

MULTICOMPONENT HEAT AND MASS TRANSFER DURING  
THE TURBULENT FLOW OF LIQUID FILMS

L. P. Kholpanov, E. Ya. Kenig,  
and V. A. Malyusov

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A method is proposed for calculating the parameters of simultaneous heat and mass transfer in turbulent multicomponent liquid films which is based on solving the system of differential equations for convective heat conduction and multicomponent convective diffusion.

There has been considerable interest in the development of the theory and methods of calculation of heat and mass transfer processes in view of their widespread occurrence in modern industrial practice. These processes are marked by their complex structures and require the simultaneous solution of the equations of momentum, mass, and energy transfer, including coupling conditions at interfaces.

Investigations of heat and mass transfer in laminar and wavy films of liquid [1], in liquid films flowing on surfaces with regular roughness elements [2], and in systems consisting of assemblies of droplets or bubbles [3] have made it possible to establish a unified functional relationship for the heat transfer (mass transfer) coefficients [1]. This relationship takes the form of a product one of the terms of which is equal to the heat transfer (mass transfer) coefficient in the absence of interactions between the heat and mass effects, while the other term is general for all the types of processes being considered.

The modeling of heat and mass transfer processes is considerably more complicated in multicomponent systems. The complexity of the theoretical description increases still further when transfer occurs under turbulent conditions.

The present paper deals with a theoretical investigation of simultaneously occurring heat and mass transfer in a turbulent multicomponent liquid film on the basis of solving the differential equations for the convective transport of heat and mass.

Let us consider a film of liquid flowing under gravity along a vertical wall. The  $x$  axis is directed downwards along the wall, and the  $y$  axis is directed perpendicularly to the wall. It is assumed as is customary [4-6] that the physical properties of the liquid phase are constant, that the overall diffusional transport of enthalpy in the bulk of the phase is negligibly small, that there are no external forces, that the condition of phase equilibrium exists at the surface of the film, and that the film thickness remains constant. It is also assumed that it is possible to neglect the dissipative term in the heat transfer equation and the transport of mass as a result of thermodiffusion [7]. The equations for the steady-state convective transfer of heat and mass in the turbulent multicomponent liquid film then have the forms:

$$u(y) \frac{\partial T}{\partial x} = \frac{\partial}{\partial y} \left( \sigma(y) \frac{\partial T}{\partial y} \right); \quad (1)$$

$$u(y) \frac{\partial \mathbf{C}}{\partial x} = \frac{\partial}{\partial y} \left( [E(y)] \frac{\partial \mathbf{C}}{\partial y} \right), \quad (2)$$

where  $\sigma(y)$  is the turbulent temperature conductivity;  $[E(y)]$  is the matrix of turbulent diffusion coefficients. These quantities depend on both the physical-chemical properties of the liquid mixture and the hydrodynamic parameters. The column vector  $\mathbf{C}$  consists of the molar concentrations of the components  $C_i$  and has dimensions of  $n - 1$ .

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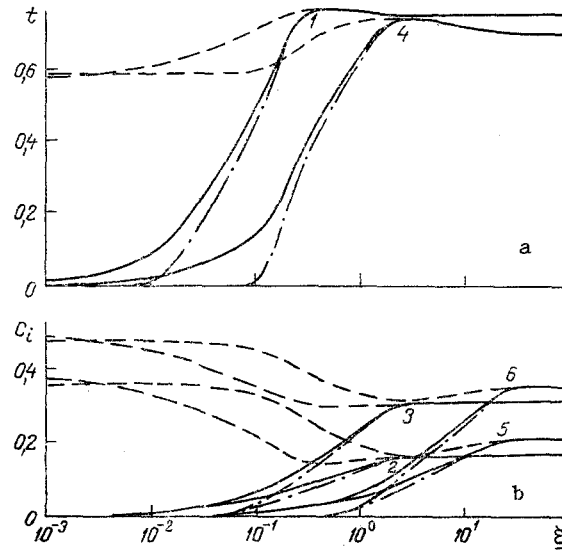


