

STUDY OF THE MASS-TRANSFER KINETICS DURING EVAPORATION IN A CYLINDRICAL  
CAPILLARY ON THE BASIS OF THE BGK EQUATION

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An approximate solution is found for a model kinetic equation for gas flow in a cylindrical capillary at whose flat bottom evaporation occurs.

A description of transport processes in capillary-porous media incorporating phase transitions requires a study of the vapor-transport kinetics in a cylindrical capillary of finite length in which evaporation occurs. Levdanskii et al. [1] have solved this problem for the case of free-molecular flow.

Much work has been done on gas flow in infinitely long capillaries; e.g., Cercignani and Sernagiotto [2] found a numerical solution for this problem over a broad range of Knudsen numbers Kn. Sone and Yamamoto [3] analyzed the asymptotic solution for small Kn, and Ferziger [4] carried out analogous calculations for large Kn (finding a series solution).

In the present paper we analyze the slow flow of a single-component gas in a cylindrical capillary of radius  $r_0$  bounded on one side (the bottom;  $Z = 0$ ) by a flat surface at which evaporation occurs. The inner surface of the capillary is assumed at a constant temperature. We assume that the gas molecules are reflected diffusely from the walls and that the evaporation (or condensation) coefficient at the bottom equals one.

We begin this analysis of the gas flow with the Bhatnagar-Gross-Krook (BGK) kinetic equation:

$$\vec{\xi}_R \frac{\partial f}{\partial \vec{R}} + \xi_z \frac{\partial f}{\partial Z} = \frac{f_0 - f}{\tau}, \quad (1)$$

where  $\vec{R} = (X, Y)$ ,  $\vec{\xi}_R = (\xi_X, \xi_Y)$ , and the  $Z$  axis is the axis of the cylinder.

Introducing the dimensionless coordinates and velocities  $z = Z/r_0$ ,  $\vec{r} = \vec{R}/r_0$ ,  $\vec{u} = \vec{\xi} \times h^{1/2}$  ( $h = m/2kT$ ), we transform Eq. (1) to

$$\vec{u}_r \frac{\partial f}{\partial \vec{r}} + u_z \frac{\partial f}{\partial z} = \alpha (f_0 - f), \quad (2)$$

where

$$\alpha = \frac{r_0 h^{1/2}}{\tau} = \frac{1}{2Kn}.$$

The boundary conditions are as follows: At the lateral surface ( $r = 1$ ), we have the condition

$$f(\vec{n} \cdot \vec{u}_r > 0) = n_\infty \exp\{-u^2\} \left(\frac{h}{\pi}\right)^{3/2}; \quad (3)$$

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for reflected molecules; at the bottom ( $Z = 0$ ), we have

$$f(u_z > 0) = n_s \exp\{-u^2\} \left(\frac{h}{\pi}\right)^{3/2}, \quad (4)$$

where  $n_s$  is the saturation vapor density at the given pressure. We also specify the density  $n_l$  at  $z = l$ .

By analogy with the problems involving slow gas flow in an infinitely long capillary under the influence of a small pressure gradient [5], we seek a solution of Eq. (2) in the form

$$f = f_l [1 + K(z-l) + u_z \psi(\vec{r}, \vec{u}_r)], \quad (5)$$

where

$$f_l = n_l \left(\frac{h}{\pi}\right)^{3/2} \exp\{-u^2\},$$

and the quantity  $K$  is to be determined, in contrast with the situation in the earlier work, where it was specified.

According to Eq. (5), the particle density  $n$  is constant over a cross section and is a function of  $z$  alone.

Substituting (5) into (2) and linearizing, we find

$$\psi + \frac{\vec{u}_r}{\alpha} \frac{\partial \psi}{\partial \vec{r}} = 2c_z(\vec{r}) - \frac{K}{\alpha}, \quad (6)$$

where  $c_z$  is the dimensionless macroscopic velocity; by virtue of the axial symmetry we have  $c_z = c_z(r)$ .

