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Balance Equations for Molecular Distillation

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ABSTRACT

We have derived balanced equations for continuous molecular (short-path) distillation of a binary mixture in a falling film evaporator. The relation of heat and mass transfer in liquid films on both the evaporating and condensing surfaces were taken into account, as well as the mass transfer in the vapor phase in the distillation gap. Individual balance equations were coupled by boundary conditions into a closed set of partial differential equations. By introducing the streams, we have transformed partial differential equations into the simple form of ordinary differential equations. These were solved numerically or approximately for some selected problems in isothermal (e.g., for turbulent film on evaporation surface) and nonisothermal regimes and for the influence of reevaporation from the condenser. These developed mathematical formulations can be used to model various operational situations in a molecular evaporator or to evaluate the influence of some parameters on the molecular distillation process.

INTRODUCTION

Molecular or short-path distillation is a gentle distillation method appropriate for the separation and purification of thermally unstable materials as well as for liquids with low vapor pressure and higher molecular weight, without the hazard of thermal decomposition. This method is characterized by a short exposure of the distilled liquid to elevated temperatures, a high vacuum in the distillation space, and a small distance between the evaporator and condenser. The short mean residence time of the liquid

on the evaporating cylinder, on the order of a few seconds to tens of seconds, is guaranteed by distributing the liquid in the form of a thin, constantly wiped film. By considerably reducing the pressure of a noncondensable gas in the evaporator to the 10^{1} to 10^{-1} Pa level, reduction of the distillation temperatures by as much as 250°C can be achieved. The combination of a small distance (20–70 mm) between the evaporator and condenser together with a high vacuum in the distillation gap results in a specific mass transfer mechanism with evaporation outputs as high as 20–40 $g \cdot m^{-2} \cdot s^{-1}$. Under these conditions the distillation of heat-sensitive materials is accompanied by only negligible thermal decomposition and proceeds at rates which can be technologically utilized.

A comprehensive model of molecular distillation has not been proposed as yet; rather, only model studies of partial stages of the process have been presented: evaporation [Kawala (1), Maa and Tsay (2), Ruckenstein and Hassink (3)], passage of molecules through distillation space [Lutišan and Cvengroš (4), Ferron and Bhandarkar (5)], and condensation on the condenser [Badin and Cvengroš (6)]. The present paper offers a simplified model of molecular distillation which accounts for processes in liquid films on both the evaporator and the condenser, and in the gas phase in the distillation gap. A system of balanced equations has been developed, and their solution for selected model examples is shown.

MATHEMATICAL DESCRIPTION OF THE PROBLEM

An apparatus for falling film molecular distillation is shown in Fig. 1. It consists of a cylindrical evaporator surrounded by a condenser jacket. The liquid to be distilled is transported to the evaporating surface. There it flows down in the form of a film and is partly vaporized. The evaporating cylinder is heated internally by the heating fluid at constant temperature T_1^*. Evaporated molecules condense on the closely positioned condenser. The condensing cylinder is cooled by the cooling fluid at constant temperature T_2^*. If both films are much thinner than the evaporator and condenser radii, the liquid films can be regarded as planar. The temperature profile in the molecular evaporator is shown in Fig. 2.

The assumption that the distilled liquid consists of two components A and B will be used in our work.

The parameters for heat and mass transfer under steady-state conditions are described by four fundamental balance equations: the Boltzmann equation for mass transfer in the vapor phase, the Navier–Stokes equation for film flow in the gravity film, an equation for diffusion, and a thermal balance equation.

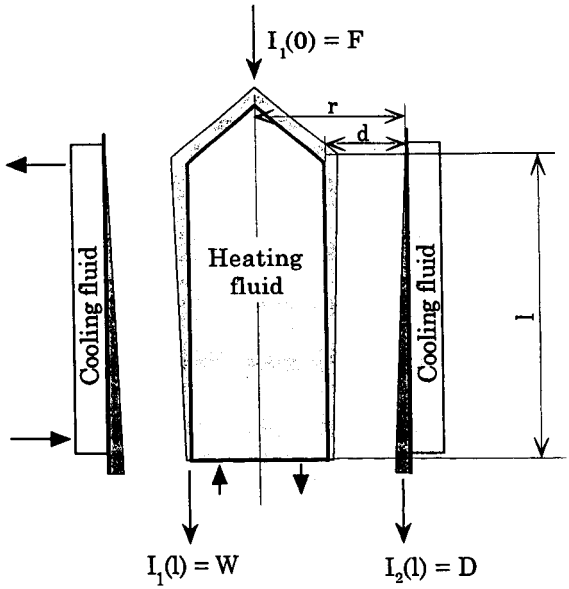

FIG. 1 Scheme of the molecular evaporator with falling film.

