

ANALYSIS OF FREE MOLECULAR FLOW IN A TUBE OF FINITE LENGTH USING THE TIME-TRANSIENT MONTE CARLO METHOD

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Results by modification of the time transient method are presented, in which the superficial average velocity (streaming velocity) can be obtained in addition to molecular number density. The molecular number flux was thus obtained by the product of molecular number density and superficial average velocity.

The results of analysis of molecular flow in a circular tube were newly studied. The study revealed that there was a distortion of molecular number density distribution affected by outer storage. It became clear that the jumps in molecular number density and superficial average velocity at inlet and outlet openings were induced by discontinuity of macroscopic transfer rate (molecular number flux) between the tube and the outer space.

For a finite length tube, using Knudsen's simple equation for a tube of infinite length, the transfer rate, i.e. the conductance, can be easily calculated by applying the slip distance.

Introduction

Many analyses of rarefied gases flow have been performed. In these analyses, the statistical indeterminate Monte Carlo method is recently becoming a powerful method.

The authors have reported the application of the Monte Carlo method to the transient flow region²⁾ by taking intermolecular collision into consideration. We have also performed an analysis of flow through complicated conduits with diverging-converging cross section⁸⁾ and equal-spheres packed bed⁵⁾ under free molecular flow.

At that time many analyses of the overall transfer coefficient, i.e. conductance, had been made, but analyses with respect to local properties in the conduit such as local molecular number density (pressure distribution) were quite few. Only Sparrow *et al.*⁷⁾ have published regarding molecular number flux*.

Later authors³⁾ have proposed the Monte Carlo method with time concept (time-transient method) to calculate the molecular number density under free molecular flow. After that, in the previous paper,⁶⁾ we have improved on the illogically low value appearing in this method for the vicinity of the inlet opening.

Since this improvement enables us to calculate stable local molecular number density in the whole tube, local properties in the finite length tube are newly studied in the present work by combining the local superficial average velocity (streaming velocity).

1. Theoretical considerations

In the time-transient Monte Carlo method, described in this paper, time histories of sample molecules are traced. Since the basic calculation technique and procedure are the same as in the previous paper,^{3,6)} only the main points are mentioned in the following.

1.1 Calculation procedure (time-transient method)

The model tube and coordinates system for the simulation are shown in Fig. 1. After determination of the geometrical conditions, trial molecular numbers, transient time interval and the like, the trial molecules start at the inlet opening. To eliminate unnecessary complexity, the molecular number density of outlet side n_o is assumed to be zero in this paper. The treatment for the case of $n_o \neq 0$ is discussed in the previous paper.³⁾

1) Initial condition and boundary condition Initial conditions are given as follows:

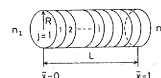


Fig. 1. Schematic diagram of the circular-section tube

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* Sparrow *et al.* reported a velocity distribution, which corresponds to molecular number flux in this paper.

$$n=0 \quad \text{at} \quad t \leq 0, \quad x=0 \sim L \quad (1)$$

The tube connects with two large reservoirs in which molecular number density $n=n_i$ in equilibrium at the inlet side and $n=n_o=0$ at the outlet side.

2) Resident probability of sample molecules in a volume element V_i Now let the number of molecules which enter the inlet opening with sectional area A during unit time interval U be N_U , which is given by conventional molecular dynamics as follows:

$$N_U = (1/4)n_i \bar{v} U A \quad (2)$$

Equation (2) means that molecular number flux through a circular orifice is the product of $(1/2)n_i$ and $(1/2)\bar{v}$.

As sample molecules, N out of N_U are chosen. The trajectory direction and velocity component are determined by the conventional method,^{5,8)} and sample molecules start one after another at equal intervals during transient time interval U . We consider the trial molecules N in unitary interval U as one group. Let the unit number of transient time interval be τ , which is an integer. The resident probability of trial molecules of one group f_i^τ is

$$f_i^\tau = N_i^\tau / N \quad (3)$$

where N_i^τ is the number of molecules which stay in a volume element V_i after τU .