Fig. 1. The dimensionless temperature (a) and the dimensionless concentrations of the components (b) as functions of the length of the contact device for  $Fr = 218$ ;  $Pr = 10$ ;  $Sc_1' = 1500$ ;  $Sc_2' = 2500$ ;  $a_1 = 1.1$ ;  $a_2 = 0.9$ ;  $b_1 = 0.3$ ;  $b_2 = -0.1$ , for various values of the Reynolds number  $Re$ : curves 1-3:  $Re = 20,000$  (curve 1 is for  $t$ , curve 2 for  $c_1$ , and curve 3 for  $c_2$ ); curves 4-6:  $Re = 5000$  (curve 4 is for  $t$ , curve 5 for  $c_1$ , and curve 6 for  $c_2$ ); solid lines are for the values in the core of the phase, dashed lines are for the values at the interface, and dot-dashed lines are for the values at the wall.

The boundary conditions are:

$$\text{at } x = 0 \quad T = T_0, \quad C = C_0; \quad (3)$$

$$\text{at } y = 0 \quad \frac{\partial T}{\partial y} = 0, \quad \frac{\partial C_i}{\partial y} = 0, \quad i = 1, 2, \dots, n-1; \quad (4)$$

$$\text{at } y = h_0 \quad C = v \cdot T + w; \quad (5)$$

$$q = \sum_{k=1}^n N_k \Delta H_k. \quad (6)$$

In order to express the heat and mass fluxes in terms of the gradients of the temperature and the concentrations of the components it is necessary to use Fourier's law and the generalized Fick's law. Besides this, additional conditions linking the mass fluxes are superimposed on the system; these conditions have various forms for the different processes.

For example, for the process of multicomponent rectification when the condition of equimolarity is used ( $\sum_{k=1}^n N_k = 0$ ) the relationship (6) assumes the form:

$$\lambda \frac{\partial T}{\partial y} = r_p^{(r)} [D] \frac{\partial C}{\partial y}, \quad (7)$$

where  $r_{pi} = \Delta H_i - \Delta H_n$ ,  $i = 1, 2, \dots, n-1$ , while for multicomponent absorption with an inert component ( $N_n = 0$ ) relationship (6) appears as follows:

$$\lambda \frac{\partial T}{\partial y} = r_A^{(T)} [D] \frac{\partial \mathbf{C}}{\partial y}; \quad (8)$$

where  $r_{Ai} = \Delta H_i$ ,  $i = 1, 2, \dots, n-1$ . For the general case we will therefore write condition (6) in the form

$$\lambda \frac{\partial T}{\partial y} = r^{(T)} [D] \frac{\partial \mathbf{C}}{\partial y}; \quad (9)$$

where  $r_i = r_{pi}$  for multicomponent rectification,  $r_i = r_{Ai}$  for multicomponent absorption with an inert component, etc.

The matrix of turbulent diffusion coefficients which appears in Eq. (2) has the following structure [8-11]:

$$[E(y)] = [D] + \varepsilon_D(y)^{-1} I, \quad (10)$$

where  $\varepsilon_D$  is the coefficient of turbulent diffusion, which is determined by the hydrodynamic conditions, and which can be obtained from the results of turbulence investigations in binary mixtures [11].

The matrix [D] is expressed in terms of the coefficients of molecular diffusion of binary pairs of the components making up the given mixture. Formulas for evaluating [D] can be obtained by use of the molecular theory of gases and liquids [7, 12, 13]. Important properties of the matrix [D] are its reducibility to diagonal form and also the fact that its eigenvalues are real and positive [4, 13]. Let us now show that the matrix [E] defined by Eq. (10) possesses the same properties.

