## TWO-PHASE ABSORPTION COMPLICATED BY A SECOND-ORDER CHEMICAL REACTION IN THE LIQUID PHASE IN IRRIGATED CHANNELS (A SOLUTION FOR THE FIRST QUADRANT OF THE HYDRODYNAMIC PLANE. THEORY. CALCULATION)

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Two-phase film absorption complicated by an irreversible chemical reaction in the liquid is studied on the basis of a solution of diffusion transfer equations in the gas and liquid phases. The concentration distribution of the soluble component and the reaction product on the interface is studied theoretically. The dimensionless diffusion flow is calculated numerically as a function of the length of the channel with arbitrary controlling parameters.

Formulation of the Problem. The general formulation of the problem of two-phase chemisorption of carbon dioxide gas (A) by solutions of amines (B) is formulated in [1] at a carbonization  $\alpha \le 0.5$ . In this case the following reaction takes place in the liquid phase between the compound being dissolved (A = CO<sub>2</sub>) and the absorbent (B = RNH<sub>2</sub>):

$$A + B \Rightarrow C^{-} + H^{+}, \tag{1}$$

where  $H^+$  and  $C^-$  are ions of hydrogen and the bound state of A (RNHCOO<sup>-</sup>). A thin film (of thickness h) of absorbent solution (the inlet concentration is B<sub>0</sub>) flows down uniformly under gravity over the walls of a plane channel (of width 2R) in contact with the gas flowing down (the inlet concentration is  $C_0$ ). The practically important case B<sub>0</sub> >>  $KC_0$  (or  $N = B_0/KC_0 >> 1$ ), i.e., the chemical capacity of the absorbent is high, is considered. If it is taken into consideration that between the concentrations [B] and [C<sup>-</sup>] local chemical equilibrium exists ([B] = B<sub>0</sub> - [C<sup>-</sup>]), the two-phase problem of chemisorption can be reduced to two-phase absorption with nonlinear conditions of conjugation on the phase interface [1]:

$$U_{g}\frac{\partial C_{g}}{\partial x_{g}} = \frac{\partial^{2} C_{g}}{\partial y_{g}^{2}}, \quad U_{\text{liq}}\frac{\partial C_{\text{liq}}}{\partial x_{\text{liq}}} = \frac{\partial^{2} C_{\text{liq}}}{\partial y_{\text{liq}}^{2}}; \quad (2)$$

$$\left(\frac{\partial C}{\partial x_{\text{liq}}}\right)_{i} = P_{\text{liq}} \left(1 - C_{i}\right)^{1/2} \frac{\tanh\left[\sqrt{M}\left(1 - C_{i}\right)^{1/2}\right]}{\tanh\sqrt{M}} C_{g,i},$$

$$\left(\frac{\partial C_{g}}{\partial y_{g}}\right)_{i} = -P_{g} \left(1 - C_{i}\right)^{1/2} \frac{\tanh\left[\sqrt{M}\left(1 - C_{i}\right)^{1/2}\right]}{\tanh\sqrt{M}} C_{g,i}$$
(3)

at  $y_{g} = y_{hiq} = 1;$ 

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Fig. 1. Hydrodynamic planes X - Y and  $X_N - Y_N$ .

$$\frac{\partial C_g}{\partial y_g} = 0 \quad \text{at} \quad y_g = 0; \quad \frac{\partial C}{\partial y_{\text{liq}}} = 0 \quad \text{at} \quad y_{\text{liq}} = 0; \quad C_g = 1, \quad C = 0 \quad \text{at} \quad X = 0, \quad (4)$$

where  $\sqrt{M} = h\sqrt{kB_0/D_{\text{liq}}}$ ;  $P_{\text{liq}} = \sqrt{M} \tanh \sqrt{M}/N$ ;  $P_{\text{g}} = \epsilon\beta^2 \sqrt{M} \tanh \sqrt{M}$ .

The dimensionless coordinates  $y_g$ ,  $y_{liq}$ ,  $x_g$ ,  $x_{liq}$  are related to the Cartesian coordinates x and y by the formulas

$$y = (R - h) y_g = R - h y_{\text{liq}}, x = (h \text{ Pe}_{\text{liq}}) x_{\text{liq}} = (R \text{ Pe}_g) x_g$$

The dimensionless concentrations of CO<sub>2</sub> in the gas ( $C_g$ ) and of the reaction product RNHCOO<sup>-</sup> in the liquid (C) are determined as follows:

$$[A] = C_0 C_g(x_g, y_g), \quad [C^-] = \frac{B_0}{2} C(x_{liq}, y_{liq}).$$

The solution of problem (2)-(4) depends on the four dimensionless parameters  $\varepsilon$ ,  $\beta$ , N, M or any four independent combinations of them.

In what follows, parameters that contain phase velocities will be referred to as hydrodynamic (for example,  $\varepsilon$ ,  $\beta$ ) and parameters containing the reaction rate constant k are called chemisorption parameters (M,  $P_{g}$ ,  $P_{liq}$ ).

In [1, 2], in studies of two-phase chemisorption, it is recommended that the two hydrodynamic parameters  $(\varepsilon N)$  and  $(\varepsilon \beta N)$  be used (in physical meaning they are dimensionless capacities of the liquid [1]). For clear representation of the solution, the rectangular coordinate system  $X_N - Y_N$  was introduced (the hydrodynamic plane for chemisorption:  $X_N = \log (\varepsilon N)$ ,  $Y_N = -\log (\varepsilon \beta N)$ ). The linear relation  $X_N = X + \log N$ ,  $Y_N = Y - \log N$  exists between these two coordinates and the corresponding hydrodynamic coordinates for two-phase absorption X - Y [3] ( $X = \log \varepsilon$ ,  $Y = -\log \varepsilon \beta$ , where  $\varepsilon$  and  $\varepsilon \beta$  are capacities of the liquid phase in absorption). This means that the planes (X, Y) and ( $X_N$ ,  $Y_N$ ) are shifted by log N along the axes (see Fig. 1).

Earlier [1, 4], the solution was studied in the second and fourth quadrants of the hydrodynamic plane  $X_N - Y_N$ , i.e., at small ( $\epsilon N \le 1$ ,  $\epsilon \beta N \le 1$ ) and large ( $\epsilon N > 1$ ,  $\epsilon \beta N > 1$ ) capacities of the liquid.

In the present work a solution of (2)-(4) is obtained in the first quadrant, where the inequalities  $\epsilon N \ge 1$ ,  $\epsilon\beta N \le 1$  ( $X_N \ge 0$ ,  $Y_N \ge 0$ ) are satisfied. At any point of the hydrodynamic plane  $X_N - Y_N$ , two other parameters (they are chosen to be chemisorption ones) should "run through" all admissible values from zero to infinity. It is evident that the choice of chemisorption parameters is arbitrary; however, following [1, 4], the dimensionless thickness of the film  $\sqrt{M}$  (*M* is the Damköhler number) will be chosen as one of them. Studies carried out in the second and fourth quadrants of the hydrodynamic plane show that  $\sqrt{M}$  has a little effect on the solution. The establishment of one or another absorption regime (kinetic absorption, an instantaneous chemical reaction, resistance in either of the phases) in the two-phase system depends mainly on the other chemisoption parameter ( $\kappa$ ), which was called controlling. The form of this parameter depends on the quadrant of the hydrodynamic plane in which the considered point  $X_N$  and  $Y_N$  lies: for example, in the second quadrant  $\kappa = P_{liq}$  [1, 2], and in the fourth one  $\kappa = P_g$  [4, 5].

