AN APPROXIMATE PHYSICAL MODEL OF MASS TRANSFER

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On the basis of an approximate physical model of mass transfer, the distribution of liquid mass in the effective diffusion boundary layer of a whirled unidirectional stream is determined, with the resistance of the liquid phase to mass transfer taken into account.

Several physical models have been proposed for describing the mass transfer in gas–liquid systems [1-8]. Without further analyzing them – they have been analyzed in [9, 10] – we will only show here that each of them more or less reliably describes a certain class of processes characterized by some basic physicochemical and hydrodynamic parameters.

There is an indisputable interest alive today in research and development concerning high-efficiency and high-output mass exchangers which consist of contact stages with the phases interacting in a parallel flow [11-13].

In order to ensure a sufficiently thorough phase separation between stages, for producing a counterflow of the phases throughout the device, and for boosting the mass transfer rate, it is worthwhile to consider a whirled two-phase stream [14-23].

On the basis of certain assumptions, we will analyze here a model of the mass transfer process in a whirled unidirectional stream, which should be useful for an engineering design of a parallel-flow contact stage of a mass exchanger.

A two-phase (gas–liquid) stream in a field of centrifugal forces is characterized by an annular flow mode.

Unlike in a free discharge of liquid or in a counterflow of phases with a negligibly low gas velocity, here the maximum tangential stress occurs at the interphase boundary (Fig. 1a).

The flow of liquid and gas in a whirled stream is rather helical and, therefore, characterized by regular vortices [24, 25] in each phase layer. Besides, the presence of an interphase boundary is also a cause of irregular vortices at that surface [10, 25].

In the case of mass transfer where the liquid phase resists it, one may assume (considering a high gas velocity and an intensive stirring of the gas by the turbulent fluctuations due to vortices) that the concentration of the gas over an entire cross section of the gas stream is equal to its mean concentration over this section, while the high-velocity gas stream should be viewed as the source of tangential stresses which ensure the forced helical motion of the liquid.

The existence of appreciable tangential stressed and forced vortices in the liquid layer causes turbulence to develop in the liquid layer and, consequently, tends to equalize both velocities and concentrations within the total mass of liquid.

The liquid layer is not turbulized uniformly throughout its entire thickness. A section of the liquid annulus contains regions where the hydrodynamic flow mode can be assumed invariable but different than in the remaining stream (Fig. 1b).

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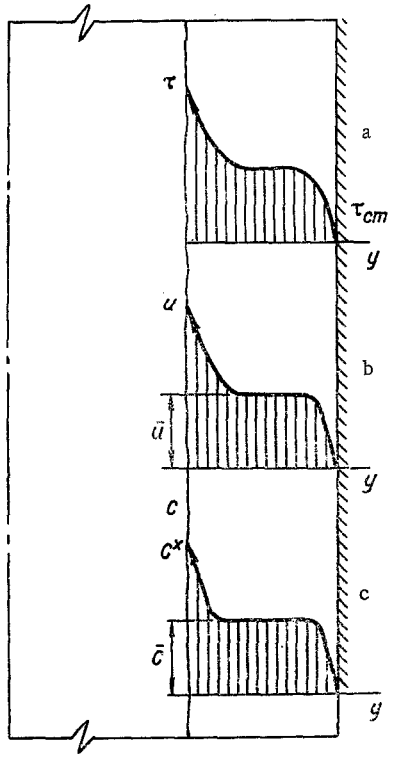

Fig. 1. Profiles: a) tangential stresses $\tau = \tau(y)$; b) mean velocity $u = u(y)$; c) concentration in the liquid phase $C = C(y)$.

Zone 1 at the wall of cylindrical channel is the viscous sublayer region (thickness δ'). Here at $y < \delta''$ the velocity varies fast from zero directly at the solid wall to the mean value $\bar{u}$ referred to the stream. The thickness of this zone can be determined from the condition given in [8] with the Reynolds number necessarily of a magnitude $Re \sim 1$.

Zone 2 is the fully turbulent mainstream in the liquid layer. Both the turbulent fluctuations and the vortices tend to make the velocity field uniform. Without a large error, the velocity of liquid in this zone may be assumed equal to the mean stream velocity $\bar{u}$.

Zone 3 at the interphase boundary is the turbulent boundary layer of liquid (thickness δ''). This region is characterized by irregular vortices. A strong interphase surface tension, however, tends to stabilize this surface somewhat and it determines the velocity profile here.

Considering that the thickness of this zone is small, we can accurately enough represent its velocity profile $u = u(\delta'')$ as

$$u = u' - \frac{u' - \bar{u}}{\delta''} y,$$

with u' denoting the velocity of the phases at their boundary.

The characteristics of the concentration profile across the liquid layer are also shown here (Fig. 1c).