Suppose that [L] is the fundamental matrix for [D], i.e., that

$$[L]^{-1}[D][L] = \text{diag } D'_i.$$

Then

$$[L]^{-1}[E(y)][L] = [L]^{-1}[D][L] + [L]^{-1}\varepsilon_D(y)^{-1}I[L] = \text{diag } D'_i + \varepsilon_D(y)^{-1}I = \text{diag } E'_i,$$

where  $E'_i = D'_i + \varepsilon_D$ ,  $i = 1, 2, \dots, n-1$ .

Since  $D'_i > 0$  and  $\varepsilon_D > 0$ , then  $E'_i > 0$  for all values of  $i$ . Consequently, the matrix [E(y)] is reduced to diagonal form with the use of the same fundamental matrix as [D], and has real, positive eigenvalues.

By analogy with the matrix [E(y)], the coefficient of turbulent temperature conductivity which appears in Eq. (1) consists of two terms [5]:

$$\sigma(y) = \kappa + \varepsilon_T(y), \quad (11)$$

where  $\varepsilon_T(y)$  is the thermal analog of the coefficient of turbulent diffusion  $\varepsilon_D(y)$ .

The system of equations (1)-(2) with the boundary conditions (3)-(5) and (9) represents a coupled system of equations of the parabolic type with boundary conditions of the fourth sort, which leads to significant difficulties in finding a solution. Hence, by making use of the property of diagonality of the matrices [D] and [E], use is made of a method proposed in [14] which makes it possible to transform the initial system into an uncoupled form:

$$u(y) \frac{\partial T}{\partial x} = \frac{\partial}{\partial y} \left( \sigma \frac{\partial T}{\partial y} \right); \quad (12)$$

$$u(y) \frac{\partial \mathbf{C}'}{\partial x} = \frac{\partial}{\partial y} \left( \text{diag } E'_i \frac{\partial \mathbf{C}'}{\partial y} \right). \quad (13)$$

The boundary conditions are:

$$\text{at } x = 0 \quad T = T_0, \quad \mathbf{C}' = \mathbf{C}'_0; \quad (14)$$

$$\text{at } y = 0 \quad \frac{\partial T}{\partial y} = 0, \quad \frac{\partial \mathbf{C}'}{\partial y} = \mathbf{0}; \quad (15)$$

$$\text{at } y = h_0 \quad \mathbf{C}' = \mathbf{v}' \cdot T + \mathbf{w}', \quad \lambda \frac{\partial T}{\partial y} = r_1^{(T)} \frac{\partial \mathbf{C}'}{\partial y}; \quad (16)$$

where

$$\mathbf{C}' = [L]^{-1}\mathbf{C}, \mathbf{C}'_0 = [L]^{-1}\mathbf{C}_0; \quad (17)$$

$$\mathbf{v}' = [L]^{-1}\mathbf{v}; \mathbf{w}' = [L]^{-1}\mathbf{w}; \mathbf{r}'^{(T)} = \mathbf{r}^{(T)}[D][L]. \quad (18)$$

Dimensionless variables are introduced through the relationships

$$\xi = \frac{4x}{\text{Re } h_0}, \eta = \frac{y}{h_0}, v = \frac{u}{\bar{u}}, t = \frac{T - T_0}{T_e - T_0}; \quad (19)$$

$$c_i = \frac{C'_i - C'_{0i}}{C'_{ei} - C'_{0i}}, \quad i = 1, 2, \dots, n-1; \quad (20)$$

where

$$C'_{ei} = v'_i T_0 + w'_i, \quad T_e = (C_{01} - w_1)/v_1. \quad (21)$$

The system (12)-(16) then assumes the final form

$$v(\eta) \frac{\partial t}{\partial \xi} = \frac{\partial}{\partial \eta} \left\{ \left( \text{Pr}^{-1} + \frac{\varepsilon_T}{v} \right) \frac{\partial t}{\partial \eta} \right\}; \quad (22)$$

$$v(\eta) \frac{\partial c}{\partial \xi} = \frac{\partial}{\partial \eta} \left\{ \left( \text{Sc}'^{-1} + \frac{\varepsilon_D}{v} \right) \frac{\partial c}{\partial \eta} \right\}; \quad (23)$$