3) Molecular number density Because under free molecular flow the sample molecules groups behave independently of each other, the resident probability of every sample molecular group after equal time lapse is consistent with those of the other groups. Therefore, time transient variation can be obtained by superposing the result for the initial group, as follows:

$$\bar{n}_i^\tau = \sum_{\tau=1}^{\tau} N_U f_i^\tau / (V_i n_i) \quad (4)$$

where $\bar{n} = n/n_i$. The steady-state value can be obtained as the ultimate result of transient calculation after τ is large enough.

4) Average velocity in the volume element V_i The time transient average velocity in the flow direction is given by averaging the velocity component of all the molecules in V_i after τU , as follows:

$$\bar{u}_i^\tau = \sum_{\tau=1}^{\tau} \sum_{N=1}^{N_i^\tau} (N f_i^\tau u_N / \bar{v}) / \sum_{N=1}^{N_i^\tau} N f_i^\tau \quad (5)$$

Where $\bar{u} = u/\bar{v}$. The steady-state value can be obtained as the ultimate value. The above value is called the "superficial average velocity" to distinguish it from macroscopic flow velocity under continuous (viscous) flow condition.

5) Molecular number flux The steady-state macroscopic molecular number flux, based on the inlet opening, is given by Clausing¹⁾ as follows:

$$F = (1/4)n_i \bar{v} \alpha \quad (6)$$

The transmission probability can be calculated as $\alpha = N_o/N$ by trial molecules N , when N_o pass out through the outlet opening.

The local molecular number flux in the tube is given by the product of a local molecular number density and a local superficial average velocity by the following equation:

$$\bar{F}_i^\tau = \bar{n}_i^\tau \bar{u}_i^\tau / F \quad (7)$$

The local value in the above equation is normalized with the steady-state macroscopic value F based on the inlet opening. The steady-state value can be obtained as the ultimate value of transient calculations.

1.2 Calculation conditions

The same conditions as described in the previous paper³⁾ are selected: a temperature of 20°C and nitrogen as the sample gas. Calculation parameters are shown below.

Sample molecules	$N = 10,000$
Model tube radius	$R = 5 \text{ mm}$
Geometric parameter	$L/R = 0.01-100$
Transient time interval	$U = 10^{-10}-10^{-6} \text{ s}$
Model tube division	axial $i = 10$

In the vicinity of openings, volume elements are divided into smaller ones when it is necessary to check in detail. A schematic diagram of the model tube is shown in Fig. 1.

2. Results and Discussion

2.1 Molecular number density

In Fig. 2 the calculated results of molecular number density in the circular-section tube are shown for various geometric parameters R/L . The plotted keys and solid lines stand for results by the time-transient

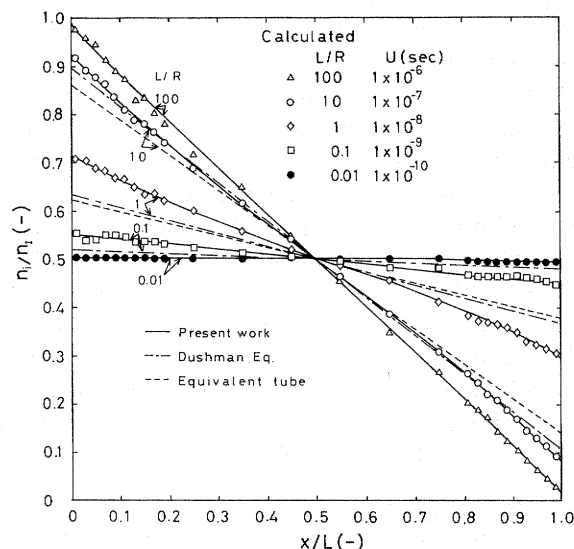


Fig. 2. Molecular number density in flow direction

Monte Carlo method in the present work.