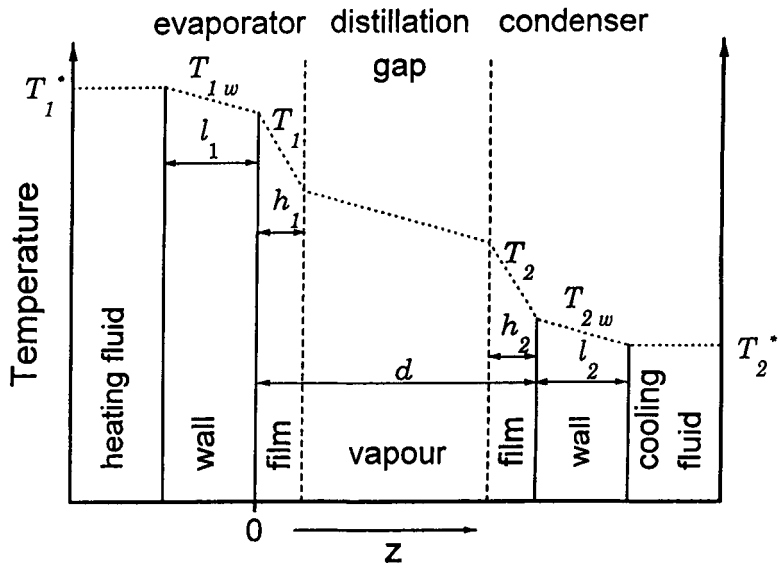

FIG. 2 The temperature profile in the molecular evaporator.

Boltzmann Equation for Mass Transfer in the Vapor Phase

The influence of the vapor phase in the process is described by the Boltzmann equation:

$$\frac{\vec{p}_A}{m_A} \text{grad}_{\vec{r}} f_A(r_A, p_A) = \hat{S}t_A(f_A, f_B) \tag{1}$$

where f_A is one-particle distribution function in phase space, $\hat{S}t_A$ is a collision integral. Since there is very low pressure in the distillation gap, the collision integrals can be neglected:

$$\hat{S}t_A(f_A, f_B) = \hat{S}t_B(f_A, f_B) = 0$$

Our previous study has shown that this assumption is fully qualified for adequate low inert gas pressures, for low evaporating rates, and for sufficiently low condenser temperatures, i.e., negligible reevaporation (4, 7). This assumption is also valid for broader distillation gaps up to 50–70 mm in the evaporator with a convex evaporating surface (4).

Then it follows for f_A, f_B that

$$f_{A,B} = \text{constant}$$

Navier–Stokes Equation for Film Flow in the Gravity Film

The Navier–Stokes equation of film flow in the gravity film is formulated as

$$(v_j \text{ grad})v_j = \nu \nabla^2 v_j + f_j \tag{2}$$

where $j = 1$ (evaporator) and 2 (condenser).

In case of a molecular evaporator, Nusslet's solution of Eq. (2) is sufficient. So, for the value of the velocity component in the direction of axis y on surface j, the expression is governed by

$$v_{yj}(z) = v_{\max j}\left[1 - \left(\frac{z}{h_j}\right)^2\right] \tag{3}$$

Equation for Diffusion

The equation of diffusion has a general shape

$$\text{div}(v_j c_{ij}) = \text{div}(D \text{ grad } c_{ij}) \tag{4}$$

where $i = A$ (component A) or B (component B) and $j = 1$ (evaporator) or 2 (condenser). Diffusion coefficient D is to be held constant.

The boundary conditions in Eq. (4) between the film and vapor are determined by the Langmuir–Knudsen relation for the rate of evaporation:

$$w_{ij} = X_{ij}k_{ij} = X_{ij}(y, h_j)p_i^0(T_j)/\sqrt{2\pi RM_iT_j(y, h_j)} \tag{5}$$

where

$$k_{ij} = \frac{p_i^0(T_j)}{\sqrt{2\pi RM_iT_j(y, h_j)}} \tag{6}$$

Relation (5) describes the flow density of evaporated molecules of component i from film j.