$$\xi = 0, \quad t = 0, \quad c_i = 0; \quad (24)$$

$$\eta = 0, \quad \frac{\partial t}{\partial \eta} = 0, \quad \frac{\partial c_i}{\partial \eta} = 0; \quad (25)$$

$$\eta = 1, \quad c_i + a_i t = 1; \quad (26)$$

$$\frac{\partial t}{\partial \eta} = \sum_{h=1}^{n-1} b_h \frac{\partial c_h}{\partial \eta}; \quad (27)$$

$$i = 1, 2, \dots, n-1,$$

where

$$a_i = v'_i \frac{T_0 - T_e}{C'_{ei} - C'_{0i}}, \quad b_i = \frac{r_{1i}(C'_{ei} - C'_{0i})}{\lambda(T_e - T_0)}, \quad (28)$$

$$\text{Sc}'_i = v/D'_i. \quad (29)$$

Let us consider a motion of the liquid with a flow-mean velocity ( $v = 1$ ) and make the assumption that the coefficients of turbulent diffusion and turbulent temperature conductivity are equal [15]:

$$\varepsilon_D(\eta) = \varepsilon_T(\eta) = \varepsilon(\eta). \quad (30)$$

The relationship (30) is quite a complex function, since the natures of the variation of the turbulent transport coefficients are not the same close to the wall, in the core of the flow, and close to the interface [16]. A large number of investigations exist dealing with the determination of the functional relationships (30) for the various layers of film flows [5, 16-18]. A detailed analysis of these investigations is contained in [15], and the use of the following three expressions is recommended.

For the zone near the wall the van Driest formula [19] is recommended:

$$\frac{\varepsilon}{v} = \frac{1}{2} \left\{ -1 + \left[ 1 + 0,04 \frac{\text{Re}^2 \eta^2}{\text{Fr}} \left( 1 - \exp \left( -\frac{\text{Re} \eta}{104 \sqrt{\text{Fr}}} \right) \right)^2 \right]^{1/2} \right\}, \quad (31)$$

where

$$0 \leq \eta \leq \eta_1, \quad \eta_1 = 120 \sqrt{\text{Fr}}/\text{Re}. \quad (32)$$

For the core of the turbulent flow, Reichardt's formula is used [20]:

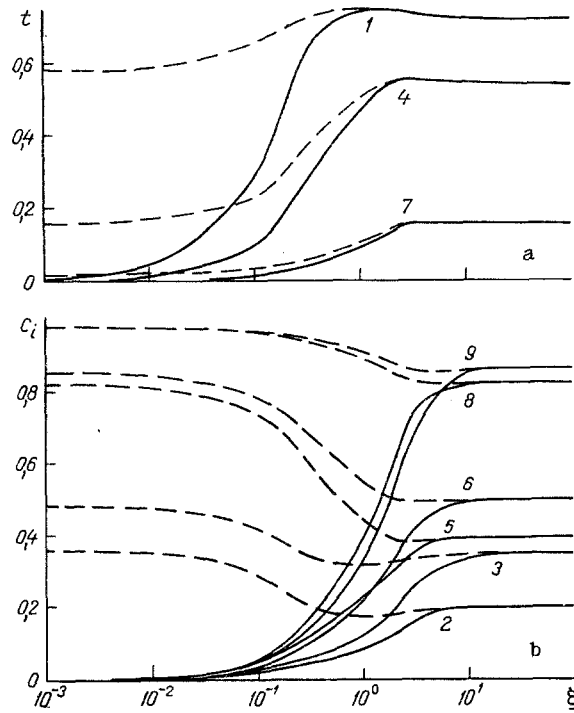


Fig. 2. The dimensionless temperature (a) and the dimensionless concentrations of the components (b) as functions of the length of the contact device for  $Re = 10,000$ ;  $Fr = 218$ ;  $Pr = 10$ ;  $Sc_1^1 = 1500$ ;  $Sc_2^1 = 2500$ ;  $a_1 = 1.1$ ;  $a_2 = 0.9$ , for various values of  $b_1$ : curves 1-3:  $b_1 = 0.3$ ,  $b_2 = -0.1$  (curve 1 for  $t$ , curve 2 for  $c_1$ , curve 3 for  $c_2$ ); curves 4-6:  $b_1 = 0.03$ ,  $b_2 = -0.01$  (curve 4 for  $t$ , curve 5 for  $c_1$ , curve 6 for  $c_2$ ); curves 7-9:  $b_1 = 0.003$ ,  $b_2 = -0.001$  (curve 7 for  $t$ , curve 8 for  $c_1$ , curve 9 for  $c_2$ ); solid lines are for values in the core of the phase, and dashed lines are for values at the interface.

$$\frac{\varepsilon}{v} = K \frac{Re}{\sqrt{Fr}} (2\eta - \eta^2)(3 - 4\eta + 2\eta^2), \quad (33)$$

in which the constant  $K$  is determined from the condition that the results calculated by Eqs. (31) and (33) should agree at the point  $\eta = \eta_1$  which is given from Eq. (32).

For the interfacial zone a modification of the formula by Lamourelle and Sandall [21] is recommended:

$$\frac{\varepsilon}{v} = 3,153 \cdot 10^{-7} Fr^{-2/3} Re^{2.758} (1 - \eta)^2, \quad (34)$$

which is used over the range of variation of the dimensionless thickness from  $\eta = 1$  to the value  $\eta = \eta_2$  at which the results of the calculations by Eqs. (33) and (34) coincide.

In order to determine the profiles of the coefficient of turbulent diffusion from relationships (31)-(34) it is necessary to set up two computational procedures. The first of these is intended for calculating the constant  $K$  in relationship (33) from the known values of  $Re$  and  $Fr$  and at  $\eta = \eta_1$ . The second procedure determines the value of the dimensionless thickness  $\eta_2$  from the known values of  $Re$  and  $Fr$  and the value of  $K$  calculated in the first procedure. In the present work both procedures were carried out using Newton's method.

Thus, the solution of the dimensionless problem (22)-(27), taking (30)-(34) into account, is determined by the dimensionless parameters  $Re$ ,  $Fr$ ,  $Pr$ ,  $Sc_i^*$ ,  $a_i$ ,  $b_i$ ,  $i = 1, 2, \dots, n - 1$ , i.e., it depends on  $3n$  quantities.

The solution is carried out by the method of marching using the finite-difference operators [22]

$$\begin{aligned} \frac{\partial W}{\partial \xi} &= \frac{W(k, j) - W(k-1, j)}{\Delta \xi}; \\ \frac{\partial}{\partial \eta} \left\{ \theta(\eta) \frac{\partial W}{\partial \eta} \right\} &= \frac{1}{(\Delta \eta)^2} \left\{ \frac{\theta(j+1) + \theta(j)}{2} [W(k, j+1) - W(k, j)] - \right. \\ &\quad \left. - \frac{\theta(j) + \theta(j-1)}{2} [W(k, j) - W(k, j-1)] \right\}, \end{aligned} \quad (35)$$

where  $k, j$  are the numbers of the steps vertically and horizontally;  $\Delta \xi, \Delta \eta$  are the corresponding sizes of the steps, and  $W$  and  $\theta$  represent respectively either  $t$  and  $\sigma$ , or  $c_i$  and  $E_i^*$ ,  $i = 1, 2, \dots, n - 1$ .

