

# MASS TRANSFER ACCOMPANIED BY CHEMICAL CONVERSION OF SUBSTANCE IN A DROP

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**Abstract**—An investigation is carried out between a spherical drop moving at  $Re < 1$  and a continuous medium with an irreversible second-order chemical reaction inside a drop.

Solutions of transfer equations are presented both for finite values of a chemical reaction rate constant with the limiting resistance of a dispersed phase and for a fast reaction with comparable phase resistances.

Numerical results are reported for mean concentrations of reactants, extraction degree and flow in dependence on dimensionless time of phase contact and problem parameters.

## NOMENCLATURE

$r$ ,	radial coordinate;
$\theta$ ,	polar angle;
$t$ ,	time;
$V_r, V_\theta$ ,	radial and tangential velocity
$c$ ,	components of liquid;
$R$ ,	radius of drop;
$U$ ,	steady velocity of drop;
$\mu = \mu_d/\mu_c$ ,	ratio of viscosities of dispersed and continuous phases;
$\rho$ ,	density;
$D$ ,	diffusivity;
$c$ ,	concentration;
$C_{10}, C_{20}$ ,	initial concentrations of surface extractant and chemisorbent inside a drop, respectively;
$Q$ ,	extractant flow;
$C_1 = c_1/C_{10}$ ,	dimensionless concentrations;
$C_2 = c_2/C_{20}$ ,	
$K$ ,	chemical second-order reaction rate constant;
$K = kR^2C_{20}/D_1$ ,	dimensionless constant of chemical reaction rate;
$m = C_{20}/C_{10}$ ;	
$n = D_2/D_1$ ;	
$\beta = D_1\psi/K_c d$ ,	where $K_c$ is mean mass-transfer coefficient for continuous phase; drop diameter;
$\psi = C_{10}/Y_0$ ,	distribution coefficient;
$Y_0$ ,	constant over height concentration of extractant in a continuous phase;
$Re = Ud\rho_c/\mu_c$ ,	Reynolds number;
$\tau = D_1 t/R^2$ ,	Fourier number (dimensionless time of phase contact);
$Pe = Ud/D_1$ ,	Peclet number;
$Pe' = Pe/4(1 + \mu)$ .	

## Subscripts

1,	extractant;
2,	chemisorbent;
$d$ ,	dispersed phase;
$c$ ,	continuous phase.

## INTRODUCTION

TRANSFER of a substance from one phase to another involving chemical reactions is one of the widespread phenomena in chemical engineering. A study of this problem extended to disperse systems of moving spherical particles is of great practical interest. Such investigations are of importance for optimization of engineering processes and prediction of chemical column-type reactors, one of the contacting phases disperses in another. When solving these problems a knowledge of the interaction mechanism of an individual chemically-reacting particle with a flow is of particular importance. Some aspects of this problem will be considered for mass transfer accompanied with an irreversible second-order chemical reaction inside a moving spherical drop.

Mass-transfer equations for a particle in an axisymmetric flow involving an irreversible chemical reaction for each of the reactants may be written in the form

$$\frac{\partial C_i}{\partial t} + V_r \frac{\partial C_i}{\partial r} + \theta \frac{V_\theta}{r} \frac{\partial C_i}{\partial \theta} = D_i \Delta C_i + q_i \quad (1)$$

where  $q_i$  characterizes a contribution of a chemical reaction to a transfer process.

Mass transfer between a moving particle and a continuous flow, complicated with a chemical reaction, is usually considered for cases when a reaction proceeds in one of the phases limiting a transfer process.

Mass transfer with a chemical reaction in a medium around a single sphere was investigated in [1] for a first-order reaction by solving steady-state equation (1) at small and great  $Re$  values with the aid of analytical and finite-difference methods. In [2] unsteady-state equation (1) is solved for  $Pe \gg 1$ , using the diffusional boundary layer method. For a second-order reaction a numerical solution of transfer equations is obtained in [3] for finite  $Pe$  and  $K$  values, and in [4] a fast reaction is considered for great  $Pe$  values in the diffusional boundary layer approximation.