The flow density for molecules A from the vapor phase to the film can be described as

$$J_{ij} = \vec{z}_j^0 \int \frac{\vec{p}_i}{M_i} f_i d^3\vec{p}_i \tag{7}$$

where $\vec{z}_j^0$ is a unit vector in the z-direction. Because the influence of collisions between the molecules in a vapor phase is neglected, J_{ij} equals the evaporation rate of molecules i from the opposite surface:

$$J_{i1} = w_{i2}$$

$$J_{i2} = w_{i1}$$

Now it is possible to describe the total evaporation rate in the form

$$W_{i1} = w_{i1} - w_{i2} = X_{i1}p_i^0(T_1)\sqrt{2\pi RM_iT_1} - X_{i2}p_i^0(T_2)\sqrt{2\pi RM_iT_2} \tag{8.1}$$

$$W_{i2} = w_{i2} - w_{i1} = X_{i2}p_i^0(T_2)\sqrt{2\pi RM_iT_2} - X_{i1}p_i^0(T_1)\sqrt{2\pi RM_iT_1} \tag{8.2}$$

The boundary condition between the wall of a cylinder and the film now has the shape

$$\left.\frac{\partial c_{ij}}{\partial z}\right|_{z=0} = 0 \tag{9}$$

Thermal Balance Equation

The thermal balance equation can be expressed in the form

$$\operatorname{div}(\vec{\nu}_j T_j) = \operatorname{div}(\Gamma \operatorname{grad} T_j) \tag{10}$$

Thermal conductivity Γ and thermal capacity C_p are regarded as constant.

The boundary conditions for Eq. (10) between the film and vapor phase can be then formulated as

$$\Gamma \left.\frac{\partial T_1}{\partial z}\right|_{z=h_1} = -\sum_{i=A}^{B} \Delta H_i (X_{i1} p_i^0(T_1)/\sqrt{2\pi R M_i T_1} - X_{i2} p_i^0(T_2)/\sqrt{2\pi R M_i T_2}) \tag{11.1}$$

$$\Gamma \left.\frac{\partial T_2}{\partial z}\right|_{z=h_2} = \sum_{i=A}^{B} \Delta H_i (X_{i1} p_i^0(T_1)/\sqrt{2\pi R M_i T_1} - X_{i2} p_i^0(T_2)\sqrt{2\pi R M_i T_2}) \tag{11.2}$$

Boundary conditions between the film and wall have the form

$$T_1(y, 0) = T_{1w}(y, 0) \tag{12.1}$$

$$T_2(y, d) = T_{2w}(y, d) \tag{12.2}$$

$$\Gamma \frac{\partial}{\partial z} T_1|_{z=0} = \lambda_{1w} \frac{\partial}{\partial z} T_{1w}(y, z)|_{z=0} \tag{13.1}$$

$$\Gamma \frac{\partial}{\partial z} T_2|_{z=d} = \lambda_{2w} \frac{\partial}{\partial z} T_{2w}(y, z)|_{z=d} \tag{13.2}$$

SOLUTION OF THE BALANCE EQUATIONS

The solution of equations describing diffusion and thermal balance is the crucial problem. The assumption that the dependence of concentration and the temperature on the coordinate z is known is used.

The first assumption is of a quadratic profile of concentration of the more volatile component in the film:

$$c_{i1}(y, z) = c_{i1}(y, 0) + \frac{c_{i1}(y, h_1) - c_{i1}(y, 0)}{h_1^2} z^2 \tag{14.1}$$

$$c_{i2}(y, z) = c_{i2}(y, d) + \frac{c_{i2}(y, d - h_2) - c_{i2}(y, d)}{h_2^2} z^2 \tag{14.2}$$

Expressions $c_{i1}(y, h_1)$, $c_{i1}(y, 0)$, $c_{i2}(y, d - h_1)$, $c_{i2}(y, d)$, $h_1(y)$, and $h_2(y)$ can then be determined as

$$2\pi r D \left.\frac{\partial c_{1A}}{\partial z}\right|_{z=h_1} + \frac{c_{1A}(y, h)}{c_1}\left(\frac{dI_{1A}}{dy} + \frac{dI_{1B}}{dy}\right) = -2\pi r\left(k_{1A}\frac{c_{1A}(h)}{c_1} - k_{2A}\frac{c_{2A}(h)}{c_2}\right) \tag{15}$$

$$I_{i1}(y) = 2\pi r \int_0^{h_1} v_1 c_{i1} dz \tag{16}$$

$$v_1(y, z) = \frac{g h_1^2}{\nu}\left(\frac{z}{h_1} - \frac{1}{2}\frac{z^2}{h_1^2}\right) \tag{17}$$

whereby analogous equations to Eqs. (15)–(17) exist for component B and for the condenser.