In order to improve the accuracy of approximating the derivatives at the interfacial surface (Eq. (27)) use is made of a finite-difference analogy making it possible to approximate with accuracies to the third order of smallness [23]:

$$\left. \frac{\partial W}{\partial \eta} \right|_{\eta=1} = \frac{1}{12(\Delta \eta)} \{8f(k) - 18W(k, N-1) + W(k, N-2) + 9W(k, N)\}, \quad (36)$$

where  $N$  is the number of steps along the horizontal direction, and  $f(k)$  is the value of the corresponding function on the interface determined for any  $k$  by the formula

$$f(k) = \frac{W(k, N-1) + W(k, N)}{2}. \quad (37)$$

Having found the fields of the dimensionless concentrations of the components and temperature by this method, it is possible to calculate the values of the wall, surface, and mean concentrations and temperature, the mass fluxes of the components and the heat flux at the interface, the coefficients of mass and heat transfer, etc.

By way of an example, in the present paper we have investigated numerically the process of non-isothermal absorption of a two-component gas mixture by a nonvolatile turbulent film of liquid. Figures 1 and 2 give the characteristic dependences of the dimensionless temperature and the dimensionless concentrations of the components on the length of the contact device for various values of the problem parameters. The solid lines show the temperature and concentration profiles in the core of the phase (the integral-mean values over the thickness of the film), the dashed lines give the profiles of the free-surface values, and the dot-dashed lines give the profiles of the wall values. It can be clearly seen from the graphs that at some definite distance from the inlet of the contact device the heat and mass transfer process ends up giving equilibrium values of the concentrations and temperature. It is clear that then the corresponding values at the wall, in the core of the flow, and at the free interface become the same.

The change from the dimensionless to the dimensional parameters of the problem is carried out by using Eqs. (19)-(21), and these in turn are converted into real values of the concentrations of the components and the temperature in the turbulent liquid film by using Eq. (17).

The proposed method of solving the problem makes it possible in the first place to determine for given initial values of the parameters the profiles of the concentrations of the components and the temperature at each cross-section of the contact device, and to determine their free-surface, wall, integral-mean, and other values; in the second place, to determine the required length of the equipment; and in the third place, to investigate theoretically the effects of the parameters of the turbulent multicomponent heat and mass transfer process on the solution.

## NOTATION

$T$ , temperature of the mixture;  $c$ , vector of the molar concentrations of the components of the mixture;  $c'$ , concentration vector transformed by means of Eq. (17);  $[D]$ , matrix of the coefficients of multicomponent molecular diffusion;  $[D']$ , diagonal matrix consisting of the eigenvalues of the matrix  $[D]$ ;  $[E]$ , matrix of the coefficients of multicomponent turbulent diffusion;  $[E']$ , diagonal matrix consisting of the eigenvalues of the matrix  $[E]$ ;  $[L]$ , fundamental matrix for  $[D]$  and  $[E]$ ;  $\lambda$ , coefficient of thermal conductivity;  $\kappa$ , coefficient of temperature conductivity;  $\sigma$ , coefficient of turbulent temperature conductivity;  $\nu$ , coefficient of dynamic viscosity;  $q$ , heat flux;  $N_i$ , molar flux of  $i$ -th component;  $v, w$ , parameters of the equilibrium relationship (5);  $\Delta H_i$ , difference of the molar enthalpies of the  $i$ -th component in the gaseous and liquid phases transported by its mass flux through the free interface;  $n$ , number of components in the mixture;  $h_0$ , thickness of the liquid film;  $u$ , velocity of liquid film;  $\bar{u}$ , mean velocity of liquid film;  $x, y$ , coordinates;  $\xi, \eta$ , corresponding dimensionless coordinates;  $[I]$ , unit matrix;  $Re = 4\bar{u}h_0/\nu$ , Reynolds number;  $Fr = \bar{u}^2/h_0g$ , Froude number;  $Pr = \nu/\kappa$ , Prandtl number;  $Sc_i^* = \nu/D_i^*$ , modified Schmidt number of the  $i$ -th component.

## SUBSCRIPTS

0, value at the inlet to the contact device;  $e$ , equilibrium value;  $i$ , value for the  $i$ -th component.

## SUPERSCRIPTS

' , value transformed using the fundamental matrix; (T), notation for line vector.

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