In what follows, from a theoretical study of the solution in different areas of the first quadrant, we find an expression for  $\kappa$  in this quadrant. Here, as the main calculated characteristic of chemisorption, we use the integral dimensionless flow expressed in terms of the concentration of CO<sub>2</sub> in the gas (1). This flow is related to the corresponding flow  $\Sigma$  expressed in terms of the concentrations in the liquid by the material-balance equation

$$I \equiv 1 - \int_{0}^{1} U_{g}C_{g}dy_{g} = \varepsilon N \int_{0}^{1} U_{liq}Cdy_{liq} \equiv \varepsilon N\Sigma.$$
<sup>(5)</sup>

We investigate the solution of general problem (2)-(4) at different points of the first quadrant where the solution is known or can be obtained analytically.

The Solution on the Axis  $Y_N (\epsilon N = 1, \epsilon \beta N \le 1)$  [2]. Since the positive axis  $Y_N$  belongs simultaneously to the first and second quadrants, on this axis the solution can be obtained as the particular case of the solution for the second quadrant at  $\epsilon N = 1$  [1]. Here,  $P_{\text{liq}}$  is the controlling parameter. As the longitudinal coordinate, we chose the dimensionless coordinate Z, which, in view of the equality  $\epsilon N = 1$ , is expressed as follows:

$$Z = \begin{cases} P_{\text{liq}} x_{\text{liq}} & \text{at } P_{\text{liq}} \leq 1 \\ P_{\text{liq}}^2 x_{\text{liq}} & \text{at } P_{\text{liq}} > 1 \end{cases} = \begin{cases} P_g x_g & \text{at } \kappa \leq 1, \\ P_{\text{liq}}^2 x_{\text{liq}} & \text{at } \kappa > 1, \end{cases}$$
(6)

where  $\kappa$  is the chemisorption parameter, determinmed from the formulas

$$\kappa \equiv \frac{P_{\text{liq}}}{\varepsilon N} = \frac{P_{g}}{(\varepsilon \beta N)^{2}}.$$
(7)

As was shown in [1], with a large chemical capacity of the absorbent (N >> 1), at a certain distance from the inlet to the channel, on the interface, the concentrations always satisfy the conditions  $C_{g,i} \simeq 1$ ,  $C_i << 1$ . This section of the channel was called the initial section of chemisorption. Here, the chemisorption resistance is concentrated in the liquid phase, and reaction (1) can be considered a chemical reaction of the pseudofirst order  $(B \simeq B_0)$ . The solution of this single-phase problem was found in [6]. In particular, for the dimensionless diffusion flow I(x), at  $x_{lig} >> 1/M$ , a linear relation was obtained, which is expressed in the adopted notation as

$$I \simeq (\varepsilon N) P_{\text{lig}} x_{\text{lig}} = P_{g} x_{g} .$$
<sup>(8)</sup>

This is the regime of a rapid chemical reaction with transfer resistance in the liquid phase. In the dimensionless coordinate Z of (6), relation (8) has the form

$$I = \begin{cases} Z & \text{at } \kappa \leq 1, \\ \frac{Z}{\kappa} & \text{at } \kappa > 1. \end{cases}$$
(9)

Formulas (9) are true until the inequality  $Z \ll 1$  is satisfied.

A monotonic increase in the concentration  $C_i(Z)$  from zero to unity in a section of dimensionless length  $Z \sim 1$  is a characteristic property of the solution of problem (2)-(4) on the vertical line  $X_N = 0$ . Outside this section (Z >> 1), when the concentration on the interface approaches saturation ( $C_i \Rightarrow 1$ ), the dimensionless flow I(Z) is determined analytically:

$$I \Rightarrow \varepsilon N \Sigma_{i} = \varepsilon N \left\{ 1 - \sum_{n=0}^{\infty} \frac{2}{\pi^{2} \left(n + \frac{1}{2}\right)^{2}} \exp \left[ -\pi^{2} \left(n + \frac{1}{2}\right)^{2} x_{\text{liq}} \right] \right\}.$$
 (10)

This means that in the system an instantaneous chemical reaction starts. Under this condition, at the interface the absorbent concentration is  $(B)_i \Rightarrow 0$  [7, 8]. Subsequently, this condition is preserved at any Z.

Thus, it is sufficient to obtain the solution of problem (2)-(4) only in the restricted range of the dimensionless length  $Z \sim 1$  in the so-called section of two-phase chemisorption. Outside this section (at small and large Z), the dimensionless flow I(x) is determined analytically from formulas (9) and (10), respectively. In the section of two-phase chemisorption, where in the general case diffusion interaction of both phases should be taken into consideration, the function I(Z) is formally a four-parameter function that depends on  $X_N$ ,  $Y_N$ ,  $\kappa$ , and  $\sqrt{M}$ . However, as was shown in [2], everywhere inside the second quadrant, for  $\Sigma(Z)$  (and, consequently, also for I(Z) on the axis  $Y_N \ge 0$ , where  $\varepsilon N = 1$ ), the number of controlling parameters can be decreased.

Indeed, at small  $\kappa$  (in practice, log  $\kappa \leq 1$ ), the function I(Z) is two-parameter, since it coincides with the solution of the ordinary differential equation

$$\frac{dI}{dZ} = \sqrt{\left(1 - \frac{I}{\epsilon N}\right)} \frac{\tanh\left(\sqrt{M} \sqrt{\left(1 - \frac{I}{\epsilon N}\right)}\right)}{\tanh\sqrt{M}} (1 - I), \quad I(0) = 0.$$
(11)

This solution is denoted subsequently by  $I_0(X_N, \sqrt{M}, Z)$ . On the axis  $Y_N \ge 0$ , it depends only on  $\sqrt{M}$ , and at large and small  $\sqrt{M}$  it can be obtained analytically [9]:

$$I_0(0, \sqrt{M}, Z) = \begin{cases} Z/(1+Z) & \text{at } \sqrt{M} \Rightarrow 0, \\ 1-1/\left(1+\frac{Z}{2}\right)^2 & \text{at } \sqrt{M} \Rightarrow \infty. \end{cases}$$
(12)

The difference between these limiting curves is within 10%. In view of the monotonic dependence of  $I_0$  on  $\sqrt{M}$ , it can be stated that on the axis  $Y_N$  the effect of the parameter  $\sqrt{M}$  on the solution is weak.

At moderate  $\kappa$  (parameters  $\log \kappa \ge -1$ ), the function I(Z) is three-parameter, depending only on  $X_N$ ,  $Y_N$ , and  $\kappa$ . This follows directly from the definition  $\kappa \equiv P_{\text{liq}} = (\sqrt{M} \tanh(\sqrt{M}))/N$  and the condition N >> 1. In this case, in the general formulation (2)-(4)  $\sqrt{M} \Rightarrow \infty$ ,  $\tanh[\sqrt{M}(1 - C_i)^{1/2}]/\tanh(\sqrt{M}) \cong 1$  can be assumed. The corresponding solution will be denoted subsequently by  $I(X_N, Y_N, \kappa, Z) \equiv I(X_N, Y_N, \infty, \kappa, Z)$ . Thus, at fixed  $X_N$ ,  $Y_N$ , it is sufficient to investigate the general problem only at  $\sqrt{M} \Rightarrow \infty$ .