Using the Newton–Leibnitz's relation and integrating it in the direction of axis z, we get

$$\frac{d}{dy} I_{i1}(y) = -2\pi r[k_{i1} X_{i1}(h_1) - k_{i2} X_{i2}(h_2)] \tag{18}$$

Simultaneously, from the material balance it follows that

$$I_{i2}(y) = I_{i1}(0) - I_{i1}(y) \tag{19}$$

The unknown surface molar fractions $X_{ij}(h_j)$ are expressed in

$$X_{ij} = \frac{c_{ij}(h_j)}{c_j} \tag{20}$$

The set of equations for X_{A1} and X_{A2} will now by obtained from the boundary conditions (8):

$$\frac{4Dc_1}{h_1} X_{A1} - X_{A1}(X_{A1}\Delta k_1 + k_{B1} - X_{A2}\Delta k_2 + k_{B2}) + k_{A1} X_{A1} - k_{A2} X_{A2} = \frac{4Dc_1}{h_1}\frac{I_{A1}}{I_1} \tag{21}$$

$$\frac{4Dc_2}{h_2} X_{A2} - X_{A2}(X_{A2}\Delta k_2 + k_{B2} - X_{A1}\Delta k_1 + k_{B1}) + k_{A2} X_{A2} - k_{A1} X_{A1} = \frac{4Dc_2}{h_2}\frac{I_{A2}}{I_2} \tag{22}$$

$$\Delta k_j = k_{Aj} - k_{Bj}$$

The solution of these equations can be expressed as

$$X_{A1} = \frac{\mathcal{D}_1 x_{A1}}{\mathcal{D}_1 + \Delta k_1} \tag{23}$$

$$X_{A2} = \frac{a_1 - \sqrt{a_2}}{2\Delta k_2} - 3\left(\frac{a_1 - \sqrt{a_2}}{2\Delta k_2} - x_{A2}\right) \tag{24}$$

where

$$\text{Đ}_j = \frac{4D_j c_j}{h_j}$$

$$a_1 = \text{Đ}_2 + \Delta k_2 - \Delta k_1 X_{A1} - k_{B1}$$

$$a_2 = a_1^2 - 4\Delta k_2 \text{Đ}_2 x_{A2}$$

Finally, substituting X_{A1} from Eq. (23) and X_{A2} from Eq. (24) into Eq. (18), we obtain the base set of the balanced equations.

Parameter k_{ij} from Eq. (6) depends on the surface temperatures of the films $T_j(h_j)$. These temperatures will be determined from Eq. (10) and boundary conditions (11)–(13) using the assumption that the profile of the temperature in the film is linear:

$$T_1(y, z) = T_1(y, 0) + \frac{T_1(y, h_1) - T_1(y, 0)}{h_1} z \tag{25.1}$$

$$T_{1w}(y, z) = T_{1w}(y, -l_1) + \frac{T_1(y, 0) - T_1(y, -l_1)}{l_1} z$$

$$T_2(y, z) = T_2(y, d) + \frac{T_2(y, d - h_2) - T_2(y, d)}{h_2} z \tag{25.2}$$

$$T_{2w}(y, z) = T_{2w}(y, d + l_2) + \frac{T_2(y, d) - T_2(y, d + l_2)}{l_2} z$$

Accepting this as a new form of thermal boundary conditions, for the evaporator we obtain

$$\Gamma \frac{T_1(y, h) - T_1(y, 0)}{h_1} = -\sum_{i=A}^{B} \Delta H_i \frac{dI_{1i}}{dy} \tag{26.1}$$

$$\Gamma \frac{T_1(y, h_1) - T_1(y, 0)}{h_1} = \lambda_{1w} \frac{T_1(y, 0) - T_1(y, -l_1)}{l_1} \tag{26.2}$$

$$T_{1w}(y, 0) = T_1(y, 0) \tag{26.3}$$

Analogous conditions can be written for the condenser:

$$\Gamma \frac{T_1(y, h) - T_1(y, 0)}{h_2} = \sum_{i=A}^{B} \Delta H_i \frac{dI_{1i}}{dy} \tag{27.1}$$

$$\Gamma \frac{T_2(y, d - h_2) - T_2(y, d)}{h_2} = \lambda_{2w} \frac{T_2(y, d) - T_1(y, d + l_2)}{l_2} \tag{27.2}$$

$$T_{2w}(y, d) = T_2(y, d) \tag{27.3}$$

Providing that $T_{1w}(y, -l_1) = T_1^*$ and $T_{2w}(y, d + l_2) = T_2^*$, a system of nonlinear equations for four unknown temperatures is obtained: $T_1(y, h_1)$, $T_1(y, 0)$, $T_2(y, d)$, and $T_2(y, d - h_2)$.