Mass transfer involving a chemical reaction inside a drop was investigated in [5]–[7] for different cases of a first-order reaction and in [8, 9] for a second-order reaction at finite values of  $K$  and  $Pe$ .

The present paper deals with mass transfer accompanied by an irreversible second-order chemical reaction in a drop both for finite  $Pe$  and  $K$  at limiting resistance of a dispersed phase and for comparable phase resistances and large  $Pe$  in the presence of a fast reaction.

#### MASS TRANSFER AT FINITE $K$ AND $Pe$ VALUES

Consider the problem of mass transfer between a moving spherical drop and a continuous flow when a substance (an extractant) diffusing into a drop enters into a chemical second-order reaction with a reagent (chemisorbent) dissolved inside a drop. At the initial time instant concentrations of extractant and chemisorbent in a drop equal 0 and  $C_{20}$ , respectively. A chemisorbent flow through a drop surface is assumed absent during a mass-transfer process. For the limiting resistance of a dispersed phase such a problem may be reduced to a system of equations in terms of dimensionless values

$$\frac{\partial C_1}{\partial \tau} + Pe' \left( V_r \frac{\partial C_1}{\partial r} + \frac{V_\theta}{r} \frac{\partial C_1}{\partial \theta} \right) = \Delta C_1 - KC_1 C_2 \quad (2)$$

$$\frac{\partial C_2}{\partial \tau} + Pe' \left( V_r \frac{\partial C_2}{\partial r} + \frac{V_\theta}{r} \frac{\partial C_2}{\partial \theta} \right) = n\Delta C_2 - \frac{K}{m} C_1 C_2 \quad (3)$$

with boundary and initial conditions

$$C_1 \Big|_{r=0} \neq \infty; \quad C_2 \Big|_{r=0} \neq \infty \quad (4)$$

$$C_1 \Big|_{r=1} = 1; \quad \frac{\partial C_2}{\partial r} \Big|_{r=1} = 0 \quad (5)$$

$$C_1 \Big|_{\tau=0} = 0; \quad C_2 \Big|_{\tau=0} = 1. \quad (6)$$

Velocity components of a liquid inside a drop,  $V_r$  and  $V_\theta$ , in equations (2) and (3) are prescribed by the Hadamard–Rybczynski formulas [10].

Equations (2)–(6) are solved using the alternating-direction finite-difference method. Numerical calculations were carried out on the computer BSEM-4 for  $Pe = 20, 40$  and different values of  $m, n, K$  parameters.

An amount of substance diffused into a drop up to the time instant  $\tau$  is determined by the formula

$$M = VC_{10}\bar{C}_1(\tau) + VC_{20}[1 - \bar{C}_2(\tau)], \quad (7)$$

where  $V$  is the drop volume and  $\bar{C}_1$  and  $\bar{C}_2$  are the mean concentrations of reactants determined by the formulas

$$C_s(\tau) = \frac{3}{2} \int_0^1 \int_0^\pi C_s(r, \theta, \tau) r^2 \sin \theta dr d\theta \quad (s = 1, 2). \quad (8)$$

For a mean value of an extractant flow we have

$$Q = C_{10} \frac{\pi d^3}{6t} [\bar{C}_1 + m(1 - \bar{C}_2)]. \quad (9)$$

An amount of the absorbed extractant referred to  $C_{10}$  is

$$A = \bar{C}_1 + m(1 - \bar{C}_2). \quad (10)$$

#### MASS TRANSFER ACCOMPANIED BY A FAST REACTION

At finite values of a velocity constant  $K$  a reaction between an extractant and chemisorbent proceeds in the volume of the whole drop. As far as  $K$  grows, the reaction zone thickness contracts, and at sufficiently great  $K$  it becomes much less than a drop radius. At  $K \rightarrow \infty$  the reaction zone thickness tends to zero and the zone itself may be approximately replaced by a front. In time the reaction front moves from a surface into a drop, thus separating the drop volume into two regions, one of them being with extractant, and another, with chemisorbent. Thus, the problem on mass transfer to a moving spherical drop with a fast chemical reaction present reduces to solution of convective diffusion equations for extractant and chemisorbent coupled by conjugation conditions on a chemical reaction front.

