DIFFUSION MODEL OF LONGITUDINAL AGITATION IN HEAT AND MASS TRANSFER PROCESSES. 1. CLASSIFICATION OF MASS TRANSFER PROCESSES – 1st-LEVEL PROBLEMS

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The application of a diffusion model is classified for describing heat and mass transfer processes. All possible combinations are formulated within the framework of the distinguished agitation models. The problems are divided into three levels of complexity of the combinations. Derivation of formulas and solutions for determining carrying capacities of a heat exchanger (mass exchanging apparatus) are considered as applied to the problems of the 1st level.

There exist a number of models allowing one to account for the structure of flows when solving problems of heat and mass transfer. "Limit models" – ideal displacement (ID) and ideal agitation (IA) – are the simplest in mathematical description. But often they cannot sufficiently accurately describe an object, thus leading to the need for more complex models, i.e., a diffusion model (DM). However, we did not find in the literature [1-5] any reasonable systematization in the presentation of DM employment for the mentioned transport processes. This paper is aimed at compensating for this deficiency.

A subsequent analysis will be made applied to heat transfer. But the obtained relations are fully valid also for mass transfer along the straight line of equilibrium. In this case the meaning of designations in equations and formulas, as will be shown below, somewhat changes.

We consider the following model (Fig. 1a): a heat exchanger with a heat transfer surface F (length L and width B); the coefficient of heat transfer K has two volumes – for cold and hot flows with cross-sections φ_1 and φ_2 , respectively. The flows moving in the heat exchanger have the following characteristics: hot – flow rate G_1 , heat capacity C_1 , temperatures T' (at the inlet) and T'' (at the outlet); cold – flow rate G_2 , heat capacity C_2 , temperature t' (at the inlet) and t'' (at the outlet).

The flows can move in forward or reverse directions. The structure of flows is DM. In this case DM can be also transformed to limiting cases: ID and IA.

Within the framework of our model we assume the coefficient of heat transfer K and specific heat capacities of flows C_1 and C_2 to be constant. In other words, in the considered process all the stages are linear. Consequently, the whole process is also linear. This makes it possible to use for the analysis the notion of carrying capacities (CC) [6, 7]. Thus, G_1C_1 and G_2C_2 are the carrying capacities of forced transfer (the stages of heat supply to the heat exchanger and withdrawal), KF is the carrying capacity of transverse transfer (the surface stage), Q/Δ is the carrying capacity of the heat exchanger as a whole, where Q is the heat transferred in the apparatus, $\Delta \equiv T' - t'$ is the difference of temperatures at the inlet to the system (further we shall call it initial). We denote the process criteria [6]: $KF/(G_1C_1) \equiv a$ is the number of transfer units (NTU) for a hot agent, $KF/(G_2C_2) \equiv b$ the same for a cold agent.

To formulate differential equations we introduce (Fig. 1a) axis f (a current heat transfer surface), whose origin is congruent with the left end of the heat transfer surface, and axis l (the current length) and axis x (the dimensionless length or dimensionless heat transfer surface x = l/L = f/F).

We consider the heat balance of an infinitely small portion of a hot flow moving from left to right in the mode of DM:

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Fig. 1. To the derivation of differential equations (a) and boundary conditions (b, c).

$$G_1C_1T + \lambda_1\varphi_1\left(\frac{\partial T}{\partial l} + \frac{\partial^2 T}{\partial l^2}dl\right) - G_1C_1\left(T + \frac{\partial T}{\partial l}dl\right) - \lambda_1\varphi_1\frac{\partial T}{\partial l} - K\left(T - t\right)df = 0, \qquad (1)$$

where λ is the coefficient of effective thermal conductivity, allowing not only for the thermal conductivity of the medium but also for longitudinal agitation of the flow.