To calculate the conductance of a finite length tube, Dushman¹⁰⁾ proposed the following equation by adding the conductance of orifice and long tube in series as follows:

$$C = (1/4)\bar{v}(\pi D^2/4)(4D/3(L + 4D/3)) \quad (8)$$

The pressure gradient, i.e. molecular number density gradient, calculated by Eq. (9) below on the basis of modified tube length is shown in Fig. 2 by dashed broken lines. The other broken line, representing an equivalent tube, is discussed later.

$$\Delta p/L = (p_i - p_o)/(L + 4D/3) \quad (9)$$

The molecular number density by present work agrees with the linear line of Dushman's Equation (Eq. (8)) for a long tube, $L/R=100$. In a medium-length tube, $L/R=10$, it is almost consistent with the linear line in the inner part of the tube, but diverges slightly in the vicinity of inlet and outlet openings where it distorts. For a short tube, $L/R=1$, the distribution diverges seriously from the linear line of Eq. (8). As L/R decreases, the tube approaches the orifice. The variation of distribution in the flow direction is so small that it superficially becomes linear and agrees with the linear line of Eq. (8).

The distribution of the finite length tube distorts toward the outer value, but values are not consistent with the outer value ($\bar{n}_{x=0} \approx 1$, $\bar{n}_{x=1} \approx 0$). Therefore, there is a discontinuity, i.e. a jump, at the inlet and outlet openings.

Even though the linear line of Eq. (8) does not completely agree with the calculated results in the present work, it can be said that Dushman's modification is reasonable supposing that a jump occurs at inlet and outlet openings.

2.2 Distribution of superficial average velocity

In Fig. 3 the distributions in the flow direction for the various L/R are shown. The keys and solid lines represent the calculated results of the present work.

The distribution of superficial average velocity of a very short tube converges to the theoretical value of orifice $(1/2)\bar{v}$. At this point, it can be said that the calculated results are appropriate. For a tube of finite length, the velocity increases generally from inlet to outlet. Around $L/R=1$ the variation is small. As L/R increases to nearly that of the long tube, the absolute value near the entrance decreases and near the outlet the value sharply accelerates to nearly sonic velocity.

It can be seen that the superficial velocity is not zero in the tube at inlet and outlet openings. Therefore, it can be said that superficial average velocity has a discontinuity or jump at both the inlet and outlet openings as well as molecular number density jumps at those locations.

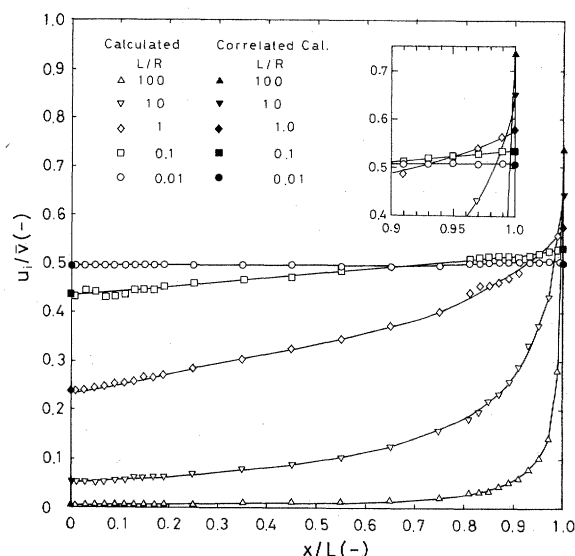


Fig. 3. Superficial average velocity in flow direction

2.3 Effect of outer space on the properties in the tube

Let us discuss the molecular number density under equal pressure in detail so as to consider the distortion of distribution which occurs near the entrance in tubes where there is flow.

Under equal pressure condition, the molecules that stay in a volume element V_i can be classified into the following groups.