For sufficiently great  $Pe$  at  $Re < 1$  the equations of convective diffusion for extractant and chemisorbent may be approximately described by the Kronig and Brink equations [11]

$$\frac{\partial}{\partial x} \left[ p(x) \frac{\partial C_1}{\partial x} \right] = \frac{q(x)}{16} \frac{\partial C_1}{\partial \tau} \quad (11)$$

$$\frac{\partial}{\partial x} \left[ p(x) \frac{\partial C_2}{\partial x} \right] = \frac{q(x)}{16n} \frac{\partial C_2}{\partial \tau}, \quad (12)$$

where  $x = 4r^2(1-r^2)\sin^2\theta$  and  $q(x)$  and  $p(x)$  are defined in [11] as functions of elliptical integrals.

Equation (11) is obtained in [11] assuming constant concentrations along streamlines that hold at  $Pe \rightarrow \infty$ . In this case the equation of convective diffusion reduces to that of unsteady-state molecular diffusion (11) in the direction normal to streamlines. At  $K \rightarrow \infty$  the condition of constant concentrations of extractant and chemisorbent along streamlines is satisfied on surfaces being as close as possible to a reaction front, thus the latter coincides with streamlines as well. Concentrations of reagents on the reaction front are equal to zero and magnitudes of their flows are the same and opposite in direction

$$C_1 \Big|_{x=l} = C_2 \Big|_{x=l} = 0 \quad (13)$$

$$\frac{\partial C_1}{\partial x} \Big|_{x=l} = -n \frac{\partial C_2}{\partial x} \Big|_{x=l} \quad (14)$$

where  $l$  is the instantaneous position of the reaction front. Once valencies of extractant and chemisorbent are not equal, the concentration of chemisorbent should be multiplied by a stoichiometric coefficient.

The boundary condition for extractant on a drop surface is of the same form as in the case of mass transfer without chemical reaction at comparable phase resistances and constant extractant concentration in a continuous phase [12]

$$\frac{\partial C_1}{\partial x} \Big|_{x=0} = \frac{3}{32\beta} \left( C_1 \Big|_{x=0} - 1 \right). \quad (15)$$

Concentrations of reactants inside a drop are limited. Initial conditions are determined by formulas (6).

At small  $\tau$  a reaction occurs on a drop surface and boundary conditions (13) through (15) are not satisfied. In the present case concentration of extractant on a drop surface is equal to zero, and instead of boundary conditions (14), (15) we have

$$\frac{\partial C_2}{\partial x} \Big|_{x=0} = \frac{3}{32\beta mn}. \quad (16)$$

Concentration of chemisorbent on a drop surface decreases with time from 1 up to 0 that is achieved at  $\tau_1$ . Just from this time instant boundary conditions (13), (14) begin to hold. Thus, a general solution of the problem reduces to a successive solution of two problems; firstly for  $0 < \tau \leq \tau_1$  equation (12) is solved provided a chemisorbent flow on a drop surface is determined according to (16), and then for  $\tau > \tau_1$  a system of equations (11) through (15) is obtained at initial boundary conditions (6). Time  $\tau_1$  is defined by solving the first problem when chemisorbent concentration on a drop surface becomes equal to zero.

For chemisorbent mean concentration  $\bar{C}_2$  at  $\tau \leq \tau_1$  use of the material balance equations

$$K_c \pi d^2 Y_0 = - \frac{\pi d^3}{6} \frac{dc_2}{dt} \quad (17)$$

also yields an analytical solution

$$\bar{C}_2 = 1 - \frac{3}{2} \frac{\tau}{\beta m}. \quad (18)$$

Beginning from  $\tau = \tau_2$  corresponding to  $C_2 = 0$  (position of a reaction front is defined by  $x = 1$ ), mass transfer is described by equation (11). Here the previous boundary conditions hold for  $C_1$ , and the initial one is defined by  $C_1$  obtained solving the problem in the range of  $0 < \tau \leq \tau_2$  at  $\tau = \tau_2$ .