The process of the evaporation is now fully described by a set of two differential equations (18) for $i = A, B$ and $j = 1, 2$ and by the set of boundary conditions described by Eqs. (23), (24) and (26), (27).

SOLVING THE BALANCE EQUATIONS AND THEIR ANALYSIS

In this part we present the set of balance equations for some selected cases of molecular distillation. We perform the analysis of these equations and find the solution for some cases.

Di-butyl-phthalate (DBP) and di-butyl-sebacate (DBS) were used as a model system. $M_{DBP} = 278.35\ g \cdot mol^{-1}$, $\log p^0_{DBP} = 12.7 - 4450/T$ Pa, $\Delta_{evp}H_{DBP} = 85.6\ kJ \cdot mol^{-1}$, $c_{p\,DBP} = 583\ J \cdot mol^{-1} \cdot K^{-1}$, $\rho_{DBP} = 1294.6 - 0.839T\ kg \cdot m^{-3}$, $M_{DBS} = 314.46\ g \cdot mol^{-1}$, $\log p^0_{DBS} = 13.22 - 4850/T$ Pa, $\Delta_{evp}H_{DBS} = 92.77\ kJ \cdot mol^{-1}$, $c_{p\,DBS} = 632\ J \cdot mol^{-1} \cdot K^{-1}$, $\rho_{DBS} = 1169.6 - 0.78T\ kg \cdot m^{-3}$, from Kawala (1).

Turbulent Films

This case represents ideally mixed films on the evaporator and on the condenser. Both the temperature and the concentration of films are constant in the direction of axis z. The temperature of the film is the same as that of the wall, $T_j = T_j^*$. The surface mol fraction X_{ij} is determined as

$$X_{ij} = \frac{I_{ij}}{I_{Aj} + I_{Bj}} \tag{28}$$

By substituting Eq. (28) into Eq. (18), we obtain the set of balance equations

$$\frac{d}{dy} I_{A1} = -2\pi r k_{A1} \frac{I_{A1}}{I_1} + 2\pi r k_{A2} \frac{I_{A2}}{I_2} \tag{29.1}$$

$$\frac{d}{dy} I_{B1} = -2\pi r k_{B1} \frac{I_{B1}}{I_1} + 2\pi r k_{B2} \frac{I_{B2}}{I_2} \tag{29.2}$$

If reevaporation from the condenser is insignificant, $k_{A2} = 0$, $k_{B2} = 0$, the set of differential Eqs. (29) has an analytical solution:

$$I_{B1}(y) + I^{\alpha_1}_{B1}(y) = I_{B1}(0) + I^{\alpha_1}_{B1}(0) - yk_{B1} \tag{30.1}$$

$$I_{A1}(y) = I_{A1}(0)\left(\frac{I_{B1}(y)}{I_{B1}(0)}\right)^{\alpha_1} \tag{30.2}$$

where

$$\alpha_1 = \frac{k_{A1}}{k_{B1}} = \frac{p_A^0}{p_B^0}\sqrt{\frac{M_B}{M_A}} \tag{31}$$

is a theoretical value of separation efficiency for molecular distillation.

In the case of distillation on continuous film evaporators, the Rayleigh equation is usually used for determining the separation efficiency of the process

$$\alpha_{film} = 1 + \frac{\ln\{x_w(1 - x_F)/[x_F(1 - x_w)]\}}{\ln\{W(1 - x_w)/[F(1 - x_F)]\}} \tag{32}$$

where $F = I_1(0)$, $W = I_1(l)$, $x_F = I_{A1}(0)/I_1(0)$, $x_W = I_{A1}(l)/I_1(l)$.

