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Kinetics of intense evaporative mass transfer through a porous layer

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Abstract—A kinetic problem of mass transfer in a model porous body in the process of intense evaporation (condensation) and vapour escape into a vacuum is considered. Two computational methods have been used: the mean free path method and the method of direct statistical simulation. With the aid of the first method the location of the condensation zone within a porous body is determined as a function of the evaporating surface-to-porous layer temperature difference and also of the condensation coefficient. The second method is employed in a one-dimensional case to obtain (without condensation) the density, velocity and temperature distributions for a gas in a porous layer and in a gas medium behind the porous body. It is shown that the agreement between the parameters obtained by both methods for the gas flow escaping the porous layer is quite satisfactory.

INTRODUCTION

THE KINETIC theory of transfer processes with intense evaporation (condensation) into a vacuum has been studied extensively (see, for example, [1–7]). A detailed molecular–kinetic description of substantially non-equilibrium processes occurring near the phase interface allows one to obtain accurate predictions for vapour streams. In particular, it is shown that in the process of steady-state evaporation from an open surface to vacuum, the magnitude of the limiting vapour stream is smaller by about 18% than that of the maximum one-sided flow. Besides, the obtained values of macroscopic parameters (density, temperature) behind the Knudsen layer (on the order of the free path of molecules) can serve as boundary conditions for gas-dynamic equations. The latest achievements in this field are being considered in reviews [8, 9].

The knowledge of the laws governing intense vapour escape into a rarefied medium during substance evaporation in porous media is necessary for describing sublimation drying [10], mass transfer in porous materials exposed to laser radiation [11] and a number of other processes. Thus, the vacuum coating technology employs a high-porous partition for controlling a molecular flux. Mass transfer in such a partition was studied in ref. [12] within the framework of the mean free path concept, but this was done without a systematic account of intermolecular collisions in pores. At the same time, in ref. [13], when studying the kinetics of mass transfer in a high-porous layer, a method of direct statistical simulation was used, in which the collisions of gas molecules with the spheres that modelled the porous body skeleton were described by employing isotropic scattering approximation.

The present work considers the kinetic problem of intense mass transfer with evaporation (and condensation) of material in a model porous body and escape of vapour into a vacuum assuming an approximate technique for taking into account intermolecular collisions in a transient (molecular–viscous) regime, which often prevails in sublimation drying, spray-coating with the use of a porous partition and in other processes. The location of the moist zone (the zone of condensation) depending on the evaporator and porous body temperatures is defined. The technique allows one to substantially simplify the calculation scheme in a two-dimensional case. For a one-dimensional problem, the method of direct statistical simulation is used, with the aid of which (in an isothermal case, i.e. without condensation) the density, velocity and temperature distributions for a gas in a porous layer and in a gaseous phase behind the porous body are obtained, and the values of the fluxes of vapour molecules are compared with corresponding quantities found by the mean free path method.

STATEMENT OF THE PROBLEM

The geometry of the problem is depicted in Fig. 1, where above the evaporation surface ($x = 0$) a high-porous layer of thickness L_ε is located which is modelled by a homogeneous system of irregularly dis-

NOMENCLATURE

I	density of resulting vapour stream
k	Boltzmann constant
L	length of calculation region
M	Mach number
m	mass of molecule
n	number density of gas particles
n_c, p_c	density and pressure of saturated vapour, respectively
q_0	energy required to evaporate one atom
r	radius of fixed spherical particles of porous body
R_ε, R_0	radii of porous body and evaporating surface
T	temperature
$U(0)$	indicatrix value at angle $\varphi = 0$
v	mean gas velocity
x	coordinate.

Greek symbols

α	evaporation (condensation) coefficient
ε	porosity
λ_0	mean free path of gas molecules
$\vec{\xi}$	velocity vector of gas molecules
σ	collision cross section of molecules.

tributed fixed spherical particles of radius r (the 'dusty-gas' model [14, 15]). The number of fixed particles and surface per volume unit are respectively given by

$$n_\varepsilon = 3(1-\varepsilon)/4\pi r^3, \tag{1}$$

$$S = 3(1-\varepsilon)/r. \tag{2}$$

The mean free path of gas molecules relative to the fixed spherical particles of the porous body skeleton is determined by the expression

$$\lambda_\varepsilon = \frac{4}{3}\frac{\varepsilon}{1-\varepsilon}r. \tag{3}$$

In the case of a two-dimensional statement of the problem, molecules evaporate from the area of a circle of a given radius, with the law of diffuse reflection of molecules being assigned on the remaining portion of the evaporating surface.