From Eqs. (3) and (5) we find that at  $r = 1$  we have

$$\psi(\vec{n} \cdot \vec{u}_r > 0) = 0. \quad (7)$$

We write Eq. (6) in integral form (the integration is carried out along the characteristics), using boundary condition (7) (Fig. 1):

$$\psi = \alpha \int_0^b \frac{1}{u_r} \exp\left\{-\frac{\alpha}{u_r} s\right\} \left[2c_z(r') - \frac{K}{\alpha}\right] ds, \quad (8)$$

where

$$s = \sqrt{(x-x')^2 + (y-y')^2}, \quad b = -r \cos \theta + \sqrt{1 - r^2 \sin^2 \theta}.$$

From (5) we find

$$c_z = \frac{1}{\pi^{3/2}} \int \exp\{-u^2\} u_z^2 \psi d\vec{u}.$$

Now multiplying (8) by  $(u_z^2/\pi^{3/2}) \exp\{-u^2\}$  and integrating over  $\vec{u}$  ( $d\vec{u} = u_r du_z du_r d\theta$ ), we find

$$c_z = \frac{\alpha}{2\pi} \int_0^{2\pi} \int_0^b \left[2c_z(r') - \frac{K}{\alpha}\right] J_0(\alpha s) ds d\theta, \quad (9)$$

where

$$J_m(s) = \int_0^\infty t^m \exp\left\{-t^2 - \frac{s}{t}\right\} dt.$$

To determine  $K$  we write another equation, which is found by equating the flux across an arbitrary cross section of the capillary to the flux at the bottom, obtained with the help of (4):

$$\int_0^1 rc_z dr = \frac{\frac{n_s}{n_i} - 1 + Kl}{2\pi^{1/2}}. \quad (10)$$

In Eq. (5) and the derivation of Eq. (10) we assumed the distribution function of the incident molecules to retain its  $z$  dependence all the way to the bottom. Consequently, the equations derived here are valid for  $z > z_0$ , where  $z_0 \approx 1/2\alpha$  is the thickness of the Knudsen layer.

We rewrite Eq. (9), introducing  $v = v_z = -2c_z/K$

$$v = \frac{\alpha}{\pi} \int_0^b \int_0^{2\pi} \left[ v(r') + \frac{1}{\alpha} \right] J_0(\alpha s) ds d\theta. \quad (11)$$

The problem has thus been reduced to one of solving integral equation (11) and then determining  $K$  from Eq. (10). In the limit  $\alpha \rightarrow \infty$  we expand  $v$  in a Taylor series in (11) and replace the integration over the cross-sectional area of the capillary by an integration over the area of a circle of radius  $A/\alpha$ , where  $J_n(A) = 0$ ; as a result we find a Poiseuille profile:

$$v = \frac{\alpha}{2}(1-r^2) + v_\omega \quad (12)$$

where  $v_\omega$  is the slip velocity.

Let us examine Solution (11) for the case of small values of  $\alpha$ .

Since  $s ds d\theta = dx' dy'$ , we can write  $J_0(\alpha s) ds d\theta$  as  $[J_0(\alpha s)/s] dx' dy'$ . In the limit  $\vec{r}' \rightarrow \vec{r}$ ,  $s$  tends toward zero, while  $J_0(\alpha s)/s$  tends toward infinity for small values of  $\alpha$ . For these small values of  $\alpha$  we can thus approximate  $v(r')$  on the right side of (11) by  $v(r)$ . An analogous procedure was used by Kogan [5] for the flow between infinite parallel plates in the case in which the kernel of the integral equation has a logarithmic singularity. As a result of this substitution we find

$$v_0(r) = \frac{1}{\frac{\pi}{a(r)} - \alpha}, \quad (13)$$

where

$$a(r) = \int_0^b \int_0^{2\pi} J_0(\alpha s) ds d\theta = \frac{2}{\alpha} \left[ \frac{\pi}{2} - \int_0^\pi J_1(\alpha b) d\theta \right].$$