Using these relations in Eq. (32), we obtain

$$\ln\frac{x_w(1 - x_F)}{x_F(1 - x_w)} = \ln\frac{I_{A1}(l)I_{B1}(0)}{I_{A1}(0)I_{B1}(l)}$$

By application of Eq. (32):

$$\ln\frac{x_w(1 - x_F)}{x_F(1 - x_w)} = (\alpha_1 - 1)\ln\frac{I_{B1}(l)}{I_{B1}(0)} \tag{33}$$

Analogically,

$$\ln\frac{W}{F}\frac{(1 - x_w)}{(1 - x_F)} = \ln\frac{I_{B1}(l)}{I_{B1}(0)} \tag{34}$$

By substituting Eqs. (33) and (34) into Eq. (32), we obtain

$$\alpha_{film} = \frac{k_{A1}}{k_{B1}} = \frac{p_A^0}{p_B^0}\sqrt{\frac{M_B}{M_A}} \tag{35}$$

This result shows that when an ideally mixed film evaporates without boiling and without reevaporation from the condenser, the separation efficiency approaches the theoretical value (31). Although intensively mixed films can almost be produced in typically nonequilibrium processes of molecular distillation by wipers, rotating at high peripheral speed, and pressing on an evaporating surface through centrifugal force, concentration and thermal gradients in the evaporating film do exist at higher evaporation rates and cannot be eliminated. The inclusion of these facts requires that a different set of balance equations be solved, a set in which the existence of gradients is taken into consideration.

Laminar Isothermal Films

Next the case of the model solution of the particular problem of molecular distillation with different condenser temperatures is shown. The temperatures of liquid surfaces in the evaporating and condensing areas do not change with the evaporator height and have the same value as that of the wall, $T_j = T_j^*$. In the distillation space a noncollision regime is proposed, concentration gradients in both films in horizontal direction are taken in account, as well as reevaporation from the condenser. The system is described by balance Eq. (18) where the surface molar fractions are determined by Eqs. (23)–(24). Because an analytical solution of these differential equations does not exist, it is necessary to use the numerical method.

As an example, the solution of these balance equations by the Runge–Kutt method of the fourth order values for streams $I_{A1}(y)$ and $x_{A1}(y)$ has been performed.

Figure 3 shows that the concentration profiles of a residual liquid film on the evaporator are significantly changed for different condenser temperatures. The evaporating temperatures is $T_1 = 373$ K. In the case of a hotter condenser, the distillate contains less of the more volatile compo-

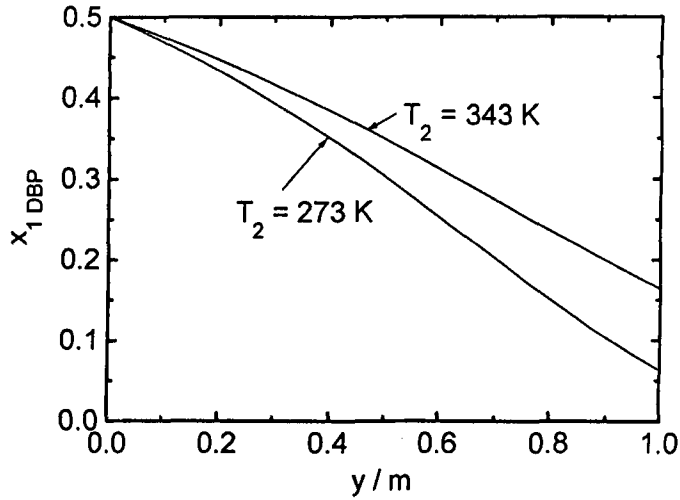

FIG. 3 Concentration profile of DBP on the evaporator vs the position in the apparatus for two different condensing temperatures at the isothermal regime. $I_1(0) = 0.015$ mol·s^{-1}, $x_{FDBP} = 0.50$, $T_1 = 373$ K.

nent, and this component remains as a residual liquid on the evaporator. It is caused by incomplete condensation and faster evaporation of the more volatile component from the condenser.

Less efficient condensation on a hotter condenser also follows as shown in Fig. 4. The liquid stream on the evaporator is larger in the case of a hotter condenser. The deleterious influence of reevaporation on the distillation process in a molecular evaporator was discussed in our previous paper (4). The phenomenon of reevaporation, which is related to the condenser temperature, and the inert gas pressure have a decisive effect on the process, while the width of the distillation gap is of less importance (7).

In some instances the thermal gradients in the liquid film on the condenser can be remarkably high, especially for intensive evaporation of viscous liquids on long condensers (6). In this case the surface temperature of the liquid film on the condenser may be rapidly elevated, and as a consequence there may be considerable reevaporation. A similar effect can occur in the distillation of components with higher melting points, where it is necessary to keep the condenser temperature high enough to secure a continuous flow of liquid distillate from the condenser.