THE MEAN FREE PATH METHOD

The mean free path method in the problem of molecular flux passage through a porous layer, as applied to the process of spray-coating in a vacuum chamber when a porous partition can serve as an additional regulator of the intensity and distributivity of vapour stream over the surface of a spray-coated product, it is important to determine this flux taking account of the gas molecules re-evaporated from the porous body.

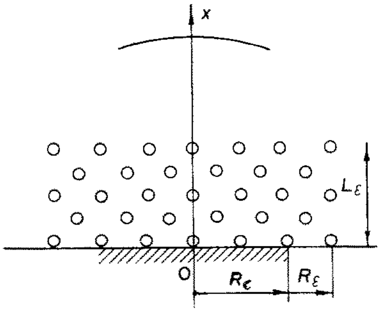

FIG. 1. Geometry of the problem.

If the temperature T_ε of the porous partition is smaller than the evaporator temperature T_0, a condensation zone (moist zone) is formed, the re-evaporation from which can exert an important influence on the spraying process. The contribution of the re-evaporated molecules into the resulting flux in a free molecular regime is determined primarily by the temperature and can be approximately estimated by the ratio of fluxes re-evaporated from the porous layer volume and coming from the evaporating surface:

$$\Delta I_\varepsilon L_\varepsilon \approx \sqrt{(T_0/T_\varepsilon)}\exp\left\{-q_0\frac{T_0-T_\varepsilon}{T_0T_\varepsilon}\right\}SL_\varepsilon.$$

Naturally, the contribution of re-evaporation increases with an increase in the temperatures T_0 and T_ε, a decrease in the difference $\Delta T = T_0 - T_\varepsilon$ and with an increase in the specific surface S and porous layer thickness L_ε.

This contribution in a free-molecular regime has already been investigated in ref. [12] when only collisions of gas molecules with the walls of a porous skeleton were taken into account. Also in that work an attempt was made to allow for the intermolecular collisions under the assumption that the field gas molecules are immobile, their distribution is known, and that test molecules scatter isotropically from them. However, as the comparison with more accurate calculations has shown (but without allowing for condensation) [13], the values of the fluxes leaving the porous partition turn out to be underestimated.

In the present work this problem is solved by the Monte-Carlo method in the mean free path approximation with allowance for the motion of field molecules over which test molecules are scattered. The use of the one-velocity mean free path approximation allows one to significantly simplify the calculation scheme and fairly quickly obtain the solution for a two-dimensional case.

As usual, in this method the mean free path length is governed by all the possible interactions of the test molecule. It is determined by the relation $1/\lambda = 1/\lambda_0 + 1/\lambda_\varepsilon$, where λ_0 is the gas-dynamic free path length. The length value is drawn from the exponential law [12], the kind of the process is obtained from the relationships:

$$P_\varepsilon = \lambda/\lambda_\varepsilon = \lambda_0/(\lambda_\varepsilon + \lambda_0), \quad P_0 = 1 - P_\varepsilon,$$

where P_ε and P_0 are the probabilities of the collision of the field molecule with the porous body skeleton and with another field molecule, respectively. The diffuse law of the reflection of gas molecules from modelling spheres has been used.

As in ref. [12], the general procedure of the solution comprises the following stages:

(1) the distribution of condensate in the porous partition due to evaporation from the bottom is computed; the condensation coefficient α is assumed to be assigned and constant throughout the porous body volume;

(2) by the sign of the resulting flux density I ($I < 0$) the location of the moist zone is determined. In this case, $I = I_a - I_e$, where $I_e = \alpha p_e(T)/\sqrt{(2\pi mkT)}$ is the flux density of evaporated molecules, I_α is the density of the flux of molecules arriving at the surface unit of model spheres from the evaporating surface and the porous layer volume;

(3) the redistribution of streams in the porous partition is calculated with account of evaporation from the moist zone;

(4) after stage 3, the location of the moist zone ($I < 0$) is redetermined;

(5) thereafter, the cycle (1)–(4) is repeated assuming a purely diffuse scattering in the dry zone until the position of the moist zone will cease varying from iteration to iteration.

