

RADIAL DISTRIBUTION OF MOLECULAR NUMBER DENSITY IN A CIRCULAR TUBE UNDER FREE MOLECULAR FLOW

MITSURU SESE AND YUTAKA MATSUMURA

Research and Development, Idemitsu Kosan Co., Ltd., Tokyo 100

YUJI KAWAMURA

Department of Chemical Engineering, Hiroshima University,
Higashihiroshima 724

Key Words: Rarefied Gas Flow, Molecular Flow, Porous Media, Molecular Density, Vacuum, Monte Carlo Method

Introduction

For derivation of the equation of rarefied gas flow, information about the molecular number density is required, in which the distribution is assumed to be negligibly small in the radial direction without positive evidence.

The authors have contrived a time-transient Monte Carlo method to calculate the molecular number density (pressure distribution)¹⁾. At that time, due to low accuracy level, we could not draw a conclusion about the radial distribution. After some improvement to obtain stable results, in the previous paper²⁾ we reported an analysis of axial distribution of flow properties without radial distribution.

In this paper, the radial distribution is newly analysed. In addition, the average radial velocity components are calculated so as to verify the radial distribution of molecular number density.

The present results will be effective for further rigorous analysis.

1. Theoretical Consideration

1.1 Calculation procedure (time-transient method)

Figure 1 shows the tube for the simulation with its coordinate system. The model tube is divided into volume elements V_{ij} , where i is the axial increment number and j is the radial increment number. To eliminate unnecessary complexity the molecular number density at the outlet, n_o , is assumed to be zero (0). The treatment for the case of $n_o \neq 0$ was reported in the previous paper¹⁾.

1) Initial condition and boundary condition The initial condition is defined as follows:

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

The tube is connected to a reservoir large enough to maintain equilibrium state during the process with

molecular density n_I at the inlet and zero (0) at the outlet.

2) Molecular number density Let the number of molecules which enter the inlet opening during unit time interval U be N_U , which can be given by the conventional kinetic theory of gases. N out of N_U are chosen as sample molecules. The resident probability f_{ij}^τ is given by N_{ij}^τ/N when N_{ij}^τ stay in volume element V_{ij} after a length of time of τU . τ is unit number of U , where τ is an integer.

Molecular number density \bar{n}_{ij}^τ in a volume element V_{ij} after a length of time τU can be obtained by integrating the time transient resident probability as follows:

$$\bar{n}_{ij}^\tau = \sum_{\tau=1}^{\tau} N_U f_{ij}^\tau / (V_{ij} n_I) \quad (2)$$

The equation is normalized with molecular number density n_I .

3) Radial velocity component Time transient average velocity of radial direction can be obtained by averaging all the radial components of sample molecules in a volume V_{ij} after a length of time τU , expressed as follows:

$$\bar{u}_{rij}^\tau = \sum_{\tau=1}^{\tau} \sum_{N=1}^{N_{ij}^\tau} (N f_{ij}^\tau u_{rN} / \bar{v}) / \sum_{N=1}^{N_{ij}^\tau} N f_{ij}^\tau \quad (3)$$

The above equation is normalized with molecular average velocity \bar{v} .

The steady-state values of n and u_r can be obtained as the ultimate value of transient calculation or as the value when τ is large enough.

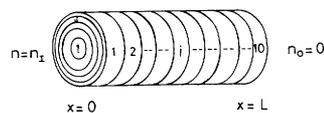


Fig. 1. Schematic diagram of the circular tube for the simulation

* Received October 20, 1990. Correspondence concerning this article should be addressed to M. Sese.

1.2 Calculation condition

The same conditions used in the previous papers are selected for this paper, using nitrogen gas as the sample gas at 20°C. Other conditions for the calculation are as follows:

Number of sample molecules	$N = 100,000$
Model tube radius	$R = 5 \text{ mm}$
Geometric parameter	$L/R = 0.1, 10$
Transient time interval	$U = 10^{-9}, 10^{-7} \text{ sec}$
Tube segmentation	$i = 10, j = 5$

In the vicinity of openings, the volume elements are divided into smaller units when it is necessary to check in detail.

