}$$  \hspace{1cm} (7)
where $l_i = i \cdot b$ and $l_j = j \cdot b$, $g_{ji}$ is the probability that a molecule which leaves element $j$ strikes directly element $i$, $g_{0i}$ is the probability that a molecule strikes directly element $i$ from inlet. $g_{ji}$ and $g_{0i}$ are expressed as follows:

$$g_{ji} = \frac{b \cdot R_j}{\pi} \int_0^{\pi} \frac{(1 - \cos \theta)^2}{\left(2R^2(1-\cos \theta) + [(j-i)b]^2\right)^2} d\theta$$

$$g_{0i} = \frac{2b \cdot R}{\pi} \int_0^{\pi} \frac{r_i \cdot (i \cdot b) \cdot (R-r_i \cdot \cos \theta)}{[(i \cdot b)^2 + R + r_i^2 + 2R \cdot r_i \cdot \cos \theta]^2} d\theta \cdot dr_i$$

### 3.3 Results

Let $b = 0.001d$ and $l_i = i \cdot b$ in calculation with the method mentioned above. The relative incident rates along the tube were computed and illustrated for different tube lengths. The result curves are shown in Fig. 4. The transmission probability of different tube lengths is also drawn in the figure.

Analyzing the results, the following conclusions can be reached. No matter how long the tube is, the nearer to inlet, the larger the relative incident rate is. Similarly, the longer the tube is, the larger the relative incident rate near inlet is, and the smaller the relative incident rate near outlet is. For the same distance $z$ under different tube lengths, the relative incident rate $h(z)$ of longer tube is larger than that of shorter tube. The graphs of the relative incident rate are a series of straight lines. No matter how long the tube is, the relative incident rate is 0.5 at $L/2$, that is $h(L/2) = 0.5$. The value of relative incident rate shows symmetrical complementarity about $z = L/2$, that means $h(L/2 - z) = 1 - h(L/2 + z)$ or $h(z) = 1 - h(L - z)$. 

![Graph showing relative incident rate along tube under different lengths](Fig.4 The relative incident rate along tube under different length)
4. The Molecular Positional Distribution

The former research has discovered that the “positional beaming effect” exists, i.e. total positional distribution of escaping molecules is not uniformly at orifices of tube [9-10]. In order to reflect the level of non-uniformity quantitatively, the local relative molecular areal density, defined as the ratio of the local molecular exitance rate at outlet to the molecular incidence rate at inlet, at a different position of orifices are calculated and illustrated, respectively for the “directly passing” molecules, “reflective” molecules and their superposition.

4.1 The areal density distribution of directly passing molecules at outlet

According to Eq. (2), the relative local areal density of “directly passing” molecules at $dA$ is given as

$$D_{S-dA}(r_o) = \frac{dN_{S-dA}(r_o)}{\gamma \cdot dA} = \frac{L^2}{\pi} \int_0^R d \theta \int_0^{2\pi} \frac{r_o}{\rho^4} d\theta$$ (10)

Based on equation (10), the density distribution of “directly passing” molecules along the radius at outlet is shown in Fig. 3 for different lengths. It is found that “positional beaming effect” really exists for “directly passing” molecules for all tubes. Molecular areal density in central area is always denser than that in marginal area at outlet section.

4.2 The areal density distribution of reflective molecules at outlet

According to Eq (4), the relative local areal density of “reflecting” molecules from whole tube wall at area element $dA$ can be obtained by

$$D_{W-dA}(r_o) = \frac{dN_{W-dA}(r_o)}{\gamma dA} = \frac{R}{\pi} \int_0^L h(z) dz \int_0^{2\pi} \frac{(R-r_o \cdot \cos \theta_o)}{\rho^4} d\theta$$ (11)

Where $\gamma(z) = h(z) \cdot \gamma$ as Eq.(5). $h(z)$ can be calculated from Eqs. (7), (8) and (9). Since discretization is applied in calculating $h(z)$, here the accumulation has to be used instead of the integration to $dz$. Let $dz = b \cdot z = L - i \cdot b$, Eq. (11) may be transformed into
\[ D_{W-d4}(r_o) = \frac{R}{\pi} \sum_{i=1}^{\infty} h(L - i \cdot b) \cdot b \cdot \int_0^{2\pi} \frac{i \cdot b \cdot (R - r_o \cdot \cos \theta_z)}{\left[(i \cdot b)^2 + R^2 + r_o^2 - 2 \cdot R \cdot r_o \cdot \cos \theta_z\right]^2} \cdot d\theta_z \]  

(12)

**Fig. 4** The distribution of molecules reflecting from the entire tube wall to outlet of different length.

Fig. 4 shows graphically the density distribution of all "reflecting" molecules along the radius at outlet for different lengths. The distribution tendency changes with tube length. For short tubes (like \( L = 0.1d \) and \( L = 0.2d \)), reflective molecules mainly escape from marginal area, though their number is few. However, for \( L > d \), the distribution is that center is dense and edge is sparse, showing "beaming effect".