To take into account the intermolecular collisions, an approximate technique is used according to which, first, a free-molecular flow is analyzed considering only interaction of molecules with the porous skeleton. In each space cell of the porous partition, a mean direction of the molecules passing through this cell is determined (field distribution). At the next step, the intermolecular collisions are taken into account, with the direction of the test molecule motion after collision with the field molecule being determined in accordance with the law of elastic interaction.

The flow of molecules passing through the partition and its angular distribution $U(\varphi)$ are determined as functions of the partition porosity and temperature. This allows one to obtain the distribution of molecular flux over the substrates of the holder and the degree of its uniformity. Besides, the flow of returning molecules $\tilde{I}_R$ at the boundary ($x = 0$) is calculated. Comparison with the data of direct statistical simulation (Fig. 5) has shown a satisfactory agreement between the values of I in the transient regime ($Kn = \lambda_0/\lambda_\varepsilon \approx 1$).

Figure 2 illustrates the disposition of moist zone boundaries in the porous partition depending on temperature and condensation coefficient. The equipotential curves correspond to the same values of the quantity $I_v = IS$. The line $I_v = 0$ corresponds to the boundary between the dry and moist zones. Calculations have shown that the moist zone contracts with a decrease in the temperature drop ΔT, and the condensation intensity in it drops. As the condensation coefficient α increases, the size of the moist zone diminishes, but the condensation intensity increases, since the molecules are being absorbed in a narrower zone. The tabulated values of overall fluxes of molecules emanating from the porous layer $\tilde{I}^+$, coming back to the $x = 0$ surface $\tilde{I}_R$ and condensed in the interior of the body $\tilde{I}_c$ are related as I_v in Fig. 2 to the flow of evaporated molecules $\tilde{I}_{e0} = I_{e0}\pi R_c^2$, where $I_{e0} = p_e(T_0)/\sqrt{(2\pi mkT_0)}$. When the temperature difference decreases, the flux $\tilde{I}^+$ increases owing to re-evaporation and approaches the case of pure scattering for $\Delta T \to 0$. As α decreases, the condensation intensity drops, but the flux of the molecules that passed through the partition $\tilde{I}^+$ can decrease due to the weakening of re-evaporation.

The flux $\tilde{I}^+$ increases at the expense of molecular collisions, the angular distribution $U(\varphi)$ extends forward, and becomes larger, the higher α and ΔT.

THE METHOD OF DIRECT STATISTICAL SIMULATION

Now, let us turn to the discussion of the results obtained by the Monte-Carlo method of direct statistical simulation using the Yanitskiy calculation scheme for predicting collisions in each cell [16]. Here, a one-dimensional problem is considered for evaporation and mass transfer through a model porous body. These calculations made it possible to find not only the fluxes of vapour molecules, but also density, velocity and temperature distributions both within the porous body, and in the region behind it.

The Maxwellian distribution function f^+ for the molecules entering into the computational domain is assigned over the whole evaporation surface $x = 0$

$$\begin{aligned} f^+ &= f_e(x, \vec{\xi}) \\ &= n_e(h_0/\pi)^{3/2} \exp(-h_0\xi^2), \quad \vec{\xi}\vec{n} > 0, \end{aligned}$$

where $h_0 = m/2kT_0$, $\vec{n}$ is a normal directed toward the inside of the computational domain, n_e is the density of saturated vapours at temperature T_0, the evaporation (condensation) coefficient α is assumed equal to unity. The computational domain consists of a porous layer of thickness L_ε and the area above it which is occupied by the vapour and at the boundary of which $x = L$ the condition of the absence of particle flow from the vacuum is assigned (the condition at infinity):