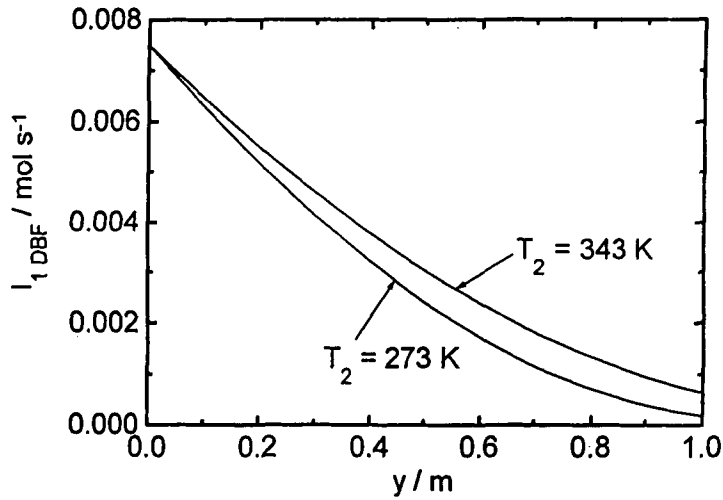

FIG. 4 Molar flows of DBP on the evaporator vs the position in the apparatus for two different condensing temperatures at the isothermal regime. $l_1(0) = 0.015$ mol·s^{-1}, $x_{FDBP} = 0.50$, $T_1 = 373$ K.

Laminar Nonisothermal Films

Figures 5 and 6 illustrate a molecular distillation approaching its real situation parameters as closely as possible for two wall temperatures of the condenser, i.e., assuming a binary mixture flowing in laminar films on both the evaporating and condensing surfaces, the existence of horizontal concentration and temperature gradients, and reevaporation on the condenser. The wall temperatures of the condenser are the same as in Figs. 3 and 4.

The concentration profiles of the more volatile component shown in Fig. 5 document the relatively higher concentration of this component in the residual liquid on the evaporation surface in a nonisothermal regime compared with the isothermal regime shown in Fig. 3. The reason for the higher concentration of the more volatile component in a nonisothermal film is its lower temperature.

The ability of our model to predict the correct consequences intuitively is demonstrated on Figs. 4 and 6 for isothermal and nonisothermal regimes. As in the previous example, the predicted flows I_{1DPB} on the evaporator at two selected temperatures clearly favor the isothermal regime, the flow I_{1DPB} at the nonisothermal regime being substantially higher.

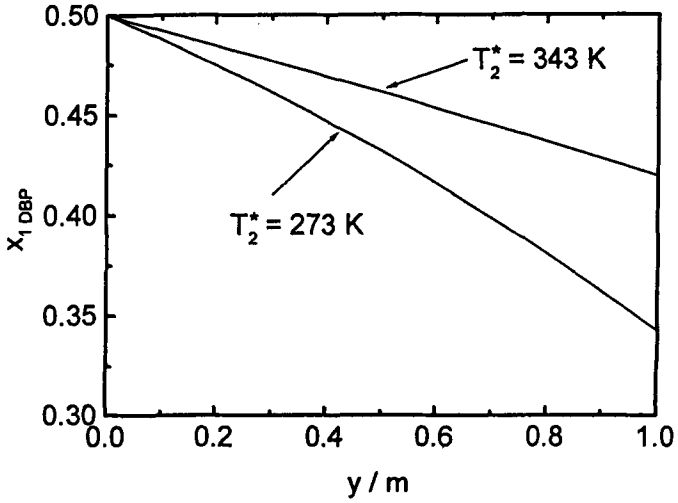

FIG. 5 Concentration profile of DBP on the evaporator vs the position in the apparatus for two different condenser temperatures at the nonisothermal regime. $I_1(0) = 0.015$ mol·s^{-1}, $x_{FDBP} = 0.50$, $T_1 = 373$ K.

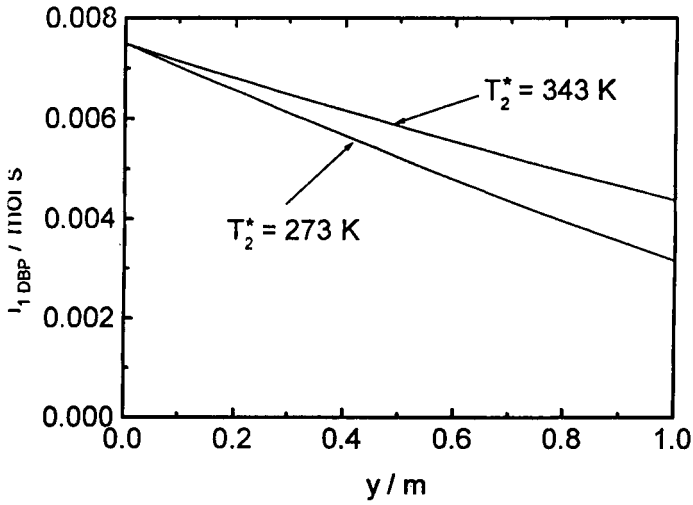

FIG. 6 Molar flows of DBP on the evaporator vs the position in the apparatus for two different condenser temperatures at the nonisothermal regime. $l_1(0) = 0.015$ mol·s^{-1}, $x_{FDBP} = 0.50$, $T_1 = 373$ K.