### 4.3 The areal density distribution of all molecules at outlet

Molecules escaping from the outlet consist of both "directly passing" ones and "reflective" ones. The total molecular areal density at outlet is expressed by

\[ D_{a4}(r_o) = D_{W-d4}(r_o) + D_{S-d4}(r_o) \]  

(13)

The superposition density distribution is sketched in Fig. 5. For any tube length, the outlet density distribution is that the local density decreases with \( r_o \) increase, showing "positional beaming effect". The value of relative density decreases along with the tube length increases, corresponding to the decrease of the transmission probability.
4.4 The molecular areal density distribution at inlet

By analogism, it is easy to calculate the relative areal density distribution of reflective molecules at inlet. Since the molecules at inlet are all reflective ones, this is the ultimate distribution at inlet. It is expressed by

\[
D_{\text{rel}}(r_i) = \frac{R}{\pi} \sum_{i=1}^{n} h(ib) \cdot b \int_{0}^{\frac{\pi}{2}} \frac{i \cdot b \cdot (R - r_i \cos \theta)}{[(i \cdot b)^2 + R^2 + r_i^2 - 2Rr_i \cos \theta]^2} d\theta
\]  

(14)

From Fig. 6, it can be summarized that molecular areal density increases with \( r_i \) increase for any tube length at inlet. For short tubes (like \( L = 0.1d \) and \( L = 0.2d \)), non-uniformity shows stronger, though their number is few. However for long tube such as \( L > 5d \), non-uniformity weakens greatly.
4.5 The superposition of outlet distribution and inlet distribution

Superimpose local molecular areal densities of corresponding positions (with same $r$) at inlet and outlet, we got

$$D_{\text{superposition}}(r) = D_{\text{in}}(r) + D_{\text{out}}(r) \quad (15)$$

The calculated results of Eq. (15) suggest that positional distributions of inlet and outlet present complementarity. Although inlet distribution and outlet distribution present "beaming effect" and "divergence" after evenly entering tube, the superposition of inlet distribution and outlet distribution returns to uniformity, which can be quantitatively expressed as $D_{\text{superposition}}(r) \equiv 1$.

5. The molecular angular distribution

The molecules leaving the tube are divided into the "directly passing" ones and the "reflective" ones as mentioned above. Fitly, at each point of the orifices, the leaving directions of two kinds of molecules are separated with each other. Two kinds of molecules occupy respectively the different azimuth solid angles. This causes that molecular angular distribution is discontinuation at every position of the orifices.

In order to reflect the 3D solid characteristics of molecular angular distribution, the relative emission probability at each point of the orifices is illustrated in a unit solid sphere which responds to the cosine distribution obeyed by the incidence molecules.

5.1 Angular Distribution at Different position on Outlet

Based on the model in Fig. 1, the molecular angular distribution at different position of orifices can be described by the relative emission intensity (probability)

$$p_{\text{outlet}}(\beta, r, \phi) = \begin{cases} \cos \beta & (\beta \leq \beta_r) \\ h(z) \cdot \cos \beta & (\beta > \beta_r) \end{cases} \quad (16)$$

where, $p_{\text{outlet}}$ is the ratio of molecule number to $\gamma / \pi$, and $\beta_r$ is the "critical polar distance angle". If $\beta \leq \beta_r$, the emitting molecule belongs to the "directly passing" one, and this kind of molecules build a eccentric cone in distribution graph. Otherwise, if $\beta > \beta_r$, molecules are the "reflective" ones which occupy the part out of the eccentric cone. $\beta_r$ is given as

$$\beta_r = \arccos \left( \frac{L}{\sqrt{L^2 + R^2 + r_o^2 - 2 \cdot R \cdot r_o \cdot \cos \theta}} \right) \quad (17)$$

where $\theta$ is calculated as follow

$$\theta = \pi - \phi - \arcsin \left( \frac{r_o}{R} \cdot \sin \phi \right) \quad (18)$$

Based on Eq. (16), Fig. 7 describes the angular distribution at different position of outlet under different tube lengths. From Fig. 7, the following regularities can be concluded.

