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NONSTATIONARY ISOTHERMAL EVAPORATION OF FLUIDS IN A CYLINDRICAL CHAMBER

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Numerical models for nonstationary isothermal evaporation of fluids in the cylindrical chamber of an experimental device are studied. The effect on the evaporation rate of the radii of the source and the output orifice is investigated. The relaxation times and the specific mass flux of the vapor are determined. The results are compared with analytic solutions for two limiting cases: the one-dimensioanl case and an infinite half-space.

The laws of mass transfer during the evaporation of solutions and melts of various types are of interest both industrially and ecologically. The most widely used information is on the temperature and concentration dependence of the evaporation rates, equilibrium partial pressures, and diffusion coefficients in gases [1, 2]. Much less attention is paid to investigating the effect of the configuration and geometric parameters of the equipment on the kinetic characteristics of the process.

Here we study the dependence of evaporation rates (average mass fluxes) on the dimensions of the liquid surface and the output orifice of a cylindrical chamber that is widely used

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in the laboratory. The circular source of liquid to be evaporated is placed in the center of the lower base of the cylinder. We examine the case of isothermal evaporation of a liquid, whose molecular weight exceeds that of the gas into which it is evaporated. This guarantees that the process is controlled by external diffusion without concentration convection inside the chamber. Also, the vapor pressure of the liquid is taken to be substantially less than the total pressure of the gas phase. These conditions correspond to most industrial processes for melts, where there is little heating above the liquidus temperature. These conditions also allow the Stefan flow to be neglected and simplify the problem substantially.

This case corresponds to a boundary problem for the diffusion equation in cylindrical coordinates:

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial z^2}\right); \tag{1}$$

$$C = C_e \quad \text{for } 0 \leqslant r \leqslant R_1,\ z = 0, \tag{2}$$

$$C = 0 \text{ for } 0 \leqslant r \leqslant R_2,\ z = H, \tag{3}$$

$$\frac{\partial C}{\partial r} = 0 \text{ for } \begin{cases} r = 0,\ 0 \leqslant z \leqslant H, \\ r = R_3,\ 0 \leqslant z \leqslant H, \end{cases} \tag{4}$$

$$\frac{\partial C}{\partial z} = 0 \text{ for } \begin{cases} z = 0,\ R_1 < r \leqslant R_3, \\ z = H,\ R_2 < r \leqslant R_3, \end{cases} \tag{5}$$

$$C = 0 \quad \text{for } t = 0. \tag{6}$$

The average mass flux (evaporation rate) from the surface of the source is defined by the expression

$$\langle j \rangle = -\frac{2D}{(R_1)^2}\int_0^{R_1} r\left.\frac{\partial C}{\partial z}\right|_{z=0} dr. \tag{7}$$

We introduce scales for dependent and independent variables: $r = R_3\rho$, $z = R_3x$, $C = C_eF$, $t = (R_3^2/D)\tau$, and reduce the problem (1)-(7) to a dimensionless form:

$$\frac{\partial F}{\partial \tau} = \frac{\partial^2 F}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial F}{\partial \rho} + \frac{\partial^2 F}{\partial X^2}; \tag{8}$$

$$F = 1 \text{ for } 0 \leqslant \rho \leqslant \rho_и,\ x = 0, \tag{9}$$

$$F = 0 \text{ for } 0 \leqslant \rho \leqslant \rho_0,\ x = X, \tag{10}$$

$$\frac{\partial F}{\partial \rho} = 0 \text{ for } \begin{cases} \rho = 0,\ 0 \leqslant x \leqslant X, \\ \rho = 1,\ 0 \leqslant x \leqslant X, \end{cases} \tag{11}$$

$$\frac{\partial F}{\partial x} = 0 \text{ for } \begin{cases} x = 0,\ \rho_и < \rho \leqslant 1, \\ x = X,\ \rho_0 < \rho \leqslant 1, \end{cases} \tag{12}$$

$$F = 0 \quad \text{for } \tau = 0. \tag{13}$$

The expression for the dimensionless flux is

$$\langle f \rangle = -\frac{2}{\rho_s}\int_0^{\rho_s} \rho\left.\frac{\partial F}{\partial x}\right|_{x=0} d\rho, \tag{14}$$

where

$$\langle f \rangle = \langle j \rangle \cdot R_1/D \cdot C_e. \tag{15}$$

The problem (8)-(14) was solved by the method of variable directions [3] by using a grid with forward differences in time and central differences in space. The integral (14) is calculated as follows. For an odd number of nodes M

$$\int_0^{\rho_s} \rho\left.\frac{\partial F}{\partial x}\right|_{x=0} d\rho = \sum_{i=1}^{M} A_i V_i, \tag{16}$$