2. Results and Discussion

The calculated radial distribution of the molecular number density for $L/R = 10$, adopted as an example of medium-length tube, is shown in Fig. 2. As we can see from Fig. 2, there is not much difference in radial direction and the distribution is almost flat. On the other hand, as shown in Fig. 3, for a very short tube of $L/R = 0.1$ a difference in radial direction clearly exists; the molecular number density increases in the vicinity of the inlet opening and decreases in the vicinity of the outlet opening.

The radial velocity components are also plotted with arrows in Figs. 2 and 3. For $L/R = 10$, the velocity components are nearly zero. On the contrary, for $L/R = 0.1$, the velocity components are not zero; the flow direction and magnitude of velocity components correspond to the gradient of molecular number density.

In the previous paper²⁾, we showed that for finite (more than medium) length tube, an effect on flow properties in the tube by outer space exists around $4R$ from inlet and outlet openings respectively.

The calculated results for very near the inlet and outlet openings of $L/R = 10$ are shown in Fig. 4. At the inlet side, a slight difference exists. At the outlet side, no difference can be seen, but radial velocity components exist. Accordingly, it can be said that a slight gradient exists in the vicinity of both openings, but these values are very small.

Thus, it can be concluded that in a finite length tube the radial distribution of molecular number density is negligibly small.

Nomenclature

f	= molecular resident probability	[—]
L	= length of model tube	[cm]
N	= molecular number	[molecules]
n	= molecular number density	[molecules/cm ³]
R	= radius of model tube	[cm]
t	= time	[s]
U	= transient time interval	[s]
u	= superficial average velocity	[cm/s]
V	= volume element of model tube	[cm ³]

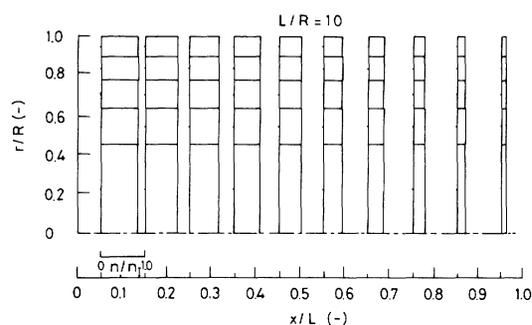


Fig. 2. Radial distribution of molecular number density and radial velocity component for $L/R = 10$

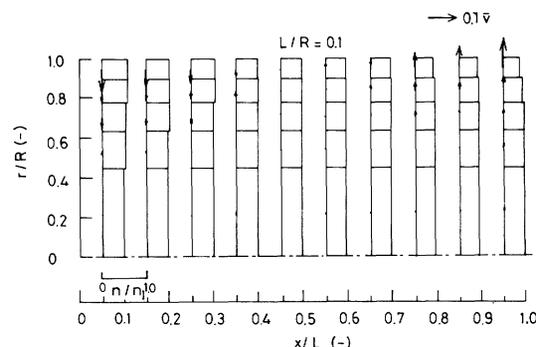


Fig. 3. Radial distribution of molecular number density and radial velocity component for $L/R = 0.1$

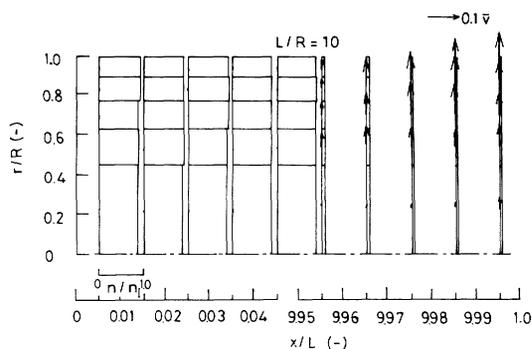


Fig. 4. Radial distribution of molecular number density and radial velocity component in the vicinity of inlet and outlet openings for $L/R = 10$

v	= molecular velocity	[cm/s]
x	= location in flow direction	[cm]

<Subscript and superscript>

τ	= time index
i	= increment number in longitudinal direction
j	= increment number in radial direction
I	= inlet side of model tube
O	= outlet side of model tube
r	= radial direction
U	= transient time interval
—	= normalized and averaged value

Literature Cited

- 1) Kawamura, Y., H. Shinagawa, M. Sese and H. Makihara: *J. Chem. Eng. Japan*, **10**(2), 104 (1977).
- 2) Sese, M. and Y. Kawamura: *J. Chem. Eng. Japan*, **23**(2), 137 (1990).