

EFFECTS OF THE CONCENTRATION-DEPENDENT  
DENSITY ON LIQUID SEPARATION IN A  
THERMAL-DIFFUSION COLUMN

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An analysis is given for the solution to a system of equations describing the separation in a liquid thermal-diffusion column. Similarity numbers are derived for the effects of concentration and thermal expansion on the separation. A method is given for calculating the thermal-diffusion constant that eliminates the effects of concentration on the density.

The concentration dependence of the density has [1] a considerable effect on the separation of liquid organic mixtures by thermogravitational diffusion. The Jones-Ferry theory [5] has formed the basis of all previous treatments of liquid separation that take this effect into account [2-4]. The theory is applicable only to isotopic mixtures and contains numerous simplifying assumptions, which have since been only partly confirmed. Here we consider the separation of a binary liquid mixture by direct solution of the equations of gas dynamics with allowance for the concentration dependence of the density. The method of [6] is used, which leads to essentially new results.

Consider a binary mixture in a planar column closed at both ends (height  $2l$ , working gap  $2d$ ,  $d \ll l$ ). The left wall is kept cooler than the right one, and the temperature difference across the column is  $2\theta$ . The following convection equations [7] define the steady-state distribution of the velocity, temperature, and concentration

$$\begin{aligned}(\mathbf{v} \cdot \nabla) \mathbf{v} &= -\frac{1}{\rho_0} \nabla P + \nu \nabla^2 \mathbf{v} + g(\beta T + \gamma c) \mathbf{k}, \\(\mathbf{v} \cdot \nabla) T &= \chi \Delta T, \\(\mathbf{v} \cdot \nabla) c &= D \nabla^2 \left[ \nabla c - \frac{\alpha}{T} c(1-c) \nabla T \right], \\ \nabla \cdot \mathbf{v} &= 0.\end{aligned}\tag{1}$$

Parameters  $\nu$ ,  $\beta$ ,  $\gamma$ ,  $\chi$ ,  $D$ , and  $\alpha$  in (1) are taken as constant and are calculated for mean values of the temperature, pressure, and concentration. The boundary conditions are as follows for the planar problem in  $x$ - $z$  coordinates:

$$\begin{aligned}\mathbf{v}(d) &= \mathbf{v}(-d) = 0, \\T(d) &= \theta, \quad T(-d) = -\theta, \\ \left[ \frac{\partial c}{\partial x} - \frac{\alpha}{T} c(1-c) \frac{\partial T}{\partial x} \right]_{-d; d} &= 0, \\ \int_{-d}^d v dx &= 0, \\ \int_{-d}^d \left\{ cv - D \left[ \frac{\partial c}{\partial z} - \frac{\alpha}{T} c(1-c) \frac{\partial T}{\partial z} \right] \right\} dx &= 0.\end{aligned}\tag{2}$$

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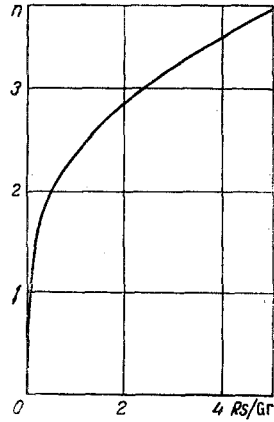


Fig. 1

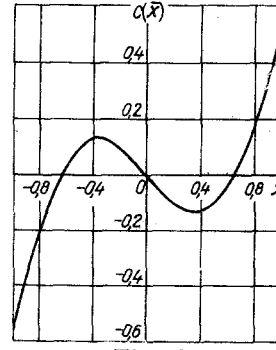


Fig. 2

Fig. 1. Dependence of  $n$  on  $Rs/Gr$  from (10).

Fig. 2. Horizontal concentration profile calculated from (7) for  $n$ -heptane mixed with benzene (mole fraction  $c_0$  of heptane 0.335);  $Gr = 13.8$ ;  $R = 132$ ;  $Sm = 176$ ;  $s = 1.68 \cdot 10^{-2}$ ;  $n = 1.53$ .