- 1) Molecules that come from the inlet opening and collide with the tube wall N_{I-W}
- 2) Molecules that come from the tube wall and flow out through the inlet opening N_{W-I}
- 3) Molecules that come from the outlet opening and collide with the tube wall N_{O-W}
- 4) Molecules that come from the tube wall and flow out through the outlet opening N_{W-O}
- 5) Molecules that come from the inlet opening and directly flow out through the outlet opening N_{I-O}
- 6) Molecules that come from the outlet opening and directly flow out through the inlet opening N_{O-I}
- 7) Molecules that come from the tube wall and collide with the tube wall again N_{W-W}

The calculated distribution of each group is shown in Fig. 4 for $L/R=10$, selected as a sample finite-length tube. The ordinate represents the location, normalized with tube radius R , in the flow direction. Since it is under equal pressure, the sum total of molecules 1-7) is constant ($\bar{n}=1$) at every location along x and each distribution is symmetrical with respect to the mid-point of the tube. In the low part of the figure molecular number densities of less than 1% are shown in detail. The calculated results were obtained by the simulation of molecules starting at an opening and the wall respectively.

As shown in Fig. 4, N_{I-W} is consistent with

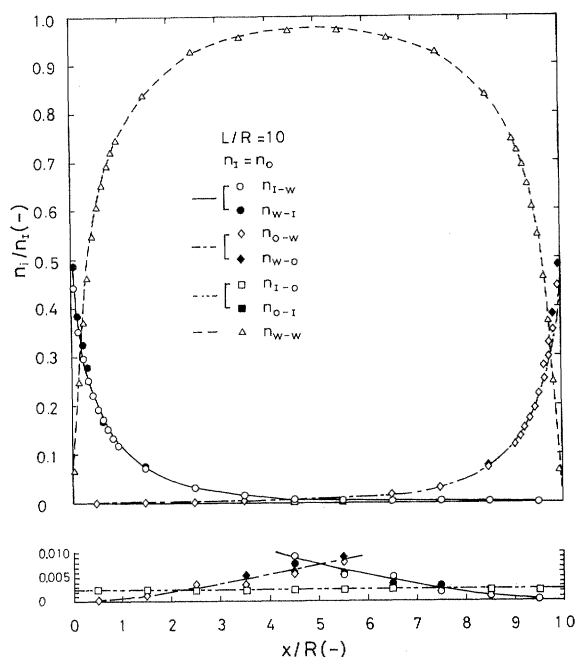


Fig. 4. Classification of molecular number density in a circular-section tube

corresponding N_{W-I} and N_{O-W} with N_{W-O} , and it can be said that the calculated results are appropriate. From the results shown in Fig. 4, it can be seen that molecules which interact with the tube wall, i.e. N_{I-W} , N_{W-I} , N_{O-W} , N_{W-O} and N_{W-W} , make up most of the molecular number density. There are very few molecules that directly pass out through the opposite opening N_{I-O} and N_{O-I} . Since the total is less than about 0.5%, the effect on the distribution is extremely small.

As the distribution is symmetrical, let us take the inlet side in the tube as an example. In the vicinity of the inlet opening, the molecules N_{I-W} and N_{W-I} are about 50% each and their total is nearly 100%; they compose almost the entire molecular number density. In the inner part of the tube, this value decreases sharply and finally, at $x > 4R$, the contribution becomes less than 1%, so the effect on the distribution is very small. Thus it may be considered that the range of distribution affected by the inlet opening, i.e. external space, is around $4R$. On the other hand, the molecules that come flying from wall to wall N_{W-W} increase sharply in the inner part of the tube, and finally at $x > 4R$ they make up nearly 100% of the molecules in the tube.

Thus it becomes clear that the external space hardly affects the distribution in the central part of the tube. We chose $L/R=10$ as a sample of finite-length tube. As L/R becomes larger, it is clear that the external reservoir has no effect on the distribution in the inner part of the tube, in the range of $4R < x < L-4R$.

In Fig. 5, the molecular number density, superficial average velocity and molecular number flux calculated