In the diffusion boundary layer, whose thickness is δ_0', directly at the wall within the viscous sublayer ($y < \delta_0' < \delta'$) the turbulent fluctuations are so small that molecular diffusion becomes the governing mode of liquid mass transfer here. The concentration in this layer varies from a minimum value at a given cross section to the mean value $\bar{C}$ referred to the entire layer.

Turbulent fluctuations and intensive vortices within the turbulent mainstream equalize the concentration over a cross section of that region, and the differential equation of convective diffusion here becomes $C = \bar{C} = \text{const}$.

The basic variation in the absorbate concentration occurs within the effective liquid-diffusion boundary layer, whose thickness is δ_0''.

A qualitative analysis of the interaction between phases, based on the theory of the diffusion boundary layer [8] and taking into account the flow characteristics of a whirled two-phase stream [18], has shown that the thickness of this diffusion boundary layer here is a function of its hydrodynamic and physicochemical parameters. At the interphase boundary the concentration of liquid C^x is equal to its mean concentration in the gaseous phase at a given cross section. At the boundary with the turbulent mainstream, however, the concentration of liquid is equal to its mean concentration in the liquid phase.

Such a model describing the mechanism of interaction between the phases of a gas–liquid system in a whirled unidirectional flow can serve as the basis for an engineering design of a parallel-flow contact stage with a prescribed velocity profile the same as in the model.

It is necessary to determine the length of the parallel-flow contact stage, where the mean concentration of the liquid phase $\bar{C}$ varies from C_e to C_f and the stipulated proximity to equilibrium

$$\eta = \frac{\bar{C}_f - C_e}{C^x - \bar{C}_e}$$

is equal to η_f.

The differential equation of mass transfer can be written as

$$\frac{\partial C}{\partial t} + \operatorname{div}(C\bar{u}) - \operatorname{div}(D \operatorname{grad} C) = 0. \qquad (1)$$

TABLE 1. Experimental Data Pertaining to the Mass Transfer in a Whirled Two-Phase Stream (CO_2 absorption in water)

Helix pitch, mm	Mean axial velocity of gas, m/sec	Mean absolute velocity of gas, m/sec	$C_e \cdot 10^8$, g/mm³	$C_f \cdot 10^7$, g/mm³	$C^* \cdot 10^7$ g/mm³	L, mm	L_c (calc.), mm	η
28	17,80	53,3	0,60	0,381	0,5606	446,0	446,8	0,642
65	18,75	29,4	0,66	0,368	0,585	234,5	232,9	0,582

In order to solve this equation, one must consider the following simplifications, which are entirely justified in terms of our model: that the medium is incompressible, the flow is steady, the diffusivity is constant, and the longitudinal concentration gradient is negligibly smaller than the transverse concentration gradient. Then

$$u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial y^2}, \tag{2}$$

where u is the vector of absolute velocity:

$$u = u' - \frac{u' - \bar{u}}{\delta''} y. \tag{3}$$

The equation of steady-state mass transfer with the given velocity profile is

$$(a - by) \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial y^2}, \tag{4}$$

where $a = u'$, $b = (u' - \bar{u})/\delta''$, and the boundary conditions are

$$C = C_e \text{ for } x = 0, \tag{5}$$

$$C = C^* \text{ for } y = \delta,\ x > 0, \tag{6}$$

$$\partial C/\partial y = 0 \text{ for } y = 0. \tag{7}$$

It must be emphasized here that the y-axis is perpendicular to the vector of absolute velocity.

For a numerical solution of Eq. (4) we use the finite-differences scheme [26]:

$$\frac{\partial^2 C}{\partial y^2} \approx \frac{C(y_{f+1}, x) - 2C(y_f, x) + C(y_{f-1}, x)}{h^2}, \tag{8}$$

with $h = \delta''/(n + 1) = \delta''/4$ when $n = 3$.

Then Eq. (4) becomes

$$(a - by_f) \frac{\partial C(y_f, x)}{\partial x} = D \frac{C(y_{f+1}, x) - 2C(y_f, x) + C(y_{f-1}, x)}{h^2} \tag{9}$$

$$\text{for } x = 0 \quad C = C_e; \quad \text{for } y = 0 \quad \frac{C_{n+1} - C_n}{h} = 0, \tag{10}$$
$$\text{for } y = \delta \quad C = C^*,$$

where $y_k = \delta''(k-1)/(n + 1)$. Finally, system (9) becomes

$$\frac{dC_1}{dx} = \frac{1}{a - b\frac{\delta''}{4}} \left[D \frac{16}{(\delta'')^2} (C_2 - 2C_1 + C_0) \right],$$

$$\frac{dC_2}{dx} = \frac{1}{a - b\frac{\delta''}{2}} \left[D \frac{16}{(\delta'')^2} (C_3 - 2C_2 + C_1) \right], \tag{11}$$

$$\frac{dC_3}{dx} = \frac{1}{a - b\frac{3\delta}{4}} \left[D \frac{16}{(\delta'')^2} (C_4 - 2C_3 + C_2) \right].$$

