APPLICATION OF THE VARIATION METHOD TO THE PROBLEM OF THERMOMOLECULAR PRESSURE DIFFERENCE IN A CYLINDRICAL CHANNEL

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The problem of thermomolecular pressure difference in a round capillary tube is solved by the variation method for the linearized BGK model. Purely diffusive dispersion of gaseous molecules at the capillary walls is stipulated in the boundary conditions. The results are compared with test data.

The problem of thermomolecular pressure difference arises, as a rule, during pressure measurements in systems where the temperature is not the same as the temperature of the pressure probes. The correction which must then be added to the instrument readings to account for this thermomolecular pressure difference may, at a sufficiently large temperature drop and high Knudsen number, amount to a high percentage of the mean pressure in the system. This does obviously explain why many researchers are so concerned about the problem. It is to be noted, however, that until now the problem of thermomolecular pressure difference was treated semiempirically and that only the extreme cases of viscous or free-molecular conditions have been analyzed theoretically.

In this study here the authors will solve the problem for any value of the Knudsen number (Kn denoting the ratio of mean free path λ to capillary radius R). For the solution, we apply the variation method [1] to the linearized BGK model, which, when diffusive reflection of molecules at the capillary walls is assumed, will, according to Sone and Yamamoto [2], transform into a linear integral equation with respect to the dimensionless velocity of the average molecule u:

$$u(r) = \frac{1}{\pi}\iint\limits_{(s)}\left[\delta u(r') - \frac{\nu R}{2} + \frac{\tau R}{2}\right]\frac{J_0(\delta|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}' - \frac{\tau R}{2\sqrt{\pi}}\iint\limits_{(s)}\frac{J_2(\delta|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}', \tag{1}$$

where

$$J_n(x) = \int\limits_0^\infty t^n \exp\left[-t^2 - \frac{x}{t}\right]dt;\ \delta = \frac{\sqrt{\pi}}{2\,\mathrm{Kn}};\ \nu = \frac{1}{p}\frac{dp}{dz};\ \tau = \frac{1}{T}\frac{dT}{dz};$$

p(z) and T(z) denote respectively the pressure and the temperature, s denotes the cross section area of a capillary, and r denotes the radial coordinate.

A linearization of the problem will make it possible to represent the average velocity u as a simple sum of two independent velocities u_1 and u_2 due to the pressure gradient and the temperature gradient respectively:

$$u = u_1 + u_2. \tag{2}$$

With (2) taken into account, Eq. (1) splits into two independent integral equations:

$$\Psi_i(r) = \Phi_i(r) + \frac{\delta}{\pi}\iint\limits_{(s)}\Psi_i(r')\frac{J_0(\delta|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}' \tag{3}$$

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TABLE 1. Numerical Values of γ

δ	Q_1	γ	δ	Q_1	γ
0	1,5045	0,5	0,5	1,3863	0,3008
0,0001	1,5043	0,4996	0,6	1,3971	0,2808
0,001	1,4996	0,4979	0,7	1,4101	0,2632
0,01	1,4763	0,4862	0,8	1,4247	0,2475
0,02	1,4603	0,4765	0,9	1,4406	0,2334
0,03	1,4483	0,4681	1	1,4576	0,2205
0,04	1,4386	0,4608	2	1,6559	0,1369
0,05	1,4305	0,4540	3	1,8772	0,0938
0,06	1,4236	0,4477	4	2,1079	0,0683
0,07	1,4177	0,4417	5	2,3438	0,0519
0,08	1,4125	0,4361	6	2,5831	0,0408
0,09	1,4079	0,4307	7	2,8246	0,0328
0,1	1,4039	0,4256	8	3,0677	0,0270
0,2	1,3815	0,3832	9	3,3121	0,0226
0,3	1,3760	0,3505	10	3,5574	0,0192
0,4	1,3788	0,3236			

for the average velocities $u_1 (i = 1)$ and $u_2 (i = 2)$. Here

$$\Phi_i(r) = \begin{cases} -1, & i = 1, \\ 1 - \dfrac{\delta}{\pi} \displaystyle\iint_{(s)} \dfrac{J_2(\delta\,|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|}\, d\mathbf{r}', & i = 2, \end{cases} \tag{4}$$

$$u_1 = \frac{\nu R}{2\delta}[1 + \Psi_1], \qquad u_2 = \frac{\tau R}{2\delta}[-1 + \Psi_2]. \tag{5}$$