$$f_L^+(x, \xi) = 0, \quad \xi\vec{n} > 0.$$

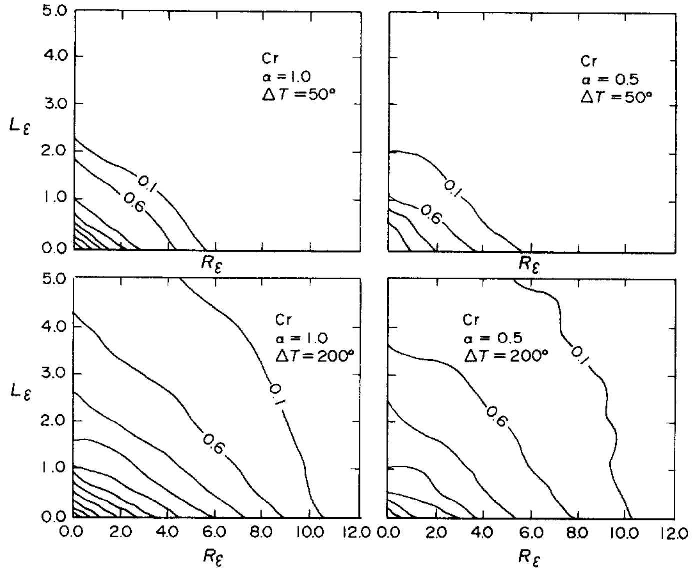

FIG. 2. Position of the moist zone in a porous body with Cr vapour condensation ($T_0 = 1830$ K, $\Delta T = T_0 - T_\varepsilon$, $R_0 = 10$, $R_\varepsilon = 12$, $\varepsilon = 0.95$, $L_\varepsilon = 5$; numerical values on the isolines I_v = const. are increased 10^3 fold for abbreviation).

For the density, temperature, velocity, and length scales the following quantities were selected: n_e, T_0, $(h_0)^{-1/2}$, λ_0, where $\lambda_0 = (\sqrt{(2)}n_e\sigma)^{-1}$, and $\sigma = \pi d^2$ is the collision cross section for the molecular model 'solid spheres'. The temperature of the porous body skeleton is assumed to be equal to the evaporating surface temperature T_0, and $L = 40\lambda_0$. Computational variants correspond to the case $L_\varepsilon/\lambda_0 = 10$, $n_\varepsilon/L_\varepsilon = 10$, $\varepsilon = 0.9$ (where n_ε is determined from equation (1)), i.e. $r = 0.13\lambda_0$. Then, for example, for Cr at $T_0 = 1830$ K the saturated vapour pressure is $P_e = 0.1$ mm Hg at which $\lambda_0 = 0.35$ cm. In this case, $r = 0.045$ cm, and $\lambda_\varepsilon = 0.5$ cm according to equation (3), i.e. $Kn = \lambda_0/\lambda_\varepsilon = 0.7$.

Numerical calculation of vapour flow through a porous layer by the method of direct statistical simulation includes two stages [13]. At the first stage, calculations are performed for the collisions between gas molecules both in the porous body and outside it, without taking into account the motion of molecules. In this case, the Yanitsky scheme is applied [16]. In contrast to the commonly used technique, the second stage is characterized by collisions with the porous body skeleton. The description of collisions comprises the determination of the normal at the point of collision of a molecule with a sphere and its reflection according to the diffuse law. Figure 3 presents distributions of dimensionless density n, mean velocity v and temperature T of the gas for the case $L_\varepsilon = 10\lambda_0$ and $\varepsilon = 0.9$. It is evident that the vapour density in the porous layer drops sharply down to the value $n \approx 0.15$, and that the function $n(x)$ decreases slowly behind the porous layer. It should be noted that in the variants considered there is no vapour oversaturation in the porous layer for $q_0/kT_0 < 5$.

Gas velocity $v(x)$ within the porous body is rather a small and almost constant quantity, but it increases sharply at the porous body–gas interface. Therefore,

Table 1. Overall molecular fluxes in a porous layer for various values of α and ΔT ($L_\varepsilon = 5\lambda_0$; $\varepsilon = 0.95$)

α	ΔT	$\tilde{I}^+$	$\tilde{I}_R$	$\tilde{I}_c$	$U(0)$
1	200	0.29	0.04	0.67	1.79
1	100	0.59	0.13	0.28	1.78
1	50	0.70	0.20	0.10	1.77
0.5	200	0.28	0.13	0.59	1.44
0.5	100	0.52	0.20	0.28	1.38
0.5	50	0.61	0.27	0.12	1.38

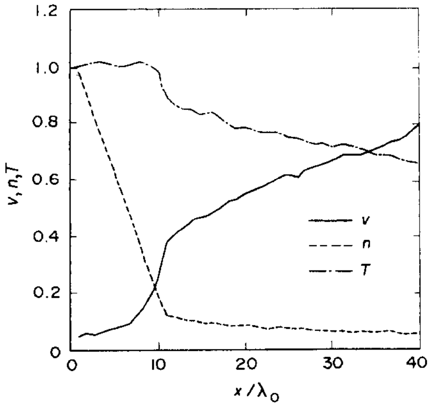

FIG. 3. Distributions of gas mean velocity, density and temperature over a porous layer and in the region behind it ($L_\varepsilon = 10\lambda_0$, $\varepsilon = 0.9$).