We transform Eq. (1)

$$\lambda_1 \varphi_1 \frac{\partial^2 T}{\partial l^2} dl - G_1 C_1 \frac{\partial T}{\partial l} dl - K (T - t) df = 0$$

Since f = Fx, l = Lx, then df = Fdx, dl = Ldx. Then

$$\lambda_1 \varphi_1 \frac{1}{L^2} \frac{\partial^2 T}{\partial x^2} L dx - G_1 C_1 \frac{\partial T}{\partial x} dx - KF (T-t) dx = 0.$$

Introducing the designations $\lambda_1/L \equiv \gamma_1$, $\partial^2 T/\partial x^2 \equiv \ddot{T}$, $\partial T/dx \equiv \dot{T}$ we obtain

$$\gamma_1 \varphi_1 \ddot{T} - G_1 C_1 \dot{T} - KF (T - t) = 0.$$
⁽²⁾

Here the highest-order coefficient $\gamma_1 \varphi_1$ represents one more carrying capacity – the CC of longitudinal transfer.

We divide expression (2) by $\gamma_1 \varphi_1$, and the third term we multiply and divide by $G_1 C_1$:

$$\ddot{T} - \frac{G_1 C_1}{\gamma_1 \varphi_1} \dot{T} - \frac{KF}{\gamma_1 \varphi_1} \frac{G_1 C_1}{G_1 C_1} (T - t) = 0$$

We designate $G_1C_1/\gamma_1\varphi_1 \equiv p$. Then the coefficient at (T-t) should involve the product of the two criteria p and a. Correspondingly, for a cold agent we introduce the criteria $KF/(G_2C_2) \equiv b$ and $G_2C_2/(\gamma_2\varphi_2) \equiv q$. As a result we have, in terms and symbols of the ratios of carrying capacities

$$\ddot{T} - p\dot{T} - ap(T - t) = 0.$$
 (3)

Model	Flow	Differential equations		Boundary conditions	
Diffusion	Hot		$\ddot{T} - p\dot{T} - ap(T-t) = 0$	at $x = 0$ $T' = T - (1/p)\dot{T}$	
				at x = 1 T = 0	
		~	$\ddot{T} + p\dot{T} - ap(T-t) = 0$	at x = 0 T = 0	
				at $x = 1$ $T' = T + (1/p)\dot{T}$	
	Cold			at $x = 0$ $t' = t - (1/q)\dot{t}$	
		->	$\ddot{t} - q\dot{t} + bq(T-t) = 0$		
				at x = 1 t = 0	
		-	$\ddot{t} + q\dot{t} + bq(T-t) = 0$	at $x = 0$ $\dot{t} = 0$	
				at $x = 1$ $t' = t + (1/q)t$	
Ideal displacement	Hot	->	$\dot{T} + a(T-t) = 0$	at $x = 0$ $T' = T$	
		-	$\dot{T} - a(T-t) = 0$	at $x = 1$ $T' = T$	
	Cold	→	$\dot{t} - b(T-t) = 0$	at $x = 0$ $t' = t$	
		<	$\dot{t} + b(T-t) = 0$	at x = 1 t' = t	

TABLE 1. Summary Table of Differential Equations and Boundary Conditions

TABLE 2. Levels of Complexity of Problems and Numbers of Computational Relations

	Cold							
Hat	ID	DM	IA	DM	ID			
HOL	→	>	⇔	←	←			
	m = +1	m = +1	m = 0	m = -1	m = -1			
ID →	6		9		12			
1=+1								
DM →								
1=+1								
IA ↔								
1=0	7		10		13			
DM ←								
1 = -1								
ID ←								
1=-1	8		11		14			

To reveal the physical meaning of the criterion p, we express the mass flow rate of the heat carrier G_1 in terms of the product of density ρ , velocity of flow w, and cross-section φ , and also take into account that $a^* \equiv \lambda/(\rho C)$ is the coefficient of effective thermal diffusivity. Then for a hot agent $p = G_1 C_1/(\gamma_1 \varphi_1) = v\rho CL/(\pi \varphi)$ = wL/a^* = Pe is the Peclet number for longitudinal agitation, which is the only parameter for DM. Of the same meaning is $q = G_2 C_2/(\gamma_2 \varphi_2)$ – the Peclet number of a cold agent.