We can put  $u = 0$  as  $d \ll l$  and end effects are neglected. We also assume that the temperature does not vary along the vertical coordinate  $z$ , that the thermal-diffusion term can be put as  $(\alpha/T_0)c(1-c)(\partial T/\partial x)$ , and that  $c(1-c) = \text{const}$  in the integration.

Then system (1) can be reduced to the following, where the unknowns are represented in dimensionless form:

$$\begin{aligned} -\frac{dP}{dz} + \frac{d^2v}{dx^2} + Gr T + Rc &= 0, \\ \frac{d^2T}{dx^2} &= 0, \\ v \frac{\partial c}{\partial z} &= \frac{1}{Sm} \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial z^2} \right). \end{aligned} \quad (3)$$

The scale factors for distance, velocity, temperature, and pressure are  $d$ ,  $v/d$ ,  $\theta$ , and  $\rho_0 v^2/d^2$ .

The above assumptions give the following form to boundary conditions (2):

$$\begin{aligned} v(-1) &= v(1) = 0, \\ T(-1) &= -1, \quad T(1) = 1, \\ \left[ \frac{\partial c}{\partial x} - s \right]_{-1;1} &= 0, \\ \int_{-1}^1 v dx &= 0, \\ \int_{-1}^1 \left( cv - \frac{1}{Sm} \frac{\partial c}{\partial z} \right) dx &= 0. \end{aligned} \quad (4)$$

The following form can be given to the solution to (3) and (4):

$$T = x, \quad (5)$$

$$v(x) = \frac{2}{n^3} \frac{Gr + Rs}{\text{sh}\sqrt{2n} + \sin\sqrt{2n}} \left[ \text{sh} \frac{n}{\sqrt{2}} (1+x) \sin \frac{n}{\sqrt{2}} (1-x) - \text{sh} \frac{n}{\sqrt{2}} (1-x) \sin \frac{n}{\sqrt{2}} (1+x) \right], \quad (6)$$

$$c(x; z) = \kappa z - \frac{Gr}{R} x + \frac{\sqrt{2}}{n} \frac{\frac{Gr}{R} + s}{\text{sh}\sqrt{2n} + \sin\sqrt{2n}} \left[ \text{ch} \frac{n}{\sqrt{2}} (1+x) \cos \frac{n}{\sqrt{2}} (1-x) - \text{ch} \frac{n}{\sqrt{2}} (1-x) \cos \frac{n}{\sqrt{2}} (1+x) \right]. \quad (7)$$

This is somewhat more convenient for analysis than the form given in [6].

One can obtain the result of passing to the limit  $\gamma \rightarrow 0$  in (6) and (7) if the functions in these expressions are expanded as series in the small parameter  $n$ , which gives known expressions for the velocity and concentration distributions without allowance for the effect of the concentration on the density:

$$v(x) = \frac{Gr}{6} x(1-x^2), \quad (6a)$$

$$c(x; z) = \kappa z + sx - \frac{Gr}{12} Sm \kappa \left( \frac{x^5}{10} - \frac{x^3}{3} + \frac{x}{2} \right). \quad (7a)$$

The longitudinal concentration gradient  $\kappa$  is constant and is defined by the last boundary condition:

$$\int_0^1 vcdx = \frac{2\kappa}{Sm}. \quad (8)$$

Integration of (8) gives

$$\begin{aligned} \frac{2n^4}{RSm^2} = & -\frac{2}{n^4} Gr \left( \frac{Gr}{R} + s \right) + \frac{2\sqrt{2}}{n^5} Gr \left( \frac{Gr}{R} + s \right) \frac{\text{ch} \sqrt{2n} - \cos \sqrt{2n}}{\text{sh} \sqrt{2n} + \sin \sqrt{2n}} - \frac{2}{n^4} R \left( \frac{Gr}{R} + s \right)^2 \frac{\text{sh} \sqrt{2n} \sin \sqrt{2n}}{(\text{sh} \sqrt{2n} + \sin \sqrt{2n})^2} \\ & + \frac{1}{\sqrt{2}n^5} R \left( \frac{Gr}{R} + s \right)^2 \frac{\text{ch} \sqrt{2n} - \cos \sqrt{2n}}{\text{sh} \sqrt{2n} + \sin \sqrt{2n}}. \end{aligned} \quad (9)$$