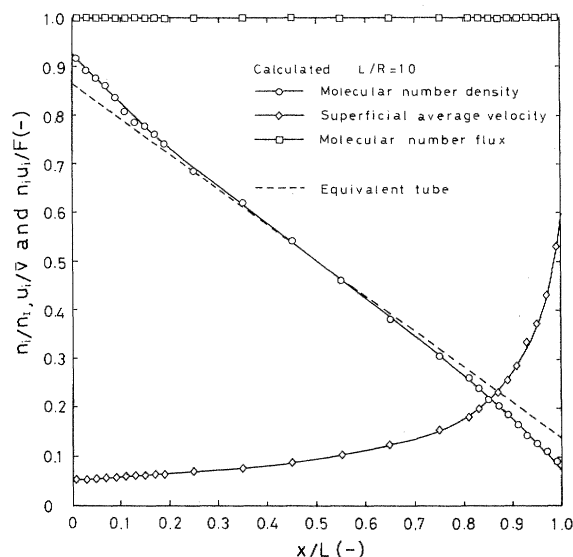


Fig. 5. Molecular number density, superficial average velocity and molecular number flux for $L/R=10$

by the present method are shown, where molecular number flux is obtained by the product of local molecular number density and superficial average velocity. The molecular number flux shows a constant value ($\bar{F}=1$) at every location, supporting the conclusion that molecular number density and superficial average velocity values obtained by the present method satisfy the law of conservation or continuity. As a result, it can be said that the calculated results of molecular number density and superficial average velocity are appropriate. The linear line along the calculated molecular number density is a gradient calculated by using Knudsen's Eq. (12) to equalize the transfer coefficient, i.e. conductance, by present work (hereafter called equivalent tube).

Although in Fig. 5 the calculated results under non-equilibrium with flow are shown, the phenomena should be based on behavior under equilibrium as in Fig. 4. As shown in Fig. 5 the density distribution agrees with the linear line of equivalent tube in the central part of the tube $4R < x < L-4R$. At the inlet side $x < 4R$ and outlet side $x > L-4R$, however, the distribution diverges from the linear line and distorts toward the external value as the location approaches the inlet and outlet openings.

As mentioned above, in the case of non-equilibrium with flow we can see the effect of external space on distribution described in Fig. 4 under equilibrium. The distortion in the vicinity of the inlet is caused by molecules that come from external space and in the vicinity of the outlet by the molecules passing out through the outlet opening.

The correctness of calculated molecular number density is verified by the fact that these values satisfy the law of conservation. It can be thus concluded that divergence of molecular number density distribution

from the linear line is an essential phenomenon.

2.4 Occurrence of jump at inlet and outlet openings

The discontinuity of molecular number density and superficial average velocity at inlet and outlet openings is generally called slip or jump. Definition of "jump" and "slip distance" are shown in Fig. 6. Slip distance is discussed later.

The jump Δ obtained by the present work and the jump of Dushman's linear gradient Δ' are plotted as a function of L/R in Fig. 7. The jump converges to the maximum theoretical orifice value $(1/2)n_I$ at $L/R=0$. As L/R increases, the jump decreases, the jump decreases and will become zero for an infinitely long tube. The jump obtained in the present work is quite consistent with Dushman's at small L/R . Around $L/R=1-10$, there is a slight difference. As L/R increases further, the values agree well. The differences at finite tube length are caused by the distortion affected by external space as discussed in the previous section.

In Fig. 7, the jump of superficial average velocity at inlet and outlet openings Δ_{ui} , Δ_{uo} is shown. The jump of inlet side Δ_{ui} converges to the maximum theoretical value of orifice $(1/2)\bar{v}$. As L/R increases, the jump value decreases. The jump of outlet side Δ_{ui} converges, at extreme tube shortness, to minimum $(1/2)\bar{v}$. As L/R increases, the jump increases and approaches sonic velocity.

Now we will discuss the mechanism of occurrence of molecular number density jump and superficial average velocity jump.

Let us consider the molecular number flux at both openings. Where the tube approaches either opening, naturally the flux should be given by Eq. (7). Therefore, at both openings the following relation between molecular number density jump and superficial average velocity jump applies.

$$F = n_I(1 - \Delta)\bar{v}\Delta_{ui} = n_I\Delta\bar{v}\Delta_{uo} \quad (10)$$

By equating Eq. (6) and Eq. (10), the following relation can be obtained:

$$(1 - \Delta)\Delta_{ui} = \Delta\Delta_{uo} = (1/4)\alpha \quad (11)$$

Using molecular number density jump Δ and calculated transmission probability, the superficial average velocity jumps Δ_{ui} and Δ_{uo} are calculated by Eq. (11). The correlated results are plotted in Fig. 3 by closed keys at $x/L=0$ and $x/L=1$. These values agree well with the calculated distribution values of the present work at both the inlet and outlet openings.