At small  $\kappa$  the corresponding solution  $I(X_N, Y_N, \kappa, Z) \Rightarrow I_0(X_N, \infty, Z)$ , i.e.,  $I(X_N, Y_N, \kappa, Z)$  continuously transforms into  $I_0(X_N, \sqrt{M}, Z)$ . In [2], this characteristic of  $I(X_N, Y_N, \sqrt{M}, \kappa, Z)$  is called the property of "splitting."

The three-parameter function  $I(X_N, Y_N, \kappa, Z)$  admits substantial simplification not only at small but also at rather large  $\kappa$ . In this case, in the section of two-phase chemisorption  $(Z \sim 1)$  there are diffusion boundary layers in both phases, and the problem is reduced to a two-phase formulation:

$$U_{g} \frac{\partial C_{g}}{\partial Z} = \frac{\partial^{2} C_{g}}{\partial y_{g,i}}, \quad U_{liq} \frac{\partial C}{\partial Z} = \frac{\partial^{2} C}{\partial y_{liq,i}},$$

$$\frac{\partial C}{\partial y_{liq,i}} = (1 - C_{i})^{1/2} C_{g,i}, \quad \frac{\partial C_{g}}{\partial y_{g,i}} = -(\epsilon\beta N) \frac{\partial C}{\partial y_{liq,i}},$$
(13)

$$\frac{\partial C_g}{\partial y_{g,i}} = 0 \quad \text{at} \quad y_{g,i} = \infty , \quad \frac{\partial C}{\partial y_{\text{liq},i}} = 0 \quad \text{at} \quad y_{\text{liq},i} = \infty ,$$
$$C_g = 1 , \quad C = 0 \quad \text{at} \quad Z = 0 ,$$

where similarity variables are introduced in the transverse  $(y_{g,i} = \beta P_{liq}(1 - y_g), y_{liq,i} = P_{liq}(1 - y_{liq}))$  and longitudinal  $(Z = P_{liq}^2 x_{liq})$  directions.

The solution of problem (13) is denoted by  $I_{lim}$  and is represented in the form

$$I \simeq I_{\text{lim}} \equiv \frac{\epsilon N}{P_{\text{liq}}} \Sigma_{\text{lim}} (Y_N, Z) = \frac{1}{\kappa} \Sigma_{\text{lim}} (Y_N, Z) \quad (\kappa >> 1)$$
(14)

or

$$I\kappa = \Sigma_{\rm lim} \left( Y_N, Z \right), \tag{15}$$

where the function  $\Sigma_{\text{lim}}(Z) \equiv \int_{0}^{\infty} CU_{\text{liq}} dy_{\text{liq.i}}$  is the integral flow in the liquid and depends only on  $Y_N$ . At Z >> 1, the asymptotic value of this function is  $(2/\sqrt{\pi})\sqrt{Z}$ .

The Solution on the Axis  $X_N$  ( $\varepsilon N \ge 1$ ,  $\varepsilon \beta N = 1$  [5]. Since the positive axis  $X_N$  belongs simultaneously to the fourth and first quadrants, the solution on this axis can be obtained as the particular case of the solution for the fourth quadrant at  $Y_N = 0$  ( $\varepsilon \beta N = 1$ ) [5]. Here  $P_g$  is the controlling parameter, which at  $\varepsilon \beta N = 1$  coincides with  $\kappa$  determined from formulas (7). Accordingly, the coordinate Z introduced in terms of  $x_g$  and  $P_g$  for points of the fourth quadrant coincides with definition (6) (the second equalities) on the considered axis, since

$$Z = \begin{cases} x_g P_g & \text{at } P_g \le 1 \\ x_g P_g^2 & \text{at } P_g > 1 \end{cases} = \begin{cases} P_g x_g & \text{at } \kappa \le 1 , \\ P_g^2 x_{\text{liq}} & \text{at } \kappa > 1 . \end{cases}$$
(16)

It can easily be shown that in the initial chemisorption section  $(C_{g,i} \simeq 1, C_i \ll 1)$  the dimensionless flow I(Z) is the linear function (9).

A monotonic decrease in the surface concentration  $C_{g,i}(Z)$  from unity to zero in the section  $Z \sim 1$  is a characteristic property of the solution of general problem (2)-(4) on the horizontal line  $Y_N = 0$ . At Z >> 1, when  $C_{g,i} \Rightarrow 0$ , the problem becomes a single-phase one, and I(x) is determined analytically:

$$I \simeq I_{\infty}(x_{\rm g}) \equiv 1 - \sum_{n=0}^{\infty} \frac{2}{\pi^2 \left(n - \frac{1}{2}\right)^2} \exp\left[-\pi^2 \left(n + \frac{1}{2}\right)^2 x_{\rm g}\right].$$
 (17)

At these large Z transfer resistance is fully concentrated in the gas phase, and in the system maximum absorption of  $CO_2$  occurs. This condition is preserved subsequently at any x.

Just as on the axis  $Y_N \ge 0$ , in the region of transition from rapid reaction (8) to maximum absorption (17), i.e., in the section of two-phase chemisorption  $(Z \sim 1)$ , it is sufficient to study the solution of general problem (2)-(4) only for the case  $\sqrt{M} \Rightarrow \infty$ , since an effect of  $\sqrt{M}$  on I(Z) is observed only at small  $\kappa = P_g(\log \kappa \le -1)$ , when I(Z) coincides with the solution of two-parameter problem (11):  $I \simeq I_0(X_N, \sqrt{M}, Z)$ . In the general case, on the axis  $X_N \ge 0$  the effect of  $\sqrt{M}$  on this function is also weak and decreases monotonically as  $X_N$  increases. It is maximum (~10%) at  $X_N = 0$  (see (12)) and almost disappears at  $X_N \ge 0.5$ . In the latter case the following analytical formula is valid:

$$I_0 \simeq 1 - \exp\left(-Z\right),\tag{18}$$

which is independent of any parameter.

In the other limiting case, at rather large  $\kappa$ , in the section  $Z \sim 1$ , in both phases there are boundary layers, and, consequently, I(Z) can be obtained from simplified formulation (13), in which it is necessary to set  $\epsilon\beta N = 1$ . In this case I(Z) is proportional to  $\kappa$ , and the product  $\kappa I$  is independent of any parameter in (14). It should be noted that simultaneous satisfaction of the conditions  $C_{g,i} \Rightarrow 0$ ,  $C_i \Rightarrow 1$  at Z >> 1 is a characteristic property of the solution of (2)-(4) on the axis  $X_N$  ( $Y_N = 0$ ). This means that in the system a regime is developed that is simultaneously maximum absorption (17) and instantaneous chemical reaction (10). It can easily be shown that this occurs in the section Z >> 1,  $x_g << 1$ . For the two regimes the dimensionless flows coincide in this region:

$$I_0(x_g) = \frac{2}{\sqrt{\pi}} \sqrt{x_g} = \varepsilon N \frac{2}{\sqrt{\pi}} \sqrt{x_{\text{liq}}} .$$

However, unlike maximum absorption, instantaneous chemical reaction takes place only in the section Z >> 1,  $x_g << 1$ . As shown in [5], in the region  $x_g \ge 1$ , the gas phase is fully depleted  $(I_0 \simeq 1)$ , and the concentration  $C_i(x)$  deviates from unity.