where

$$V_i = \frac{\rho}{2\Delta x}(-3F^n_{i,1} + 4F^n_{i,2} - F^n_{i,3}).$$

The A_i are coefficients for Simpson's quadrature formula: $A_1 = A_M = \Delta\rho/3$, $A_2 = A_4 = \ldots = 4\Delta\rho/3$, $A_3 = A_5 = \ldots = 2\Delta\rho/3$. If the number M is even

$$\int_0^{\rho_s} \rho \left.\frac{\partial F}{\partial x}\right|_{x=0} d\rho = \sum_{i=1}^{M} B_i V_i, \tag{17}$$

where $B_1 = \Delta\rho/3$, $B_{M-1} = \Delta\rho/3 + \Delta\rho/2$, $B_M = \Delta\rho/2$, $B_2 = B_4 = \ldots = 4\Delta\rho/3$, $B_3 = B_5 = \ldots = 2\Delta\rho/3$.

The following condition is used as a criterion for reaching the stationary regime

$$\max_{i,k} \left| \frac{F^{n+1}_{i,k} - F^n_{i,k}}{\Delta\tau g} \right| \leqslant E, \tag{18}$$

where

$$g = \begin{cases} F^n_{i,k}, & \text{for} \quad F^n_{i,k} \neq 0, \\ 1, & \text{for} \quad F^n_{i,k} = 0. \end{cases} \tag{19}$$

Numerical experiments (a rectangular 51 × 51 grid and a time step $\Delta\tau = 0.01$) established that as the accuracy is increased (that is, the quantity E is decreased), the value of the stationary flux <f> monotonically decreases. Starting with $E = 5\cdot10^{-4}$, the concentration and flux hardly change; that is, there is no point in increasing the accuracy further.

Figure 1 shows calculated results for the dimensionless relaxation time τ_r and the average mass flux <f>. The time for reaching the stationary regime is almost independent of the source radius, if its value is comparable with the chamber radius ($\rho_s > 0.6$), and increases for small radii as the radius of the output orifice is decreased. Evaporation kinetics usually are investigated under conditions where the radius of the vessel with the liquid is much less than the chamber radius; therefore, this behavior cannot be ignored. It is even more important for studying the concentration-dependence of the evaporation rates of multicomponent solutions and melts, because the relaxation time depends on the vapor composition (it changes the diffusion coefficient in the vapor–gas mixture, which in turn enters into the expression for the dimensionless relaxation time τ_r). As an example, we present values of τ_r for water and alcohol in a chamber whose dimensions are typical for laboratory equipment ($H = 8$ cm, $R_3 = 2$ cm). As the radii of the source and the exit orifice are changed in the range of 0.2-2.0 cm, the output time for water varies in the range of 258-1853 sec, and 530-3810 sec for alcohol (at a temperature of 273 K). The required diffusion coefficients for water and alcohol vapor are $2.16\cdot10^{-5}$ and $1.05\cdot10^{-5}$ m^2/sec respectively [4].

In the limiting case, where $\rho_s = \rho_0 = 1$, the problem becomes one-dimensional and can be solved analytically [5]:

$$F(\tau, x) = (1 - x/X) - 2\sum_{n=1}^{\infty} \frac{\sin(\pi n x/X)}{\pi n} \exp[-\tau(\pi n/X)^2], \tag{20}$$

$$\langle f \rangle = \frac{1}{X} + \frac{2}{X}\sum_{n=1}^{\infty} \exp[-\tau(\pi n/X)^2]. \tag{21}$$

Calculations showed a maximum difference of 0.024% between these formulas and the numerical results for the dimensionless concentrations at $\tau = \tau_r$; the maximum difference was 0.054% for the dimensionless flux.

The dependence of <f> on the radii of the source and the output orifice (Fig. 1b) displays three different features: a) <f> increases as ρ_s is decreased for all values of ρ_0; b) <f> increases rapidly as the radius ρ_0 of the output orifice is increased (for ρ_s = const) for small values of ρ_0, with very little dependence on ρ_0 for $\rho_0 > 0.6$; c) the dependence of <f> on ρ_s changes qualitatively for large values of ρ_0: for $\rho_s < 0.2$, the derivative dj/dr ceases to increase and begins to drop rapidly.

It is worthwhile to examine this last feature more closely. From Eq. (15) it follows that for <f> = const, the dependence of the flux <j> on the source radius is hyperbolic.