According to the general rules of variational calculus, we set up the following functionals for Eqs. (3):

$$F_i\{\tilde{\Psi}_i(r)\} = \iint_{(s)} \tilde{\Psi}_i(r)\left[\tilde{\Psi}_i(r) - 2\Phi_i(r) - \frac{\delta}{\pi}\iint_{(s)} \tilde{\Psi}_i(r')\,\frac{J_0(\delta\,|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|}\, d\mathbf{r}'\right] d\mathbf{r}. \tag{6}$$

It can be easily shown that each functional in (6) becomes minimum as soon as the trial functions $\tilde{\Psi}_i$ represent the exact solutions to Eqs. (3). The referred flow rates Q_1 due to the pressure gradient and Q_2 due to the temperature gradient are related to the functionals (6) as follows:

$$Q_1 = \frac{2\langle u_1 \rangle}{\pi R^3 \nu} = \frac{1}{s\delta}\left[-\iint_{(s)} \Phi_1(r)\, d\mathbf{r} + \min F_1\{\tilde{\Psi}_1\}\right] \tag{7}$$

and

$$Q_2 = \frac{2\langle u_2 \rangle}{\pi R^3 \tau} = \frac{1}{s\delta}\left[-\iint_{(s)} \Phi_2(r)\, d\mathbf{r} + \min F_2\{\tilde{\Psi}_2\}\right], \tag{8}$$

where the $\langle\ \rangle$ symbol denotes averaging over the capillary section.

The choice of quadratic trial functions $\tilde{\Psi}_i = A_i r^2 + B_i$ and the subsequent minimization of functionals (6) with respect to the unknown coefficients A_i, B_i leads, after a few simplifications, to the following expressions for the referred flow rates:

$$Q_1 = \frac{1}{\delta}\left[1 + \pi\,\frac{C_{12} - 0{,}25C_{22} - C_{11}}{C_{11}C_{22} - C_{12}^2}\right], \tag{9}$$

$$Q_2 = \frac{1}{\delta}\left[-1 + \frac{0{,}5\,(C_1C_{22} - C_2C_{12}) + C_2C_{11} - C_{12}C_1}{C_{11}C_{22} - C_{12}^2}\right], \tag{10}$$

where

$$C_{11} = 8\left\{I_1^0(\delta) + \frac{8}{3}[I_1^2(\delta) - I_1^4(\delta)] + \frac{4}{\delta^2}\left[I_1^2(\delta) + \delta I_0^3(\delta) + 2\delta I_2^3(\delta) - \frac{\pi}{32}\right]\right\};$$

$$C_{12} = 8\left\{I_1^0(\delta) + \frac{1}{\delta^2}\left[I_3^0(\delta) + 2\delta I_2^1(\delta) - \frac{\pi}{8}\right]\right\};$$

$$C_{22} = 8I_1^0(\delta); \qquad C_2 = 8I_3^0(\delta);$$

$$C_1 = 8\left\{I_3^0(\delta) + \frac{2}{\delta^2}\left[I_3^0(\delta) + 2\delta I_2^1(\delta) + \delta^2 I_1^2(\delta) - \frac{\pi}{8}\right]\right\}.$$

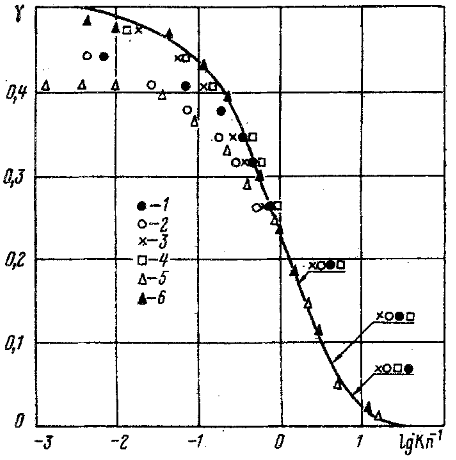

Fig. 1. Comparison between the theoretical γ-curve and test data for: 1) H_2, 2) Ne, 3) Xe, 4) Ar, 5) He at a smooth surface, 6) He at a rough surface.