The Solution of the Problem near the Origin of Coordinates  $(X_N = Y_N = 0)$ . In this area of the hydrodynamic plane, characteristics dimensions for the gas  $(RPe_g)$  and liquid  $(hPe_{liq})$  phases coincide  $(\varepsilon N \simeq \varepsilon \beta N \simeq \beta^2 \simeq 1)$ , and, consequently, the dimensionless lengths Z introduced for the second and fourth quadrants, respectively, also coincide (see (6) and (16)). At Z >> 1, the conditions  $C_i \Rightarrow 1$ ,  $C_{g,i} \Rightarrow 0$  are satisfied almost simultaneously, and therefore, in the system, chemisorption occurs, which can be considered both an instantaneous chemical reaction and maximum absorption. It is evident that in this case the equality  $I_0(x_g) \simeq \varepsilon N \Sigma_i(x_{liq})$  is valid and is not violated as the length of the channel increases further.

We investigate the solution of system (2)-(4) at interior points of the first quadrant, where the inequalities  $\epsilon N > 1$  and  $\epsilon \beta N < 1$  are satisfied.

The Solution at  $\beta^2 \ll 1$ . The relation  $\beta^2 = R \operatorname{Pe}_g / h \operatorname{Pe}_{liq}$  remains constant on inclined straight lines parallel to AC (Fig. 1). We obtain a series of analytical solutions on the straight lines  $\beta^2 = \operatorname{const} \ll 1$  for the following cases: a)  $x_g \ll 1$ ; b)  $x_g \gg 1$ ,  $x_{liq} \ll 1$ ; c)  $x_{liq} \gg 1$ .

It is evident that in case (a)  $x_g \ll 1$  (consequently,  $x_{liq} \ll 1$ ), there are boundary layers in both phases. In the initial section ( $C_{g,i} \simeq 1$ ,  $C_i \ll 1$ ), a solution of (2)-(4) exists in the form [1]

$$1 - C_g \simeq P_g (x_g)^{1/2} \frac{2}{\sqrt{\pi}} \left\{ \exp\left(-\eta_g^2/4\right) - \frac{\sqrt{\pi}}{2} \eta_g \operatorname{erfc}(\eta_g) \right] + \dots , \qquad (19)$$

$$C \simeq P_{\rm liq} \left( x_{\rm liq} \right)^{1/2} \frac{2}{\sqrt{\pi}} \left\{ \exp\left( -\eta_{\rm liq}^2/4 \right) - \frac{\sqrt{\pi}}{2} \eta_{\rm liq} \, {\rm erfc} \left( \eta_{\rm liq} \right) \right] + \dots , \qquad (20)$$

where  $\eta_g = (1 - y_g)/\sqrt{x_g}$ ,  $\eta_{liq} = (1 - y_{liq})/\sqrt{x_{liq}}$ . On the surface of the film at Z << 1

$$C_{g,i} \simeq 1 - P_g \frac{2}{\sqrt{\pi}} \sqrt{x_g} = 1 - (\epsilon \beta N) \frac{2}{\sqrt{\pi}} \sqrt{Z} ; \qquad (21)$$

$$C_{\rm i} \simeq P_{\rm liq} \frac{2}{\sqrt{\pi}} \sqrt{x_{\rm liq}} = \frac{2}{\sqrt{x}} \sqrt{Z} . \tag{22}$$

Here  $Z = P_{\text{liq}}^2 x_{\text{liq}}$ . Since  $C_i \le 1$ , from (22) it can be suggested that at  $Z \Rightarrow 1$  the concentration  $C_i \Rightarrow 1$ . In the latter case at Z >> 1 a solution of (2)-(4) exists in the form

$$1 - C_{g} = (\epsilon\beta N) \operatorname{erfc}(\eta_{g}), \quad C = \operatorname{erfc}(\eta_{\operatorname{liq}}), \quad (23)$$

and the concentrations on the interface are

$$C_{g,i} = 1 - \epsilon \beta N, \quad C_i = 1.$$
<sup>(24)</sup>

Formulas (23) and (24) are not asymptotic and are valid on a limited interval of length  $x_g \ll 1$ . Subsequently, at a distance from the inlet  $x_g \gg 1$ ,  $x_{lig} \ll 1$ , when the diffusion layer grows in the gas, the equality

 $C_g \simeq C_{g,i}(x)$  is satisfied in this region formulas (23), (24) for the gas phase become invalid. The concentration distribution in the gas can be obtained from material-balance equation (5):

$$C_{g,i} = 1 - \varepsilon N \frac{2}{\sqrt{\pi}} \sqrt{x_{\text{liq}}} \quad \text{at} \quad x_g \gg 1 , \quad x_{\text{liq}} \ll 1 .$$
(25)

It follows from (24) and (25) that in the gas phase, in the section  $x_g >> 1$ ,  $x_{liq} \le 1/(\epsilon N)^2 < 1$ , the concentration falls from an intermediate value  $(1 - \epsilon\beta N)$  to zero. Subsequently,  $1/(\epsilon N)^2 << x_{liq}$ , in view of the fact that the gas phase is fully depleted ( $C_g \Rightarrow 0$ ,  $I \Rightarrow 1$ ), and in the liquid the distribution C(x, y) is obtained from a simplified single-phase formulation:

$$U_{\text{liq}} \frac{\partial C}{\partial x_{\text{liq}}} = \frac{\partial^2 C}{\partial y_{\text{liq}}^2}, \quad \int_0^1 U_{\text{liq}} C \partial y_{\text{liq}}^2 = \frac{1}{\varepsilon N}.$$
 (26)

It can be verified that in the section  $x_{lig} \ll 1$  a solution of this problem exists in the form

$$C \simeq \frac{1}{\varepsilon N} \frac{1}{\sqrt{\pi}} \frac{\exp\left(-\eta_{\text{liq}}^2/4\right)}{\sqrt{x_{\text{liq}}}}, \quad C_{\text{i}} \simeq \frac{1}{\varepsilon N} \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{x_{\text{liq}}}}.$$
(27)

At  $x_{lin} >> 1$ , when the boundary layer grows in the liquid as well, the solution of (26) is trivial:

$$C_{\rm i} \simeq \frac{1}{\varepsilon N}$$
 (28)

We find necessary and sufficient conditions whose satisfaction ensures approximations (19)-(28). In view of the fact that the transition from a rapid reaction to an instantaneous one occurs at  $Z \sim 1$  ( $x_{liq} \sim 1/P_{liq}^2$ ) (see (21), (22)) and the transition to solutions (27) and (28) occurs at  $x_{liq} \sim 1/(\epsilon N)^2$ , it can be concluded that a necessary condition for the existence of the suggested mechanism of absorption is satisfaction of the inequality:

$$1/P_{\text{liq}}^2 \ll 1/(\varepsilon N)^2 \quad \text{or} \quad \kappa \gg 1.$$
<sup>(29)</sup>