We have  $(2n^4/RSm^2) \ll 1$ , and the term is much less than the terms on the right in (9), for liquids with realistic temperature gradients, and so (9) can be put as

$$\left( 5 + \frac{Rs}{Gr} \right) \frac{1}{\sqrt{2n}} \frac{\text{ch} \sqrt{2n} - \cos \sqrt{2n}}{\text{sh} \sqrt{2n} + \sin \sqrt{2n}} - 2 \left( 1 + \frac{Rs}{Gr} \right) \frac{\text{sh} \sqrt{2n} \sin \sqrt{2n}}{(\text{sh} \sqrt{2n} + \sin \sqrt{2n})^2} = 2, \quad (10)$$

when one gets  $n$  and hence  $\kappa$ . It follows directly from (10) that  $\kappa$  is governed by  $Rs/Gr = [\alpha c_0(1-c_0)]\gamma/\beta T_0$  for a liquid; in particular, it is not dependent on  $\theta$ . We can consider  $Rs/Gr$  as a similarity number for thermal diffusion. Figure 1 shows  $n(Rs/Gr)$ .

The concentration dependence of the density thus alters the longitudinal concentration gradient and the transverse concentration distribution, which casts doubt on the conclusion [4] that there are no such effects, which was drawn from a computer solution to a system of equations for a liquid mixture in a thermal-diffusion column.

We performed a numerical calculation for benzene + n-heptane with allowance for the concentration dependence and found that it reduced the longitudinal concentration gradient by 12% and the maximum transverse difference between the concentrations by 8%.

Figure 2 gives the transverse concentration distribution given by (7). The curve relates to a particular mixture, but the form is largely independent of this for liquids, though its shape is very different from that for gases [6], which confirms a numerical calculation [4] for the nonstationary state. The liquid curve has a special shape because the diffusion term on the right in (8) is small for a liquid whereas it is substantial for a gas.

Our solution takes account of the concentration effect and allows one to calculate the thermal-diffusion constant from results for a column: one determines the vertical concentration gradient  $\kappa$ , from which  $n$  is calculated, which is used with the curve of Fig. 1 to find  $Rs/Gr$ , which gives  $\alpha$ .

#### NOTATION

$v$	is the velocity of mixture;
$u$	is the horizontal component of velocity;
$v$	is the vertical component of velocity;
$T, c$	are the deviations of temperature and concentration from initial mean values of $T_0$ and $c_0$ ;
$P, \rho$	are the deviations of pressure and density from their equilibrium values at $T_0$ and $c_0$ ;
$\nu$	is the kinematic viscosity;
$\beta$	is the thermal expansion coefficient;

$\gamma = -1/\rho_0(\partial\rho/\partial c)_{T,P}$	is the coefficient for concentration effect on density;
$k$	is the unit vector along z axis;
$\chi$	is the thermal diffusivity;
$D$	is the diffusivity;
$\alpha$	is the thermal-diffusion constant;
$Gr = g\beta d^3\theta/\nu^2$	is the Grashof number;
$R = g\gamma d^3/\nu^2$ ;	
$Sm = \nu/D$	is the Schmidt number;
$\kappa = \partial c/\partial z$ ;	
$s = (\alpha\theta/T_0)c_0(1-c_0)$ ;	
$n^4 = g\gamma d^3\kappa/\nu D$	is the diffusion Rayleigh number.

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