The presented model for the molecular distillation process was also utilized in a study of the efficiency of an entrainment separator placed in the distillation gap between the evaporation and condensation surfaces in a molecular evaporator. A sieve acting as an inner condenser efficiently intercepts the splashing, improving the composition of the distillate although it decreases the distillation rate (8).

Analysis of the fractionation processes in a one-stage molecular evaporator with a divided condenser is another example of the described model application (9). The distillate from the upper condenser zone is rich in the more volatile component whereas the last condenser zone acts like a depletion unit. Thus the yield, but not the content of the more volatile compound, is raised in the distillate.

CONCLUSIONS

A system of balance equations for molecular distillation in a film evaporator has been formulated. The arranged set of balance equations enables various operational situations in the molecular evaporator to be modeled and the influence of some of the parameters of the molecular distillation process to be evaluated.

In the case of an ideally mixed liquid film on an evaporating surface (turbulent film) with negligible reevaporation from the condenser, the separation efficiency of the process is equal to the theoretical value.

The difference between operating a molecular evaporator in an isothermal or a non-isothermal regime is shown most clearly in the volume and composition of the residual liquid on the evaporating surface. In an nonisothermal regime the lower temperature of the film causes less evaporation, and hence there is a higher concentration of the more volatile component in the residual liquid.

Reevaporation from the condenser deteriorates the separation efficiency of molecular distillation.

NOTATION

Variables and Constants Used

C_p	thermal capacity ($J \cdot K^{-1} \cdot mol^{-1}$)
c_{ij}	molar concentration of component i on surface j ($mol \cdot m^{-3}$)
c_j	molar concentration of the liquid on surface j ($mol \cdot m^{-3}$)
D	diffusion coefficient ($m^2 \cdot s^{-1}$)
f_i	one-particle distribution function of component i
g	gravity, 9.81 $m \cdot s^{-2}$
$\Delta_{evp}H$	heat of evaporation ($J \cdot mol^{-1}$)
h_j	the thickness of the film on surface j (m)
I_{ij}	molar flow of component i on surface j ($mol \cdot s^{-1}$)
I_j	total molar flow on surface j ($mol \cdot s^{-1}$)
J_{ij}	flow density of component i from the vapor phase to surface j ($mol \cdot m^{-2} \cdot s^{-1}$)
k_{ij}	evaporation constant of pure component i on surface j ($mol \cdot m^{-2} \cdot s^{-1}$)
M_i	molar mass of component i ($kg \cdot mol^{-1}$)
p	pressure (Pa)
p_i	partial pressure of component i (Pa)
p_i^0	saturation pressure of component i (Pa)
R	universal gas constant, 8.314510 $J \cdot K^{-1} \cdot mol^{-1}$
r	radius of the evaporating cylinder (m)
$\hat{St}_i$	collision integral
T_j	temperature of surface j (K)
T_j^*	temperature of a heat exchange fluid for surface j (K)
T_{jw}	temperature of jth wall (K)
v_j	velocity of the flow on surface j ($m \cdot s^{-1}$)
W_{ij}	total evaporation rate of component i on surface j ($mol \cdot m^{-2} \cdot s^{-1}$)

w_{ij} evaporation rate of component i on surface j ($mol \cdot m^{-2} \cdot s^{-1}$)
X_{ij} the surface mole fraction of the component i on the surface j
x_{ij} mole fraction of component i on surface j
y axis direction parallel with the evaporation surface (m)
z axis direction radial to the evaporation cylinder (m)

Greek Letters

α_1 theoretical value of separation efficiency for molecular distillation
α_{film} value of separation efficiency for molecular distillation calculated from Rayleigh equation
Γ temperature conductivity coefficient of the film ($J \cdot m^{-1} \cdot K^{-1} \cdot s^{-1}$)
π 3.141593
ρ density ($kg \cdot m^{-3}$)
ν kinematic viscosity ($m^2 \cdot s^{-1}$)

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