It can easily be seen that the last condition is simultaneously sufficient. This will be shown for distances  $x_g >> 1$  from the inlet, since at  $x_g \le 1$ , the approximate equality  $C_i \simeq 1$  (Z >> 1) is unquestionable (see (24)). Integrating the transfer equation in the gas phase (2) with respect to  $y_g$  from zero to unity, we have

$$\left(\frac{\partial C_g}{\partial y_g}\right)_i \simeq \frac{\partial C_{g,i}}{\partial x_g} \text{ at } x_g >> 1$$

Substituting the above equality into boundary condition of conjugation (3), we obtain an equation for C(x):

$$-\frac{dC_{g,i}}{dx_g} / C_{g,i} = P_g \left(1 - C_i\right)^{1/2} \frac{\tanh\left[\sqrt{M} \left(1 - C_i\right)^{1/2}\right]}{\tanh\sqrt{M}},$$
(30)

where  $C_{g,i}(x)$  is determined from (25).

In the region Z >> 1 at  $\kappa >> 1$ , the approximate solution of Eq. (30) is equal to

$$1 - C_{\rm i} \simeq \frac{1}{\pi} \frac{1}{Z} \left/ \left( 1 - \varepsilon N \frac{2}{\sqrt{\pi}} \sqrt{x_{\rm liq}} \right)^2 \right.$$

It can be seen that  $C_i(x) \simeq 1$  almost everywhere at  $x_{liq} \leq (\pi/4)(\epsilon N)^2$ . A noticeable deviation of  $C_i$  from unity occurs only in the region  $x_{liq} >> 1/(\epsilon N)^2$  (see (27)).

We have proved that the mechanism of absorption suggested above really takes place at  $\kappa >> 1$  and that this condition in necessary and sufficient for its existence. As can be seen, at rather large  $\kappa >> 1$ , in the section of two-phase chemisorption ( $Z \Rightarrow 1$ ), the function I(Z) depends only on  $Y_N$  and  $\kappa$ . In the case in which boundary layers exist in both phases, the dimensionless coordinates  $Z = P_{liq}^2 x_{liq}$ ,  $y_{liq,i} = P_{liq}(1 - y_{liq})$ , and  $y_{g,i} = P_{liq}\beta(1 - y_g)$  can be introduced in (2)-(4). After that, we arrive at simplified formulation (13) and, consequently, at formula (15). Since at  $\kappa >> 1$ , in the section of two-phase chemisorption ( $Z \Rightarrow 1$ ) the inequality I << 1 is valid, this implies that the gas phase is mainly depleted at distances Z >> 1 from the inlet in the case of instantaneous chemical reaction (10).

The solution of general problem (2)-(4) will be studied at  $\beta^2 \ll 1$  and in the case of rather "weak" chemical interactions ( $\kappa \ll 1$ ). In this case substantial simplifications can also made. It can be assumed that at rather small  $\kappa \ll 1$ , in the initial section of chemisorption ( $C_{g,i} \simeq 1$ ,  $C_i \ll 1$ ), the inequality  $x_{\text{liq}} \gg 1/(\epsilon N)^2$  (or  $x_g \gg 1/(\epsilon N)^2 > 1$ ) is satisfied. This inequality implies that the boundary layer grows through the entire gas phase and, consequently,  $C_g \simeq C_{g,i}(x)$ . It is evident that in the initial section the concentration distribution is determined by formulas (20) and (22). Here, it is assumed that  $x_{\text{liq}} \ll 1$ . Taking (5) into consideration and introducing the dimensionless coordinate  $Z = P_g x_g$ , we obtain

$$C_{g,i} \simeq 1 - Z$$
,  $C_i \simeq \sqrt{\kappa} \frac{2}{\sqrt{\pi}} \sqrt{Z}$  at  $Z \gg 1$ ,  $x_{liq} < 1$ . (31)

If it is assumed that in the section  $Z \sim 1$  the gas phase is depleted almost completely  $(C_{g,i} \Rightarrow 0, I \Rightarrow 1)$ , then in the region Z >> 1, in the liquid, the concentration distribution can be obtained from simplified single-phase formulation (26). In particular, on the interface (see, (27), (28))

$$C_{i}(Z) = \begin{cases} \frac{1}{\epsilon N} \frac{1}{\sqrt{\pi}} \frac{1}{x_{\text{liq}}} = \sqrt{x} \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{Z}} & \text{at } Z \gg 1, \quad x_{\text{liq}} < 1, \\ \frac{1}{\epsilon N} & \text{at } x_{\text{liq}} \gg 1. \end{cases}$$
(32)

As can be seen from formulas (31) and (32), at  $Z \simeq 1$ , on the curve  $C_i(Z)$  a maximum with order of magnitude  $1 > C_{i,max} \simeq \sqrt{\kappa} \ge 1/\epsilon N$  is observed. This means that with rather weak chemical interactions instantaneous chemical reactions ( $C_i \sim 1$ ) are not observed at any lengths of the channel. Since  $1/\epsilon N$  is an asymptote for  $C_i(x)$ , and at  $\kappa > 1$  the equality  $C_{i,max} \simeq 1$  holds, it can be assumed that the condition  $\sqrt{\kappa} > 1/\epsilon N$ is sufficient for the existence of a maximum on the curve  $C_i(x)$ . If the reverse inequality  $\sqrt{\kappa} < 1/\epsilon N$  is satisfied, the maximum disappears from this curve and the surface concentration becomes a monotonically increasing function of Z. In this case it can easily be shown that in the section of two-phase chemisorption, boundary layers completely occupy both phases, the flow I(Z) satisfies problem (11), and the following equalities are satisfied:

$$C_{i} \simeq I_{0}(Z, X_{N}, \sqrt{M})/\varepsilon N, \quad C_{g,i} \simeq 1 - I_{0}(X_{N}, \sqrt{M}, Z)$$

In this case the chemical reaction has the same rate throughout the entire thickness of the film (the kinetic regime).

It should be noted that at  $\kappa \ll 1$ , the equality  $I \simeq I_0(X_N, \sqrt{M}, Z)$  is always true, irrespective of the presence of a maximum on the curve  $C_i(Z)$ .

The foregoing analysis suggests that on the straight lines  $\beta^2 = \text{const} \ll 1$  (just as on the vertical  $Y_N \ge 0$  and horizontal  $X_N \ge 0$  lines) the dimensionless complex  $\kappa$  has all the properties of a controlling parameter. The type of absorption regime that will be established in the two-phase system depends on its value, and the effect of the second chemisorption parameter  $\sqrt{M}$  can be virtually neglected.