The integrals

$$I_n^m(\delta) = \int_0^1 t^m (1 - t^2)^{1/2} J_n(2\delta t)\, dt$$

may be calculated to any desirable accuracy, by using the asymptotic representation of function J_n [3].

It is to be noted that the results obtained by the variation method agree closely with the numerical solution obtained by Loyalka [4] (the maximum discrepancy between both solutions is 0.15%, when $\delta \sim 1$).

Under stabilized steady conditions the total average velocity $\langle u \rangle = \langle u_1 \rangle + \langle u_2 \rangle$ vanishes. Then we have the expression

$$\frac{dp}{p} = \gamma(\delta)\frac{dT}{T}; \qquad \gamma(\delta) = \frac{Q_2(\delta)}{Q_1(\delta)},$$

which, when integrated from p_1, T_1, to p_2, T_2 along the capillary, yields a simple relation for the effect of thermomolecular pressure difference:

$$\frac{p_1}{p_2} = \left(\frac{T_1}{T_2}\right)^{\gamma}. \tag{11}$$

In the case of free-molecular conditions we have $\gamma(\delta = 0) = 0.5$, i.e., the well known Knudsen formula applies; in the other extreme case of a continuous medium we have $\gamma(\delta \to \infty) = 0$; there is no thermomolecular effect. Numerical values of γ for δ from 0 to 10 have been tabulated.

A comparison between the theoretical results obtained for a capillary tube and for a plane gap [5] indicates a weak dependence of the thermomolecular effect on the geometry of the channel section.

The theoretical γ-curve is compared in Fig. 1 with the test data in [6] and in [7]. We note a very close agreement (within test accuracy) for heavy gases (Xe, Ar) over the entire test range of the Knudsen number.

In the case of light gases, however, the maximum discrepancy between theoretical and test values under free-molecular conditions is as high as 5% for H_2, 10% for Ne, and 18% for He at a Knudsen number $Kn \geqslant 10^2$, which can, apparently, be explained by the different character of the interaction between gas and capillary surface. This conclusion is based on a comparison between Hobson's test data for He in capillaries with smooth and rough surfaces respectively.

On the basis of this discussion, we conclude that the functional relation derived here for the thermomolecular pressure difference is correct, which permits us to recommend this relation (11) for the calculation of the thermomolecular effect over the entire range of the Knudsen number.

If two volumes of a gas V_1 and V_2 at different temperatures T_1 and T_2 respectively are connected through a capillary tube with a radius R and length L, then the requirement that the number of particles in a system remain conserved will easily yield the law according to which the thermomolecular pressure difference varies with time:

$$\gamma(\delta, t) = \frac{Q_2}{Q_1}\left\{1 - \exp\left[-\frac{\pi R^3}{VL}\left(\frac{2kT}{m}\right)^{1/2} Q_1 t\right]\right\}, \tag{12}$$

where $1/V = 1/V_1 + 1/V_2$, k is the Boltzmann constant, and m denotes the mass of molecules.

It follows from (12) that the relaxation time of the process is

$$\tau_r = \frac{VL}{\pi R^3 Q_1}\left(\frac{m}{2kT}\right)^{1/2}.$$

Values of Q_1 for various values of δ are given in Table 1.

Formulas (11) and (12) together with Table 1 are useful for practical calculations of the thermomolecular pressure difference and the relaxation time, for any gas and for tubes with any cross section.

NOTATION

γ	is the index of the effect of thermomolecular pressure difference;
δ	is the rarefaction number for a gas;
λ	is the mean free path of gas molecules;
$\nu = (1/p)dP/dz$;	
$\tau = (1/T)dT/dz$;	
$\tilde{\Psi}_i$	are the trial functions;
F_i	is the functional for the integral equation;
Kn	is the Knudsen number;
k	is the Boltzmann constant;
m	is the mass of molecules;
p	is the pressure;
Q_1, Q_2	are the referred flow due to the pressure and temperature gradient;
R	is the capillary radius;
s	is the cross-sectional area;
T	is the temperature;
u	is the velocity of an average molecule.

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