We introduce one more criterion: the ratio of the carrying capacity of the heat exchanger Q/Δ to the carrying capacity of transverse transfer KF – criterion R, which is convenient for describing processes in dimensionless form: $R \equiv Q/(\Delta KF) = Q/(G_1C_1\Delta a) = Q/(G_2C_2\Delta b)$.

As applied to the processes of mass transfer the corresponding criteria have the form:

 $a \equiv K_x F/W = K_y F/W/m - NTU \text{ in } x \text{ phase };$ $b \equiv K_y F/D = K_x F/(Dm) - NTU \text{ in } y \text{ phase };$ $p \equiv W/(\gamma_1 \varphi_1) - \text{ for } x \text{ phase };$ $q \equiv D/(\gamma_2 \varphi_2) - \text{ for } y \text{ phase };$ $\Delta_x = x_{\text{in}} - x_{\text{in}}^{\rho} - \text{ initial moving force in } x \text{ phase };$ $\Delta_y = y_{\text{in}}^{\rho} - y_{\text{in}} - \text{ initial moving force in } y \text{ phase };$ $R = M/(\Delta_x K_x F) = M/(\Delta_y K_y F) = M/(\Delta_x Wa) = M/(\Delta_y Db), \quad \gamma_1 = d_1/L; \quad \gamma_2 = d_2/L.$ To obtain boundary conditions we consider the heat balance (Fig. 1b) for a "zero" volume of the set balance (Fig. 1b) for a "zero

To obtain boundary conditions we consider the heat balance (Fig. 1b) for a "zero" volume of a hot agent at the inlet to the heat exchanger:

$$G_1 C_1 T' - G_1 C_1 T + \lambda_1 \varphi_1 \frac{\partial T}{\partial l} = 0$$

or

$$T + pT - pT = 0,$$

hence T' = T - (1/p)T at x = 0.

The heat balance for a "zero" volume of a hot agent and the outlet from the heat exchange (Fig. 1b) has the form

$$-G_1C_1T'' - G_1C_1T'' + \lambda_1\varphi_1\frac{\partial T}{\partial l} = 0, \ \lambda_1\varphi_1\frac{\partial T}{\partial l} = 0$$

hence $\dot{T} = 0$ at x = 1 (the Dancwerts condition).

In a similar way we can obtain a differential equation for other cases (motion from right to left, a cold agent flow).

The differential equations and the boundary conditions for ID are obtained as particular cases of the relations derived for D when $p, q \rightarrow \infty$. On the other hand, when $p, q \rightarrow 0$ the relations for DM change over to differential equations for ID: $\ddot{T} = 0$ and $\ddot{t} = 0$ (we do not use these equations in what follows).

Allowing for the fact that hot and cold flows can be directed to the heat exchanger both from left to right (\rightarrow) and from right to left (\leftarrow), four differential equations are obtained for DM (Table 1). The same number of versions is also possible for a limiting state – ID.

Each flow in the heat exchanger can move in any of the modes DM, ID or IA. The combination of the structures of both flows determines the complexity of the problem: as has been already mentioned, the transition from the limit models ID and IA to DM makes the mathematical description more complex. Therefore, it is expedient to introduce the subdivision of the problems by the levels. The notion "level" does not involve any physical meaning and is introduced only for classification of problems according to the complexity of description: the 1st level includes cases when one of the flows is not presented by DM (only ID and IA); the 2nd level includes cases when only one of the flows moves in DM mode; the 3rd level corresponds to the case when both flows move in DM mode.

In general, R is a function of four variables:

$$R = f(a, b, p, q)$$

Depending on the specific situation (the level of the problem, the flow direction, a hot or cold agent) the characteristic equations and the equations for R will contain different combinations of these variables.

We find the total possible number of formulas for R allowing for the fact that each of the variables of p and q can participate in the formula in the case of DM; it tends to infinity $(\rightarrow \infty)$ in the case of ID; it tends to zero $(\rightarrow 0)$ in the case of IA.