System (11) with the boundary conditions (10) is solved numerically by the Euler method, according to which the computation step H is established on the basis of the equation

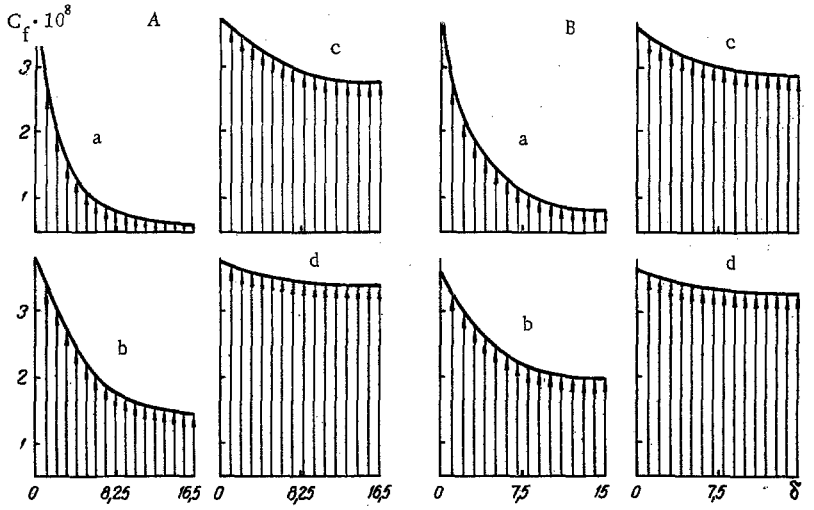

Fig. 2. Concentration distribution C(x, y) in the effective liquid-diffusion boundary layer along the height of a simulated contact stage. Simulation I (A): a) L = 20.99 mm; b) 104.99 mm; c) 446.99 mm. Simulation II (B): a) L = 20.99 mm; b) 83.99 mm; c) 232.99 mm. Concentration $C_f \cdot 10^8$ (g/mm^2), layer thickness δ (μ).

$$C_{i,f}(x_0 + H) = C_{i,f}(x, 0) + \frac{dC_{i,f}}{dx} H, \tag{12}$$

where H is the interval.

The algorithm for a numerical solution yields the concentration profile along the apparatus height, with a prescribed proximity to the equilibrium concentration at the interphase boundary C^x. Furthermore, one can determine with it the length of a parallel-flow contact stage and the optimum thickness of the effective liquid diffusion layer δ_0'' at the interphase boundary. On the basis of this algorithm, a program has been set up for the "Minsk-22" digital computer and numerical results are available. It is to be noted that questions concerning the evaluation of simulated experiments are of interest in their own right and are the subject of a separate article. Available calculations and results of computer experiments pertaining to the mass transfer in a two-phase stream whirled throughout the entire channel length yield an estimate of many important parameters characterizing the hydrodynamics and the mass transfer in such a stream. Using the data of a computer experiment ("Minsk-22" digital computer) shown in Table 1 as an example, the authors have calculated the mean flow velocity in the liquid layer and thus its mean thickness, also the thickness δ_0'' of the effective diffusion layer.

Such a calculation yielded an estimate of the basic parameters where a laboratory determination would have been extremely difficult. We obtained: a mean thickness of the liquid layer $\delta = 572\ \mu$ and a thickness of the liquid diffusion layer $\delta_0'' = 16.15\ \mu$ for the first simulated experiment, $\delta = 408.5\ \mu$ and $\delta_0'' = 15\ \mu$ for the second simulated experiment. In addition, this method has made it possible to plot curves representing the concentration of absorbed gas along the height of a contact stage.

NOTATION

δ	is the thickness of the liquid layer, μ;
δ_0''	is the thickness of the effective liquid-diffusion boundary layer, μ;
u	is the mean velocity, m/sec;
u'	is the mean velocity at the interphase boundary, m/sec;
$\overline{C}_f(x, y)$	is the mean (finite) concentration in the liquid phase, g/mm^3;
$\overline{C}_e(x, y)$	is the mean concentration in the liquid phase at the channel entrance, g/m^3;
$C^x(x, y)$	is the mean concentration of liquid at the interphase boundary, g/mm^3, in equilibrium with the mean concentration in the gaseous phase at a given cross section;
η	is the proximity to equilibrium;
D	is the diffusivity in the liquid phase, mm^2/sec.

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