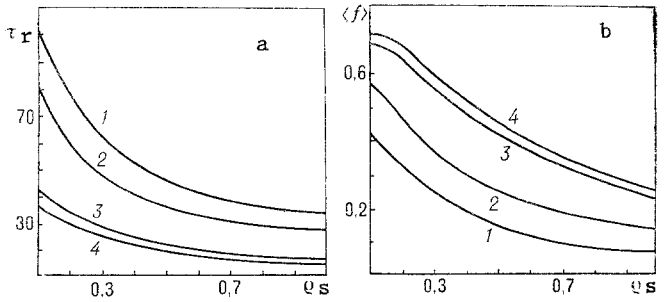

Fig. 1. The relaxation time (a) and the average flux (b) as a function of the source radius (X = 4): 1) $\rho_0 = 0.1$; 2) $\rho_0 = 0.2$; 3) $\rho_0 = 0.6$; 4) $\rho_0 = 1.0$.

Then for $\rho_s > 0.2$, $\langle j \rangle \sim 1/R_1^n$, where $n > 1$; that is, in this region, the evaporation rate increases even more as the surface radius of the liquid is decreased. This indicates that it is impossible to use the average flux (evaporation rate) as a rate characteristic dependent only on the nature of the liquid and on thermodynamic parameters, as has been suggested [2, 6], mainly to study how the volatility of solutioins and melts depends on their composition.

The cessation of the growth of $\langle f \rangle$ for small ρ_s indicates that when the source radius is an order of magnitude less than the chamber radius, the position of the chamber walls hardly affects the evaporation rate; that is, evaporation occurs under conditions close to those for an infinite half space. An analytical solution can also be obtained in this case. Analogous curves for the problem with stationary temperature distributions and electric fields was solved in [7] and [8]. Various methods (using improper discontinuous integrals and elliptical coordinates) were used to obtain identical expressions for the corresponding temperature and potential field characteristics. Differentiating these expressions and then averaging them for the desired case (evaporation in a half space from the surface of a circular source) yields the expressions

$$j(r) = \frac{2DC_e}{\pi \sqrt{R_1^2 - r^2}}, \tag{22}$$

$$\langle j \rangle = \frac{4DC_e}{\pi R_1}. \tag{23}$$

The last formula shows that for a half-space the dimensionless flux $\langle f \rangle$ is actually constant and equal to $4/\pi$. However, the formula (22), which leads to this, gives an infinitely large local flux near the source for $r = R_1$, which obviously does not exist in a real process and which should lead to increased results for $\langle f \rangle$. Earlier experiments on the evaporation of a series of liquids [9, 10] showed that the average mass flux is actually inversely proportional to the source radius; for $R_1 \ll R_3$, the $\langle f \rangle$ lies in the range of 0.65-0.75, which is close to that obtained from the numerical model. Figure 2 shows the radial distribution of the local fluxes for various values of ρ_s. For small source radii the local fluxes, obtained both numerically and analytically, are practically the same in the central portion of the evaporation surface, but the differences grow rapidly away from the center.

The actual flux distribution evidently is closer to the numerical results, because, as the source radius is decreased, the central and peripheral zones of the evaporation surface approach each other. These zones are substantially different with respect to the concentration gradient. This leads to a gradual flattening of the fluxes, which is actually

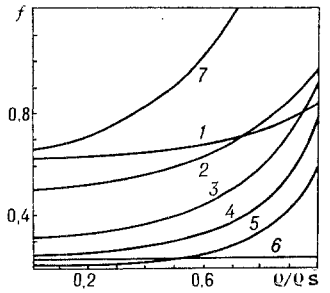

Fig. 2. Radial distribution of the local fluxes (X = 4, $\rho_0 = 1$): 1) $\rho_s = 0.1$; 2) $\rho_s = 0.2$; 3) $\rho_s = 0.4$; 4) $\rho_s = 0.6$; 5) $\rho_s = 0.8$; 6) $\rho_s = 1.0$; 7) infinite half-space.

observed in the evolution of the curves $\langle f(\rho_s)\rangle$ as the source radius is decreased; that is, the evaporation surface approaches a point source to an even greater degree.

Thus, the model presented for nonstationary isothermal evaporation of a liquid can display the characteristic features which are recorded experimentally. It correlates well with limiting analytical cases and makes it possible to calculate the concentration fields, mass fluxes, and relaxation times. It can also be used to determine the diffusion coefficients of liquid vapors in gases with known values of the vapor pressures and measured evaporation rates.

NOTATION

$\langle j\rangle$) average mass flux, kg/(m^2·sec); D) diffusion coefficient, m^2/sec; C) vapor concentration in the gas, kg/m^3; C_e) equilibrium vapor concentration, kg/m^3; R_1) source radius, m; R_2) radius of the output orifice at a height H, m; R_3) chamber radius, m; H) chamber height, m; F) dimensionless concentration; ρ_s) dimensionless source radius; ρ_0) dimensionless orifice radius; X) dimensionless chamber height; $\langle f\rangle$) dimensionless mass flux; f) dimensionless local mass flux.

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