First we consider the formulas with p (a hot agent). There will be five of them: two formulas for flow motion (\rightarrow) and (\leftarrow) at finite p; one case when $p \rightarrow 0$; two formulas for (\rightarrow) and (\leftarrow), where $p \rightarrow \infty$. The same quantity of formulas exist, correspondingly, for q (a cold agent). The total number of possible formulas is $5 \times 5 = 25$ (Table 2). They include 9 schemes for the 1st level, 12 schemes for the 2nd level, and 4 schemes for the 3rd level.

We note that formally we found the total number of schemes; among them there are physically similar schemes for which the final expressions will coincide (straight flows (\Rightarrow) and (ϵ)).

A similar analysis can be performed for limiting cases applied to criteria a and b.

We consider the technique for derivation of the formulas for R of the 1st-level model using the example: a hot agent moves from right to left in the ID mode, a cold agent moves from left to right in the ID mode. In short form we write this as

hot (ID)
$$\leftarrow$$
 cold (ID) \rightarrow

For this case we take the differential equations and the boundary conditions from Table 1:

$$T - a (T - t) = 0$$
 at $x = 1$, $T = T'$;
 $t - b (T - t) = 0$ at $x = 0$, $t = t'$. (4)

We solve the system of differential equations by the higher-order technique

$$\ddot{T} + (-a+b)\dot{T} = 0.$$
 (5)

The characteristic equation is

$$k^{2} + (-a + b) k = 0,$$

its roots are $k_0 = 0$, $k_1 = a - b$.

The solution of Eq. (5) is $T = \lambda_0 + \lambda_1 \exp(k_1 x)$. Having substituted it into the equation of system (4) and allowing for the boundary conditions, we express t', T', and then $\Delta \equiv T' - t'$:

$$T' = \lambda_0 + \lambda_1 \exp k_1, \quad t' = \lambda_0 + \lambda_1 \left(-\frac{k_1}{a} + 1 \right), \quad \Delta = \lambda_1 \left(\exp k_1 + \frac{k_1}{a} - 1 \right).$$

Then

$$\lambda_1 = \frac{\Delta}{\exp k_1 + \frac{k_1}{a} - 1}.$$

We write the expression for the heat flux which is received by a cold agent from a hot agent as a result of heat transfer:

$$Q = G_1 C_1 (T' - T') = G_1 C_1 (-\lambda_1 + \lambda_1 \exp k_1).$$

We divide this expression by $G_1C_1\Delta a$ and, allowing for $R = Q/(G_1C_1\Delta a)$, we have

$$R = \frac{-1 + \exp k_1}{a \exp k_1 + k_1 - a},$$

or in final form

$$R = \frac{\frac{1}{a-b} (1 - \exp(-a+b))}{1 + \frac{b}{a-b} (1 - \exp(-a+b))}.$$

Similarly we obtain formulas for other cases of the 1st level (all nine formulas are given in Table 2 in the form of the numbers of the corresponding computational relations):

hot (ID)
$$\rightarrow$$
 $k^{2} + (a + b) k = 0$ $R = \frac{\frac{1}{a + b} (1 - \exp(-(a + b)))}{1 + \frac{0}{a + b} (1 - \exp(-(a + b)))}$, (6)

hot (IA)
$$\Leftrightarrow$$

cold (ID) \rightarrow $k + b = 0$ $R = \frac{\frac{1}{b}(1 - \exp(-b))}{1 + \frac{a}{b}(1 - \exp(-b))},$ (7)

hot (ID)
$$\leftarrow$$
 $k^{2} + (-a+b)k = 0$ $R = \frac{\frac{1}{a-b}(1-\exp(-a+b))}{1+\frac{b}{a-b}(1-\exp(-a+b))}$, (8)

hot (ID)
$$\rightarrow$$

cold (IA) \leftrightarrow $k + a = 0$ $R = \frac{\frac{1}{a}(1 - \exp(-a))}{1 + \frac{b}{a}(1 - \exp(-a))}$, (9)

hot (IA)
$$\Leftrightarrow$$
 $k = 0$ $R = \frac{1}{1 + a + b}$, (10)