Summarizing the foregoing theoretical study, it can be suggested that irrespective of  $\kappa$ , beyond the section of chemisorption (Z >> 1), inside the first quadrant the dimensionless flow I(Z) is determined analytically, and

$$I(Z) \Rightarrow \min \left\{ \varepsilon N \Sigma_{i}(x_{\text{liq}}), I_{\infty}(x_{g}) \right\} \text{ at } Z >> 1.$$
 (33)

The above relation answers the question about the possibility of realization of an instantaneous chemical reaction. It is evident that this regime occurs only for rather strong chemical interactions  $(\kappa >> 1)$  at distances Z >> 1 from the inlet. It should be emphasized that it is preserved almost until complete depletion of the gas phase:  $I \simeq \epsilon N \Sigma_i \leq 1$ . In particular, at the boundary between the first and second quadrants  $(X_N = 0)$ , irrespective of x, the inequality  $\epsilon N \Sigma_i \leq I_{\infty}$  is satisfied, and consequently,  $I \Rightarrow \epsilon N \Sigma_i (x_{liq})$  if Z >> 1. This is reasonable since this transition is observed everywhere inside the second quadrant [1] and, consequently, for points on its boundary.

Accordingly, at  $Y_N = 0$  the reverse inequality  $I_{\infty} \leq \epsilon N \Sigma_i$  is satisfied, and consequently,  $I \Rightarrow I_{\infty}(x_g)$  if Z >> 1. This transition is typical of the whole interior of the fourth quadrant [5].

In a numerical investigation of problem (2)-(4), in the section of two-phase chemisorption  $(Z \simeq 1)$ , it is sufficient to consider only the case  $\sqrt{M} \Rightarrow \infty$ , i.e., to obtain a solution of just the three-parameter problem  $I(X_N, Y_N, \kappa, Z)$ . The effect of the parameter  $\sqrt{M}$  is observed only at  $\kappa << 1$  (in practice, at log  $\kappa \le -1$ ), where  $I(X_N, Y_N, \kappa, \sqrt{M}, Z) \simeq I_0(X_N, \sqrt{M}, Z)$ . This follows directly from the last equality and definition (7) of  $\kappa$  expressed in the form  $\sqrt{M}$  tanh  $\sqrt{M} = N\epsilon N\kappa$ . This property of the solution of (2)-(4) was called the property of "splitting" [1, 4].

Numerical Approximation of the Two-Parameter Problem (11). Equation (11) was integrated by the Runge-Kutta numerical method in [5] for the following ranges of the controlling parameters:  $-0.4 \le \log \sqrt{M} \le 0.6$ ,  $0 \le X_N \le 0.5$ . The results of the calculations were presented in the form of the following approximating formula:

$$I_0(X_N, \sqrt{M}, Z) = I_0(X_N, 0, Z) + (\log \sqrt{M} + 0.4) [I_0(X_N, \infty, Z) - I_0(X_N, 0, Z)]$$
  
at  $-0.4 \le \log \sqrt{M} \le 0.6$ , (34)

where the analytical expressions for the corresponding flows for large  $(\sqrt{M} \Rightarrow \infty)$  and small  $(\sqrt{M} \Rightarrow 0) \sqrt{M}$  values of are equal to [9]

$$\left(1 - \frac{I_0}{\varepsilon N}\right)^{1/2} = \left(1 - \frac{1}{\varepsilon N}\right)^{1/2} \frac{1 + \varepsilon N \left[1 - (1 - 1/\varepsilon N)^{1/2}\right]^2 \exp\left[-(1 - 1/\varepsilon N)^{1/2}Z\right]}{1 - \varepsilon N \left[1 - (1 - 1/\varepsilon N)^{1/2}\right]^2 \exp\left[-(1 - 1/\varepsilon N)^{1/2}Z\right]}$$
at  $\sqrt{M} \Rightarrow \infty$ .
(35)

$$I_{0}(X, 0, Z) = \frac{1 - \exp\left[-\left(\frac{\varepsilon N - 1}{\varepsilon N}\right) Z\right]}{1 - \exp\left[-\left(\frac{\varepsilon N - 1}{\varepsilon N}\right) Z\right] / \varepsilon N} \quad \text{at} \quad \sqrt{M} \Rightarrow 0.$$
(36)

In spite of the fact that the above formulas seem bulky, the difference between them is not large: it is maximum  $(\Rightarrow 10\%)$  at  $X_N = 0$  (see (12)) and decreases monotonically as this parameter grows. At  $X_N \ge 0.5$  this difference almost disappears, and formula (18) is valid. A check shows that at  $\log \sqrt{M} \le -0.4$ , the relation  $I_0 \Rightarrow I_0(X_N, 0, Z)$  holds, and at  $\log \sqrt{M} \ge 0.6$ , the relation  $I_0 \Rightarrow I_0(X_N, \infty, Z)$  is valid.

A Numerical Study of the Three-Parameter Problem ( $\sqrt{M} \Rightarrow \infty$ ). The dimensionless flow  $I(X_N, Y_N, \kappa, Z)$  was calculated at discrete points of the first quadrant  $0 \le X_N \le 1$ ,  $0 \le Y_N \le 1$  ( $\Delta X_N = \Delta X_N = 0.125$ ) by the method described in [1]. The solutions obtained are almost the same as the corresponding ones for the fourth quadrant [3]: results of calculations of I(Z) at any fixed point of the hydrodynamic plane will be expressed in the form of one-parameter curves (the parameter  $\kappa$ ). Here, it is necessary to distinguish between the cases of "large" (log  $\kappa \ge 0$ ) and "small" chemical interactions (log  $\kappa \le 0$ ). In the first case the logarithm of the product log ( $\kappa I$ ) of (14) is plotted on the ordinate, and in the second, log I(Z). The abscissa is log Z.

In the case of "large" chemical interactions (log  $\kappa \ge 0$ ) the calculations show that the effect of  $X_N$  and  $Y_N$  on  $\kappa I(Z)$  is not very strong and in the general case it is monotonic, because of which it was possible, just as in [5],



Fig. 2. Numerical calculation of the dimensionless flow at  $\log \kappa \ge 0$  on the horizontal lines  $Y_N = 0$  (a), 0.25 (b), 0.5 (c),  $\ge 1$  (d): even curves are  $X_N = 0$ , odd curves are  $X_N = 0.25$ ; 1, 2)  $\log \kappa = 0$ ; 3, 4) 0.2; 5, 6) 0.4; 7, 8) >0.6; inclined lines I and II are asymptotic relations (9) and (15), respectively.

to present clearly the functions log ( $\kappa I$ ) at constant  $Y_N$  in separate figures. For  $Y_N = 0$ , 0.25, 0.5, 1 this shown in Fig. 2.

As can be seen, all the curves  $\log (\kappa I)$  are monotonically increasing relative to  $\log Z$ , whose asymptotic values are known: if  $\log Z \le -1$ , then  $\kappa I \simeq Z$  (curves I); if  $\log Z \ge \log (P_{liq}^2 / \epsilon N) \simeq 2\kappa$ , then  $\kappa I \Rightarrow \kappa$ , since at  $x_{liq} \ge -1/(\epsilon N)^2$  the function  $I \Rightarrow 1$  (25). Moreover, at rather small Z ( $\log Z \le \log Z^*$ ), the dependences  $\kappa I \Rightarrow \sum_{lim} (Y_N, Z)$  (curves 8 in Fig. 2), i.e., in accordance with the general theory we arrive at approximation (14), when it is possible to assume that boundary layers exist in both phases. The value  $Z^*$  at which this transition occurs depends mainly on  $\kappa$  and increases monotonically with this parameter. In the case of rather intense chemical interactions (in practice, at  $\log \kappa \ge 1$ ), in the entire section of two-phase chemisorption  $-1 \le \log Z \le 1.5$ , the equality  $\kappa I \simeq \sum_i (Y_N, Z)$  is satisfied, and consequently, numerical calculations are not needed since at  $\log Z \le 1.5$  curves 8 can be used, and at  $\log Z \ge 1.5$  the approximation  $\sum_i \Rightarrow (2/\sqrt{\pi})\sqrt{Z}$  always holds (curves II in Fig. 2), i.e., in accordance with the general theory I  $\Rightarrow \epsilon N \sum_i (x_{iiq})$  (10). This regime is an instantaneous chemical reaction.