For larger values of  $\alpha$ , an approximate analytic solution  $v(r)$  can be found by expanding the function  $v(r')$  in a Taylor series in  $x'$  and  $y'$ , retaining the second derivatives, and setting  $x = 4, y = 0$ :

$$\begin{aligned} \frac{\partial v}{\partial x'} \Big|_{x'=x, y'=y} &= \frac{dv}{dr}, \quad \frac{\partial v}{\partial y'} \Big|_{x'=x, y'=y} = 0, \\ \frac{\partial^2 v}{\partial x'^2} \Big|_{x'=x, y'=y} &= \frac{d^2 v}{dr^2}, \quad \frac{\partial^2 v}{\partial y'^2} \Big|_{x'=x, y'=y} = \frac{1}{r} \frac{dv}{dr}, \\ \frac{\partial^2 v}{\partial x' \partial y'} \Big|_{x'=x, y'=y} &= 0, \\ x' - x &= s \cos \theta, \quad y' - y = s \sin \theta \end{aligned}$$

and

$$v(r') = v(r) + \frac{dv}{dr} \left( s \cos \theta + \frac{1}{2r} s^2 \sin^2 \theta \right) + \frac{1}{2} \cdot \frac{\partial^2 v}{\partial r^2} s^2 \cos^2 \theta. \quad (14)$$

Substituting (14) into (11) and replacing  $dv/dr$ ,  $d^2v/dr^2$  by their values from (12), we find

$$v_1(r) = v_0(r) - \alpha^2 \frac{ra_1(r) + 0.5a_2(r)}{\pi - \alpha a(r)}, \quad (15)$$

where

$$\begin{aligned} a_1(r) &= \int_0^{2\pi} \int_0^b s \cos \theta J_0(\alpha s) ds d\theta = -\frac{2}{\alpha} \int_0^\pi \cos \theta \left[ bJ_1(\alpha b) + \frac{1}{\alpha} J_2(\alpha b) \right] d\theta, \\ a_2(r) &= \int_0^{2\pi} \int_0^b s^2 J_0(\alpha s) ds d\theta = \\ &= 2 \int_0^\pi \left[ -\frac{1}{\alpha} J_1(\alpha b) b^2 - \frac{2}{\alpha^2} J_2(\alpha b) b - \frac{2}{\alpha^3} J_3(\alpha b) + \frac{1}{\alpha^3} \right] d\theta. \end{aligned}$$

The dimensionless volume flow rate per unit area, divided by  $-K/2$ , is

$$N^* = -\frac{2}{K} N = 2 \int_0^1 rv(r) dr. \quad (16)$$

We are dividing the flow rate by  $-K/2$  for convenience below in comparing the values found for  $N$  with the results of previous papers on capillary flow in which dimensionless mass fluxes divided by  $-K$  were calculated; they are equal to the volume flow rates divided by  $-K/2$ .

The integrals in the functions  $a(r)$ ,  $a_1(r)$ , and  $a_2(r)$ , and thus the flux  $N$  have been found numerically. The values of  $J_n(t)$  for  $t \leq 1$  were approximated by series [6], while those for  $t > 1$  were approximated by the sum of two exponential functions (the interval  $t = 1-10$  was split into two parts).

The calculations show that up to  $\alpha$  values on the order of one, the values of  $v_0(r)$  and  $v_1(r)$  (and thus  $N^*$ ) are essentially the same. With a further increase in  $\alpha$ , the difference between  $v_0(r)$  and  $v_1(r)$  increases.

In Table 1 we compare the values of  $N^*$  calculated from Eqs. (13) and (15) with the results of the numerical solution of [2]. For  $\alpha \leq 1$  the values of  $N^*$  found from  $v_0$  (or  $v_1$ ) agree well with the corresponding values from [2]; in the limit  $\alpha \rightarrow 0$  we find a value of  $N^*$  which is approximately the free-molecular value,  $8/3\sqrt{\pi}$ . At larger values of  $\alpha$ , the values of  $N^*$  determined from  $v_1(r)$  also agree with the results of [2]; in addition, the  $v_1(r)$  profile for  $\alpha = 5$  agrees well with the velocity profile given in [3]. On the basis of all this agreement, we conclude that Eq. (15) is valid for calculating both the velocity profile and the flow rate up to  $\alpha = 5$ .