Therefore it becomes clear that the molecular number density jump and the superficial average velocity jump are related to the molecular number flux, i.e. the macroscopic transfer rate.

In the external reservoir there is no flow, there is flow in the tube. This means that the occurrence of

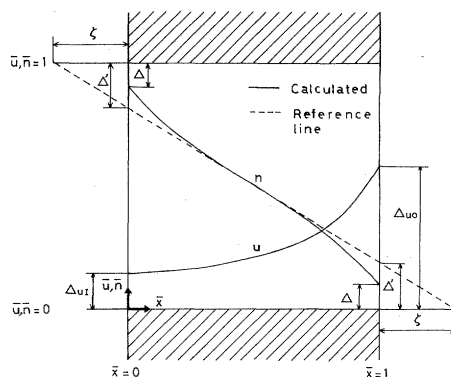


Fig. 6. Definition of jump and slip distance

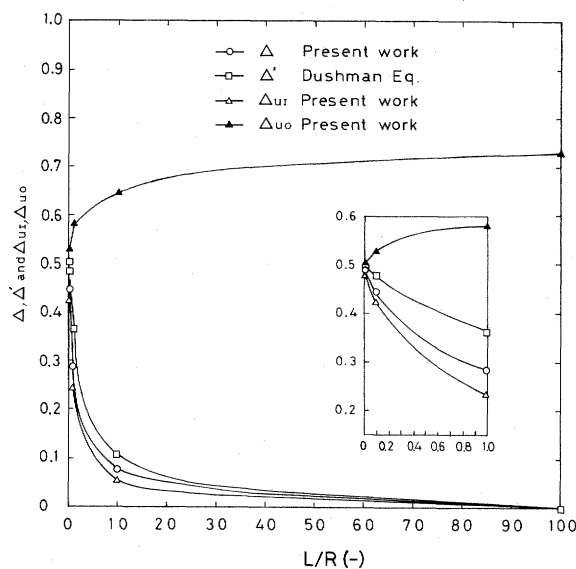


Fig. 7. Jump of molecular number density and superficial average velocity

pre-flow in the vicinity of the inlet opening of the external reservoir and the jet stream at the outlet opening connects the discontinuity between the tube and the outer space.

The pre-flow and jet stream near the two openings are interesting phenomena, but a detailed analysis will be left for the future.

2.5 Simple equation for finite-length tube

Generally, for a long tube, Knudsen's equation is used:

$$C = (1/4)\bar{v}(\pi D^2/4)(4D/3L) \quad (12)$$

Since this equation neglects the effect of inlet and outlet opening, for a tube of finite length its usage is limited of its own accord. To improve this point, Dushman proposed the previously mentioned Eq. (8). Now we modify Eq. (12) by introducing slip distance, ζ , as follows:

$$C = (1/4)\bar{v}(\pi D^2/4)(4D/(3(L + 2\zeta))) \quad (13)$$

Using Eq. (12), the molecular number density gradient is obtained by equalizing the transfer

Table 1. Comparison of transmission coefficient by Dushman and equivalent tube with Clausing

L/R	Clausing	Demarcus	Dushman diff.	Equivalent diff.
0.1	0.9524	0.9524	0.9639 +1.2%	0.9507 -0.2%
1.0	0.6720	0.67198	0.7273 +8.2%	0.6749 +0.4%
10.1	0.1973	0.19099	0.2105 +6.7%	0.1938 -1.8%
100.0	0.02658	—	0.0260 +0.7%	0.0266 +3.1%

Table 2. Constants in correlated Eq. (14)

<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>	<i>f</i>	<i>g</i>
2.9283	-3.3428	0.9009	-0.9767	0.4346	-0.7454	0.3997

coefficient values calculated in the present work, which are shown in Fig. 2 by the broken line. The slip distance in Eq. (13) can be determined by these gradients for every L/R . In Eq. (8), the modification of length $4D/3$ corresponds to slip distance 2ζ .