A solution was obtained on the computer BESM-4 by the finite-difference technique. During computation  $\tau_1$ ,  $l$ , volume-averaged concentrations of reactants and their derivatives were determined. Calculations were carried out for  $m = 1; 2; 10; n = 0.1; 0.5; 1; 5; 10; \beta = 0.0005; 0.005; 0.05$ .

By  $\bar{C}_1$  and  $\bar{C}_2$  according to formula (9) a mean value of an extractant flow  $Q$  and its relation with the maximum flow  $Q_m = K_c \pi d^2 Y_0$

$$Q/Q_m = \frac{2\beta}{3\tau} [\bar{C}_1 + m(1 - \bar{C}_2)], \quad (19)$$

and  $A/A_m$  characterizing a ratio of extractant absorbed by a drop to maximum possible absorption with chemisorption is found

$$\frac{A}{A_m} = \frac{C_1 + m(1 - C_2)}{1 + m}. \quad (20)$$

## DISCUSSION

Numerical results are presented graphically in Figs. 1–8 for  $A$ ,  $C_1$ ,  $C_2$ ,  $Q/Q_m$  and  $A/A_m$  depending on  $\tau$  and problem parameters.

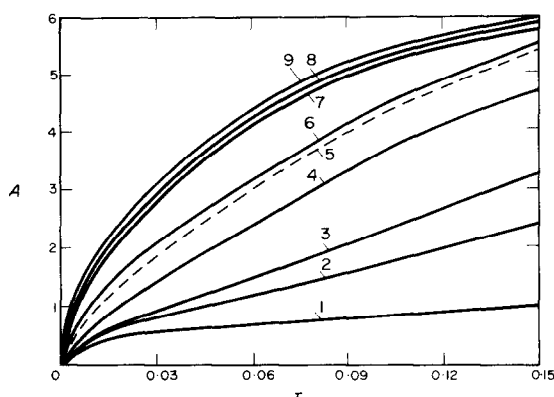


FIG. 1.  $A$  vs  $\tau$  at  $Pe = 40$ ,  $m = 5$ ,  $n = 1$  and different  $K$  values. 1,  $K = 0$ ; 2,  $K = 40$ ; 3,  $K = 100$ ; 4,  $K = 400$ ; 5,  $K = 640$  (curve is built by data of [8]); 6,  $K = 1000$ ; 7,  $K = 10000$ ; 8,  $K = 100000$ ; 9,  $K \rightarrow \infty$  [curve is built by formula (23)].

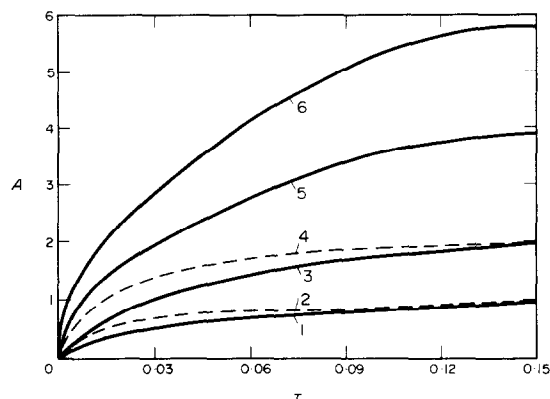


FIG. 2.  $A$  vs  $\tau$  for different  $Pe^1$ ,  $K$  and  $m$  values. 1,  $K = 0$ ,  $Pe^1 = 40$ ; 2,  $K = 0$ ,  $Pe^1 \rightarrow \infty$ ; 3,  $K = 10^5$ ,  $Pe^1 = 40$ ,  $m = n = 1$ ; 4,  $K \rightarrow \infty$ ,  $Pe^1 \rightarrow \infty$ ,  $m = n = 1$ ,  $\beta = 0.0005$ ; 5,  $K = 10$ ;  $Pe^1 = 40$ ,  $n = 1$ ,  $m = 3$ ; 6,  $K = 10^5$ ,  $Pe^1 = 40$ ;  $n = 1$ ,  $m = 5$ .