In the limit  $\alpha \rightarrow \infty$  we find from (12)

$$N^* = \frac{\alpha}{4} + v_\omega. \quad (17)$$

This equation is the same as that given in [3], with

$$v_\omega = 1.016 + \frac{0.548}{\alpha}.$$

From (10) and (16) we find

$$K = \frac{1 - \frac{n_s}{n_l}}{l + \frac{\pi^{1/2} N^*}{2}}, \quad N = \frac{\frac{n_s}{n_l} - 1}{\frac{2l}{N^*} + \pi^{1/2}}. \quad (18)$$

For large values of  $\alpha$  we find from (17) and (18)

$$N = \frac{\frac{n_s}{n_l} - 1}{\frac{8l}{\alpha + 4v_\omega} + \pi^{1/2}}.$$

TABLE 1. Volume Flow Rate  $N^*$  as a Function of  $\alpha$

$\alpha$	0,1	0,2	0,3	0,4	1	2	3	4	5
$N^*$ from (15)	1,404	1,383	1,379	1,383	1,482	1,726	1,997	2,274	2,554
$N^*$ from [2]	1,404	1,382	1,377	1,380	1,459	1,661	1,885	2,119	2,358
$N^*$ from (13)	1,404	1,383	1,379	1,385	1,501	1,865	2,424	3,240	4,411

TABLE 2.  $N/(n_s/n_l - 1)$  and  $N_0/(n_s/n_l - 1)$  as Functions of  $\alpha$  for  $l = 20$

$\alpha$	0,1	0,4	1	3	5	10	50	100	500	$\infty$
$\frac{N}{(n_s/n_l - 1)}$	0,0330	0,0326	0,0348	0,0459	0,0574	0,0766	0,211	0,302	0,479	0,564
$\frac{N_0}{(n_s/n_l - 1)}$	0,0351	0,0346	0,0370	0,0499	0,0638	0,0893	0,338	0,650	3,15	$\infty$

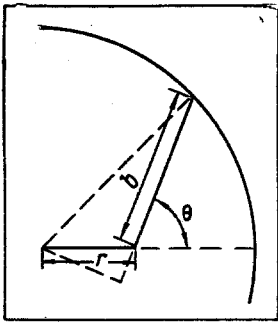


Fig. 1. Geometry of the problem.

$$N = \frac{\frac{n_s}{n_l} - 1}{\frac{8l}{\alpha + 4v_\omega} + \pi^{1/2}} \quad (19)$$

We thus see from (19) that in the case  $l \ll \pi^{1/2}\alpha/8$  we can use the Hertz-Knudsen equation for evaporation from a free surface, with the mass velocity  $v_z$  taken into account in the distribution function of molecules incident on the bottom [7]; i.e., in the limit  $\alpha \rightarrow \infty$  ( $l \ll \pi^{1/2}\alpha/8$ ), the flux  $N$  tends toward a constant value in contrast with the case of an infinite capillary [2].

Table 2 shows  $N/(n_s/n_l - 1)$  for various values of  $\alpha$  ( $l = 20$ ); shown for comparison here are the values of this quantity in the case  $K_0 = (1 - n_s/n_l)/l$ . It should be noted that the parameters  $n_l$ ,  $l$ , and  $\alpha$  cannot be chosen independently: When  $\alpha$  is changed,  $n_l$  or  $r_0$  must also be changed. If we wish to change  $\alpha$ , while holding  $r_0$  and  $n_s/n_l$  constant, we must allow the appropriate change in  $n_s$ , i.e., the temperature of the system ( $n_s$  and  $T$  are related by the equation for the saturation vapor density). Accordingly, in order to transform to dimensional velocities and flow rates we must multiply the corresponding dimensionless quantities by different factors, which are dependent on the temperature, i.e., on  $\alpha$ . Since there is an exponential dependence on  $T$  in the equation for the saturation vapor density, however, the difference is only slight: for ice, e.g., as  $\alpha$  is varied from 0.1 to 5 the temperature increases by a factor of only 1.17.

#### NOTATION

$f$ , distribution function;  $\vec{\xi}$ , molecular velocity;  $\vec{n}$ , unit vector along the normal to the lateral surface;  $\tau$ , scale time between molecular collisions;  $L$ , length of capillary;  $l = L/r_0$ ,  $N_0 = -K_0/2 N^*$ ; Indices: "w" corresponds to the lateral surface of the capillary.

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