We study the effect of the hydrodynamic parameter  $Y_N$  on the solution  $I(X_N, Y_N, \kappa, Z)$  at log  $\kappa > 0$ . Numerical calculations show that it occurs only at  $Y_N \le 1$ . At rather large  $Y_N$ , in formulation (2)-(4), assuming formally  $\epsilon N\beta \Rightarrow 0$ , we can neglect transverse changes in the concentration in the gas phase, since the concentration  $C_{g,i}$  starts to deviate from unity at distances  $x_g >> 1$  from the inlet (see, for example (21), (24), and (25)). As a result, system (2)-(4) is reduced to a single-phase problem:

$$U_{\rm liq} \frac{\partial C}{\partial x_{\rm liq}} = \frac{\partial^2 C}{\partial y_{\rm liq}^2}.$$
 (37)

$$\left(\frac{\partial C}{\partial y_{\text{liq}}}\right)_{i} = P_{\text{liq}} \left(1 - C_{i}\right)^{1/2} C_{g,i} (x) \text{ at } y_{\text{liq}} = 1,$$

$$\frac{\partial C}{\partial y_{\text{liq}}} = 0 \text{ at } y_{\text{liq}} = 0, \quad C = 0 \text{ at } x_{\text{liq}} = 0,$$
(38)

where  $C_{g,i} = 1 - \epsilon N \Sigma(x_{liq})$ . With account for definitions (16) and (7) for Z and  $\kappa$ , it can easily be seen that at rather large  $\epsilon \beta N >> 1$ , the dimensionless flow I(Z) actually depends on just one hydrodynamic parameter  $X_N$ . Calculations show that everywhere above the horizontal line AB the plots shown in Fig. 2d can be used. Analysis of the curves presented in Fig. 2 shows that in the range  $0 \le Y_N \le 1$ , the effect of  $Y_N$  on the solution is not very strong, and with high accuracy a linear approximation can be used for intermediate  $Y_N$ . As regards the effect of the second hydrodynamic parameter  $X_N$  on the solution at  $\log \kappa \ge 0$ , it can easily be seen from Fig. 2 that it is observed in practice only in the narrow band  $0 \le X_N \le 0.25$ . In the general case it can be assumed that the effect is also linear and the approximating formula

$$\log [\kappa I (X_N, Y_N, \kappa, Z)] = \log [\kappa I (0, Y_N, \kappa, Z)] + 4X_N \{ \log [\kappa I (0.25, Y_N, \kappa, Z)] - \log [\kappa I (0, Y_N, \kappa, Z)] \} \text{ at } 0 \le X_N \le 0.25$$
(39)

is valid.

At any fixed  $Y_N$  and  $\kappa$ , in the range  $X_N \ge 0.25$  the function  $I(X_N, Y_N, \kappa, Z)$  ceases to depend on  $X_N$  and coincides with  $I(\infty, Y_N, \kappa, Z)$  (curves 1, 3, 5, 7 in Fig. 2). Such solutions that do not depend on  $X_N$  were denoted by  $I_Y(\kappa, Y_N, Z)$  in [4]. Just as in the cited work, it can be easily shown that this function is a solution of the simplified diffusion formulation depending only on  $Y_N$  and  $\kappa$  and obtained from (2)-(4) formally at  $\epsilon N \Rightarrow \infty$ .

The domain of definition of the function  $I_Y(Z)$  depends mainly on  $\kappa$ . For example, as was noted above, at log  $\kappa \ge 0$ , this is the half-band  $X_N \ge 0.25$ . At rather small  $\kappa$  (in practice, log  $\kappa \le -1$ ), when in accordance with theoretical results (11) the approximation  $I(X_N, Y_N, \kappa, Z) \simeq I_0(X_N, \infty, Z)$  is valid, the domain of definition of  $I_Y$  is  $X_N \ge 0.5$  (see (18) and (34)), i.e., it can be assumed that as  $\kappa$  decreases, the domain of definition of  $I_Y(Y_N, \kappa, Z)$  is narrowed in the general case. However, it can easily be seen that the maximum difference between the functions log  $[\kappa I(\kappa, 0.25, Y_N, Z)]$  and log  $[\kappa I(\kappa, 0, Y_N, Z)$  is not very large (less that 10%), so that at log  $\kappa \ge 0$ , everywhere inside the first quadrant  $I \simeq I_Y$  (curves 1, 3, 5, 7 in Fig. 2) can be assumed in practical calculations, i.e., the effect of  $X_N$  on the solution can be neglected.

As concerns "small" chemical interactions (log  $\kappa \le 0$ ), just as was shown in [2, 4] for the second and fourth quadrants, in this case numerical calculations are absolutely unnecessary, since at any point of the hydrodynamic plane  $X_N$ ,  $Y_N$ , I(Z) can be expressed with sufficient accuracy in terms of the corresponding functions for two values of the chemisorption parameter  $\kappa$ : log  $\kappa = 0$  and log  $\kappa = -1$  by means of the approximation formula

$$\log I(\kappa, X_N, Y_N, Z) = \log I(1, X_N, Y_N, Z) + (\log \kappa) [\log I_0(X_N, Z) - \log I(1, X_N, Y_N, Z)] \quad \text{at} \quad -1 \le \log \kappa \le 0,$$
(40)

where  $I(1, X_N, Y_N, Z)$  is the target function at  $\log \kappa = 0$  (for example, for  $X_N = 0$  and 0.25, curves 1 and 2 in Fig. 2). At fixed  $Y_N$ , for any  $X_N$  these dependences can be determined from formula (39) if  $0 \le X_N \le 0.25$ , while if  $X_N \ge 0.25$ , then  $I(1, X_N, Y_N, Z) \simeq I(1, \infty, Z) = I_0$  (the odd curves in Fig. 2). As was noted above, in practice, the dependence on  $X_N$  can be neglected and the last equality can always be used. As an example, in Fig. 3 one can see typical calculations of  $I(\kappa, X_N, Y_N, Z)$  at the central point  $X_N = Y_N = 0$ . As can be seen, at  $-1 \le \log \kappa \le 0$ , the effect of  $\log \kappa$  on the solution is almost linear, and at rather small  $\log \kappa \le -1$  the dimensionless flow coincides with the two-parameter function  $I_0(X_N, Z)$  (curve 3). The absolute error in calculation of  $I(x, X_N, Y_N, Z) \simeq I_Y$  is usually within 0.02.



Fig. 3. Numerical calculation of the dimensionless flow at log  $\kappa \le 0$  at the point  $X_N = 0$ ,  $Y_N = 0$ : 1) log  $\kappa = 0$ , 2) -0.4, 3) log  $\kappa \le -1$ ; inclined straight line I is asymptotic relation (9).