To calculate the transfer rate, i.e. conductance, Clausing's transmission probability is well known and was verified with numerical calculation by Demarcus⁹⁾. We choose the Clausing coefficient as the reference. A comparison between Eq. (8) and the equivalent tube is shown in Table 1. It can be seen that in the case of the equivalent tube the difference is 0.2–3.1%, while in the case of Dushman it is 1.2–8.2%. Thus it can be said that a more accurate transfer rate can be calculated by Eq. (13) using the slip distance ζ .

The slip distance of the equivalent tube is shown in Fig. 8. The plotted keys stand for the values obtained by the above-mentioned method and the curve represents the correlated Eq. (14) below. The slip distance converges to zero at infinite tube length and becomes infinite at extreme shortness of tube, i.e. at the orifice. To calculate the conductance using equivalent tube Eq. (13) the slip distance can be obtained from Fig. 8 or by correlated Eq. (14). The constants of Eq. (14) are shown in Table 2.

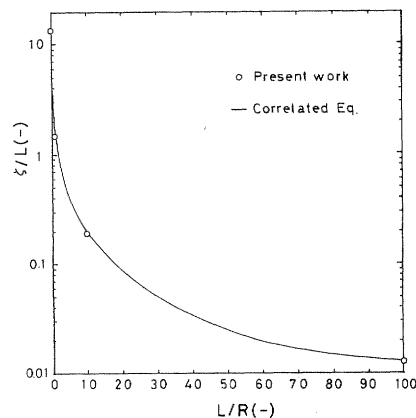
$$\zeta = \exp(a + b(L/R) + c(L/R)^2 + d(L/R)^3 + e(L/R)^4 + f(L/R)^4 + g(L/R)^6) \quad (14)$$

For the finite-length tube the transfer rate can be obtained by use of the Clausing coefficient, but the function is complex. The slip distance ζ defined in this paper gives the equivalent transfer rate as the present Monte Carlo method by a simple equation. If Knudsen's diffusion coefficient, derived for long tubes, is used for the transfer rate for a finite-length tube, it is recommended that the slip distance be used.

Conclusion

From a theoretical analysis using the time-transient Monte Carlo method for free molecular flow in a tube of finite length, the following results are obtained.

- 1) In the finite-length tube, a distortion of

**Fig. 8.** Slip distance of equivalent tube

molecular number density distribution, affected by external space, exists at around $4R$ from the inlet and the outlet openings.

- 2) In the case of superficial average velocity, a discontinuity or jump exists at inlet and outlet openings, along with a jump in molecular number density.
- 3) The jumps in molecular number density and superficial average velocity are caused by discontinuity of macroscopic transfer rate at the inlet and outlet openings between the tube and the outer space.
- 4) Applying the concept of slip distance for finite length in this paper, the transfer rate, i.e. conductance, can be calculated easily by using the simple Knudsen's equation for long tubes.

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Nomenclature

<i>C</i>	= Conductance	[cm ³ /s]
<i>f</i>	= molecular resident probability	[—]
<i>F</i>	= molecular number flux	[molecules/cm ²]
<i>k</i>	= Boltzmann constant	[erg/K · molecule]
<i>L</i>	= length of model tube	[cm]

N	= molecular number	[molecules]
n	= molecular number density	[molecules/cm ³]
p	= pressure	[dyne/cm ²]
R	= radius of model tube	[cm]
T	= absolute temperature	[K]
t	= time	[s]
U	= transient time interval	[s]
u	= superficial average velocity	[cm/s]
V	= volume element of model tube	[cm ³]
v	= molecular velocity	[cm/s]
x	= location in flow direction	[cm]
α	= transmission probability	[—]
Δ	= jump or difference	[—]
ζ	= slip distance	[—]

<Subscripts and superscripts>

τ	= time index
i	= increment number in longitudinal direction
I	= inlet side of model tube
O	= outlet side of model tube

U	= transient time interval
u	= superficial average velocity
—	= normalized and averaged value

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