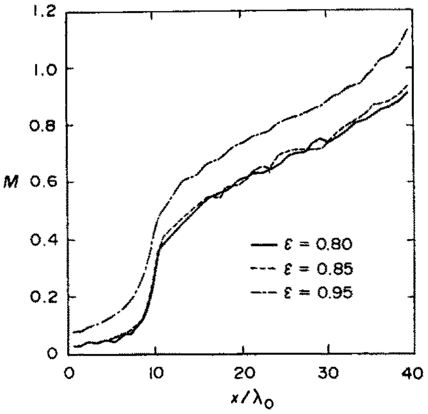

FIG. 4. Local Mach number M vs the coordinate.

the Darcy law, strictly speaking, does not hold in the case under consideration. The gas temperature in the interior of the porous body remains practically constant.

Figure 4 presents the plot of the local Mach number $M(x)$ vs the coordinate for several values of the layer porosity (note that these data correspond to the case when not the entire surface $x = 0$ is involved in evaporation, but only its part ε). It is important to emphasize that the value $M = 1$ is attained in the given computational domain ($x < 40\lambda_0$) only at $\varepsilon = 0.95$ and at a significant distance from the porous body boundary $x = L$, whereas with evaporation from an open surface into vacuum [1, 2], $M = 1$ immediately downstream of the Knudsen layer (for $n \approx 0.31$).

Let us analyze the behaviour of the vapour flux densities, the magnitudes of which are related to the maximum one-sided flow $I_{e0} = n_e\bar{\xi}/4 = \sqrt{(kT_0/2\pi m)}n_e$ (Fig. 5). The density of the resulting flux of particles at the exit from the porous layer ($x = L$) $I = \int_{-\infty}^{\infty} \xi_x f(x, \xi)\,\mathrm{d}\xi$ depends substantially on the layer thickness L_ε. In particular, for $L_\varepsilon = 10\lambda_0$ at $\varepsilon = 0.9$ $I/I_{e0} \sim 0.18$, whereas at $\varepsilon = 0.95$, $I/I_{e0} \sim 0.25$. We note for comparison, that in the process of evaporation into a vacuum from an open surface [1, 2], the value of the dimensionless limiting flow rate ($M = 1$) equals $I/I_{e0} \sim 0.82$, whereas in case of strong evaporation of a filler in a porous two-dimensional body with $2.5\lambda_0$-thick periodic channels [17] this very quantity is equal to $I/I_{e0} \approx 0.31$. More to the point, almost the same result as in ref. [17] is obtained if I/I_{e0} is calculated from an approximate equation for a free molecular flow of particles with filler evaporation from a cylindrical channel [18].

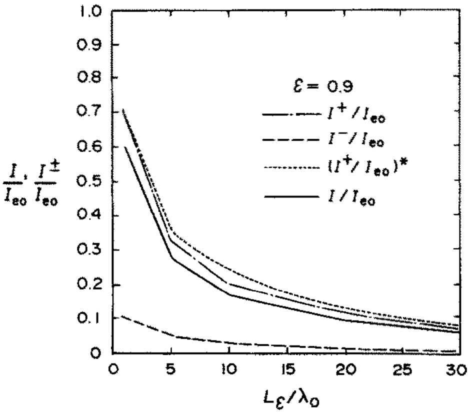

FIG. 5. The resulting gas flow I/I_{e0} and the reverse molecular flow at the boundary $x = L_\varepsilon$ vs the porous layer thickness; $(I^+/I_{e0})^*$ is the density obtained for the one-sided escaping flow by the mean free path method.

Thus, the presence of solid surfaces in a porous layer leads to a significant decrease in the gas density and velocity at the exit from the porous body in comparison with the case of evaporation from an open surface, when only intermolecular collisions take place. It is worth noting, however, that for rather thin porous layers the density of the reverse flow of molecules $I^- = \int_{-\infty}^{0} \xi_x f(x, \xi)\,\mathrm{d}\vec{\xi}$ at the interface of a gas–porous body ($x = L_\varepsilon$) amounts to about 15% of the one-sided flow I^+ escaping the body, i.e. the value I^-/I^+ at $x = L_\varepsilon$ is close to the similar quantity in case of evaporation from an open surface.

From Fig. 5 is also evident that there is a satisfactory coincidence between the values for the gas flow I^+/I_{e0} obtained by the approximate mean free path method and the method of direct statistical simulation.

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