Conclusions. A theoretical and numerical study of two-phase chemisorption was carried out in the first quadrant of the hydrodynamic plane  $(X_N \ge 0, Y_N \ge 0)$  at large chemical capacities of the liquid phase (N >> 1). The features of absorption were found for this region.

It is shown that the occurrence of one or another regime in the system that is, as a rule, known from the literature depends mainly on two criteria: the dimensionless length of the nozzle device Z of (6) and the chemisorption parameter  $\kappa$  of (7).

In particular, at small Z (log  $Z \le -1$ ) chemisorption resistance is fully controlled by the liquid phase ( $C_{g,i} \ge 1$ ), and the concentration of the absorbent is [B]  $\ge B_0$ . The latter means that these "short" channels are characterized by a chemical reaction of the pseudofirst order. A general study of this problem (at arbitrary x) was carried out in [6]. For the particular case  $\sqrt{M} >> 1$  an analytical solution is known [10].

In the other extreme case (where  $\log Z \ge 1$ ), solution of the problem of chemisorption in two-phase formulation (2)-(4) is unnecessary, since the dimensionless flow I(x) is determined analytically by (33). It can be stated that in a sense at large Z the solution in the first quadrant takes an "intermediate" position between the corresponding solutions for the second [1, 2] and fourth [4, 5] quadrants. It should be remembered that in the second quadrant at Z >> 1 the transition  $I \Rightarrow \epsilon N \Sigma_i(x_{liq})$  occurs (an instantaneous chemical reaction) and in the fourth quadrant the transition  $I \Rightarrow I_{\infty}(x_g)$  takes place (maximum absorption, transfer resistance is concentrated in the gas). Both transitions occurred irrespective of the valve of the controlling parameter  $\kappa$ .

In the region considered (the first quadrant) one or another transition is observed, depending on the value of  $\kappa$ : at log  $\kappa \ge 0$  the flow  $I \Rightarrow \epsilon N \Sigma_i(x_{\text{lig}})$ , while at log  $\kappa \le 0$ ,  $I \Rightarrow I_0(x_g)$ .

Thus, it is sufficient to carry out numerical studies of two-phase chemisorption for the limited range  $-1 \le \log Z \le 1$  in the so-called section of two-phase chemisorption. Diffusion interaction takes place only in this region, i.e., on the phase interface the concentrations  $C_{g,i}$  or  $C_i$  cannot be constant. As follows from general formulation (2)-(4), formally, the target function, which is equal to I(Z) if  $\log \kappa \le 0$  and to  $\kappa I(Z)$  if  $\log \kappa \ge 0$ , depends on the four dimensionless parameters  $X_N$ ,  $Y_N$ ,  $\kappa$ ,  $\sqrt{M}$ ; however, as was shown by the foregoing theoretical studies and numerical calculations, depending on the concrete values of these parameters, substantial simplifications can be made, which consist in the following:

1. The effect of the hydrodynamic parameter  $Y_N$  is not very strong and is observed only in the limited range  $0 \le Y_N \le 1$ . Above the horizontal line AB (Fig. 1), one can use the limiting solution  $I_X(X_N, \kappa, Z)$  (see (37), (38)): the plots in Fig. 2d if  $\log \kappa \ge 0$ , or formula (40) if  $\log \kappa \le 0$ .

2. In the general case the second hydrodynamic parameter  $X_N$  has an effect in the limited range  $0 \le X_N \le X_{NY}$ . Its width  $(X_{NY})$  depends mainly on the chemisorption parameter  $\kappa$ : at log  $\kappa \ge 0$ ,  $X_{NY} \simeq 0.25$  (see Fig. 2), and as  $\kappa$  decreases (in the range log  $\kappa \le 0$ )  $X_{NY}$  increases monotonically, reaching its maximum  $X_{NY} = 0.5$  at log  $\kappa \le -1$  (see (18), (34)).

3. The chemisorption parameter  $\kappa$  exerts the main effect on the dimensionless flow I(Z). At rather high values of it (in practice, at log  $\kappa \ge 1$ ),  $\kappa I \simeq \Sigma_{\text{lim}}(Y_N, \kappa, Z)$  (curves 8 in Fig. 2, formula (15)). In the range

 $0 \le \log \kappa \le 1$ , the plots shown in Fig. 2 can be used with the help, if necessary, of linear approximations in  $\log \kappa$ ,  $Y_N$ , and  $X_N$ . It should be noted that for most technological calculations the effect of the hydrodynamic parameter  $X_N$  can be neglected in the region  $\log \kappa \ge 0$ , i.e., approximation (39) is practically the same as  $I_Y(\kappa, Y_N, Z)$ . In the case of "weak" chemical interactions (in practice,  $\log \kappa \le 0$ ), in the general case  $X_N$  cannot be neglected; however, in this region numerical calculations are unnecessary since I(Z) can be obtained from the approximating formula (40) if  $-1 \le \log \kappa \le 0$ , and  $I(Z) \simeq I_0(X_N, \sqrt{M}, Z)$  if  $\log \kappa \le -1$  (see (34)). It should be noted that due to the property of "splitting" of problem (2)-(4) the effect of the second chemisorption parameter  $\sqrt{M}$  is observed only at rather small  $\kappa$  ( $\log \kappa \le -1$ ), when the solution is practically independent of  $Y_N$  ( $I \simeq I_0(X_N, \sqrt{M}, Z)$ ).

The foregoing results allow one to obtain quite easily a solution of two-phase problem (2)-(4) at arbitrary physicochemical, geometric, and hydrodynamic parameters, without computer calculations. The only limitation is that the parameters  $X_N$  and  $Y_N$  be within the first quadrant of the hydrodynamic plane.

## NOTATION

[A], [B], [C<sup>-</sup>], concentrations of the absorbed component in the gas, absorbent, and product of reaction (1) in the liquid, mole/liter; D, diffusion coefficient, m<sup>2</sup>/sec; K, coefficient of distribution of material A; k, directreaction constant, liter/(mole sec); l, length of the channel, m; U', phase velocity, m/sec;  $\overline{U}$ , average phase velocity, m/sec;  $U = U'/\overline{U}$ , dimensionless phase velocity;  $Pe_g = R\overline{U}_g/D_g$ ,  $Pe_{liq} = h\overline{U}_{liq}/D_{liq}$ , Peclet numbers for the

gas and the liquid;  $\epsilon = h \overline{U}_{liq} K / R \overline{U}_g$ ,  $\beta^2 = R P e_g / h P e_{liq}$ , dimensionless parameters;  $I = 1 - \int_0^1 U_g C_g dy_g$ ,  $\Sigma = 0$ 

 $\int U_{\text{liq}}Cdy_{\text{liq}}, \text{ dimensionless integral flows of materials; tanh (x), hyperbolic tangent; erfc (x), error function; <math>\Sigma_i$ ,

 $I_{\infty}$ , dimensionless flows in the case of transfer resistance in the liquid and the gas, respectively (formulas (10) and (17)). Subscripts: g, gas; liq, liquid; 0, value at the inlet; i, interface; lim, limiting.

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