No matter how long the tube is, there is an area, $\beta \leq \beta_r$, always overlapping unit sphere. This is the distribution of "directly passing" molecules which obey the cosine distribution. Oppositely, when $\beta > \beta_r$, since $h(z)$ makes the emission intensity smaller than cosine, distribution graphs are smaller than the sphere. Therefore, relative incident rate is considered to be the root cause of angular beaming effect.

With tube length growth, the area overlapping unit sphere becomes smaller, corresponding to the "directly passing" molecules decrease; and the relative emission intensity of large angle lessens considerably, which makes the distribution graph looks thinner.

Other than outlet center, the distribution graphs at other positions are not axisymmetric.
5.2 Angular Distribution at Different position on inlet

By analogism, the angular distribution of molecules returning back to inlet can be obtained. All of the molecules are "reflective" ones, and the relative emission ratio (probability) is expressed by

\[ p_{\text{inlet}}(\beta, r, \varphi) = \begin{cases} 0 & (\beta \leq \beta_h) \\ h(L-z) \cdot \cos \beta & (\beta > \beta_h) \end{cases} \]  \hspace{1cm} (19)

According to equation (19), Fig. 8 describes the molecular angular distribution at different position of inlet under different tube lengths. Following conclusions could be summarized from the Fig. 8. At every point of inlet, there is no molecule returning back in the eccentric cone \( \beta \leq \beta_h \), for all of the molecules are "reflective" ones. With tube length growth, the distribution graph is changing plump, which indicates more molecules returning back. Other than inlet center, the distribution graphs at other position are not axisymmetric.
Noting that \( h(L-z) = 1 - h(z) \) and comparing Eq. (16) with Eq. (19), we obtain

\[
p_{\text{inlet}}(\beta, r, \phi) = \cos \beta \cdot p_{\text{outlet}}(\beta, r, \phi)
\]

(20)

It is stated that the angular distribution of molecules returning back to a point of inlet is complementary to that at the corresponding point of outlet. This also causes that the angular distribution of inlet and outlet are complementary with each other about whole orifice.

5.3 The Angular Distribution of Whole Orifice

Since the molecular angular distribution at any point of orifices has been calculated, the average angular distributions of whole outlet or inlet can be obtained by integration to all points on orifices. The calculating formula for the angular distribution of whole orifices is given as equation (21), and some of its computing results are shown in figure 9.

\[
\bar{p}(\beta) = \frac{1}{\pi \cdot R^2} \int_0^R \int_0^{2\pi} p(\beta, r, \phi) \cdot d\phi \cdot 2\pi \cdot r \cdot dr
\]

(21)

The angular distribution of whole outlet is just what former scholar has been researched, so some of the results may be compared with that obtained by former scholar. K Nanbu acquired the distribution under the length \( (0.5 < L/d < 2) \) by Monte Carlo method, and generated fitting formulas by the data collected [6]. In Fig. 9, the angular distribution graphs of \( L = 0.5d \) and \( L = 1d \) are compared with those fitted by K Nanbu. The results are a little smaller than those of K Nanbu.
6. Conclusion

The calculated numerical results demonstrate that after entering the inlet uniformly, molecules show "positional beaming effect" at outlet. Meanwhile, the positional distribution of molecules returning to inlet is opposite. Inlet positional distribution and outlet positional distribution are complementary with each other, i.e. the superposition of them at corresponding points becomes uniform precisely regardless of length-diameter ratio of the tube.

For molecular angular distribution, the directional distribution graphs at different positions are drawn as the curved surfaces within a unit sphere which corresponds to the cosine distribution style. In the graphs, the “directly passing” molecules occupy an eccentric cone part around the normal line, while the “reflecting” molecules occupy the other part out of the cone. The angular distributions of two kinds of molecules are discontinuation at every position of the orifices. Other than inlet center, the distribution graphs at other position are not axisymmetric and perform more and more asymmetric with the distance growth. Calculating results demonstrate that angular distribution depends on not only the length-diameter ratio, but also the position on orifice. For either the corresponding points or the whole section of the inlet and the outlet, the angular distributions are complementary with each other, i.e. the superposition of them obeys the cosine distribution.

7. Reference