hot (ID)
$$\leftarrow$$

cold (IA) \Leftrightarrow $k - a = 0$ $R = \frac{\frac{1}{a}(1 - \exp(-a))}{1 + \frac{b}{a}(1 - \exp(-a))}$, (11)

hot (ID)
$$\rightarrow$$
 $k^{2} + (a - b) k = 0$ $R = \frac{\frac{1}{a - b} (1 - \exp(-a + b))}{1 + \frac{b}{a - b} (1 - \exp(-a + b))}$, (12)

hot (IA)
$$\Leftrightarrow$$

cold (ID) \leftarrow $k-b=0$ $R = \frac{\frac{1}{b}(1-\exp{(-b)})}{1+\frac{a}{b}(1-\exp{(-b)})},$ (13)

hot (ID)
$$\leftarrow k^2 - (a+b)k = 0$$
 $R = \frac{\frac{1}{a+b}(1 - \exp(-(a+b)))}{1 + \frac{0}{a+b}(1 - \exp(-(a+b)))}$ (14)

It is seen that the formulas for different cases contain a combination of criteria; nevertheless some regularities are vividly seen. This makes it possible to reduce all formulas to a general form.

For this purpose we introduce some sign variables I and m, which characterize the direction of flows. Let I = +1 if a hot flow moves from left to right; I = -1 if it moves from right to left; I = 0 if the flow is in IA mode. Similarly for a cold flow: m = +1, m = -1, m = 0.

Using the introduced variables, we present all the formulas for R in a general form

$$R = \frac{H}{1 + \frac{a+b-s}{1+|\mathbf{m}||}H},$$
(15)

where

$$s = ||a + mb||; H = \frac{1}{s}(1 - \exp(-s)).$$

A formula close to (15) was derived earlier [7], but in our opinion it is less convenient in practical application. In fact, to obtain any specific solution from (15) it is only necessary to place the corresponding sign variables in it, whereas the formula from [7] requires the choice of a kernel for each specific case.

Thus, we obtained differential equations for motion of flows and expressions for R. The latter are reduced to one general formula for calculating R models of the 1st level.

Equations for R and the sequence of derivation are demonstrated to confirm the correctness of equations of the 2nd and 3rd levels in their limit transitions given in other works, rather that to determine the formulas themselves.

NOTATION

B, width of heat transfer surface, m; K, coefficient of heat transfer, $W/(m^2 \cdot K)$; $K_{x,y}$, coefficients of mass transfer in phases x and y, kg of phase $x(y)/(m^2 \cdot \sec)$; $\varphi_{1,2}$, cross-section area of volumes for hot and cold flows in the heat exchanger, m^2 ; $G_{1,2}$, mass flux of a hot and a cold agent, respectively, kg/sec; $C_{1,2}$, heat capacity of hot and cold flows, J/(kg·K); T', T", temperatures of a hot agent at the inlet to and outlet from the heat exchanger, K; t', t', similarly for a cold agent, K; Q, flux of heat transferred in the apparatus, W; Δ , difference of temperatures at the inlet to the heat exchanger, K; $\Delta_{x,y}$, initial moving force in phases x and y, kg of component/kg of phase; a, b, number of transfer units (NTU) for hot and cold agents; l, L, length of the heat exchanger, current and final, m; f, F, heat transfer surface of the heat exchanger, current and final, m²; x, current dimensionless length; λ , coefficient of effective thermal conductivity, W/(m·K); p, q, Peclet numbers for hot and cold flows; ρ , density, kg/m³; w, flow velocity, m/sec; a*, coefficient of effective thermal diffusivity, m²/sec; v, volumetric flow rate of heat carrier, m³/sec; R, criterion equal to the ratio of the carrying capacity of the heat exchanger (Q/ Δ) to the carrying capacity of transverse transfer (KF); W, D, mass flow rates of x and y phases in mass transfer, kg/sec; m, equilibrium constant; M, flux of mass transferred from one phase to another, kg/sec; d_{1,2}, coefficients of effective diffusion in x and y phases, m²/sec; l, m, sign variables characterizing flow direction.

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