Figure 1 presents  $A$  vs  $\tau$  at  $Pe = 40$ ,  $m = 5$ ,  $n = 1$  and different values of  $K$ . Curve 1 built at  $K = 0$  (no chemical reaction) coincides with the appropriate calculations obtained by Johns and Beckman [13] when solving the equation of convective mass transfer inside a drop. A dotted curve is built for  $K = 640$  by data of [8]. Curve 9 is built when  $K \rightarrow 640$ . In this case  $A$  is sought by the formula

$$A = A_0(1 + m) \quad (21)$$

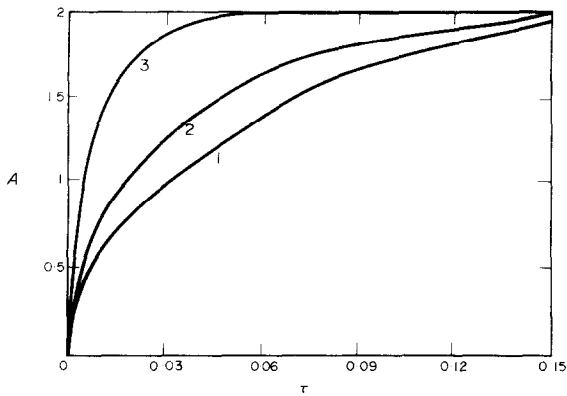


FIG. 3.  $A$  vs  $\tau$  at  $Pe = 40$ ,  $m = 1$ ,  $K = 10^5$  and different  $n$  values. 1,  $n = 1$ ; 2,  $n = 2$ ; 3,  $n = 10$ .

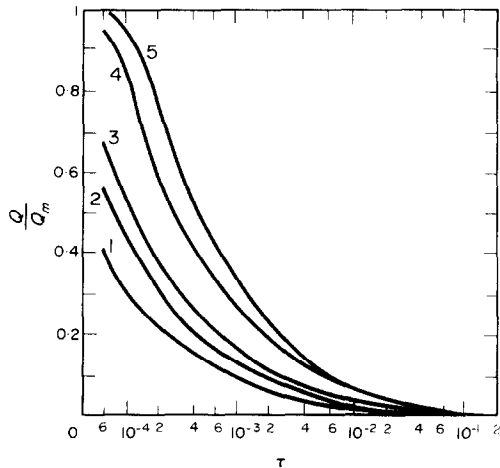


FIG. 6.  $Q/Q_m$  vs  $\tau$  at  $\beta = 0.0005$ ,  $m = 2$  and different  $n$  values. 1,  $n = 0.1$ ; 2,  $n = 0.5$ ; 3,  $n = 1$ ; 4,  $n = 5$ ; 5,  $n = 10$ .

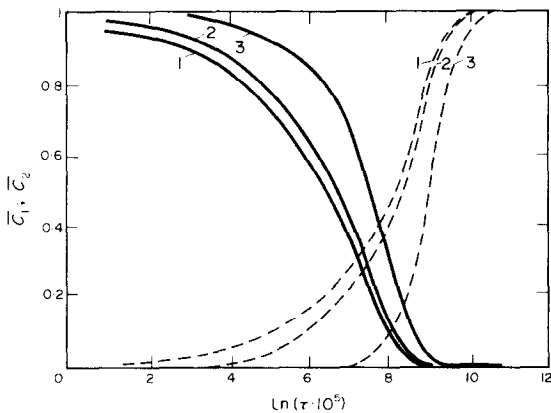


FIG. 4.  $\bar{C}_1$  and  $\bar{C}_2$  vs  $\tau$  at  $m = 1$ ,  $n = 0.5$  and different  $\beta$  values. 1,  $\beta = 0.0005$ ; 2,  $\beta = 0.005$ ; 3,  $\beta = 0.05$ .

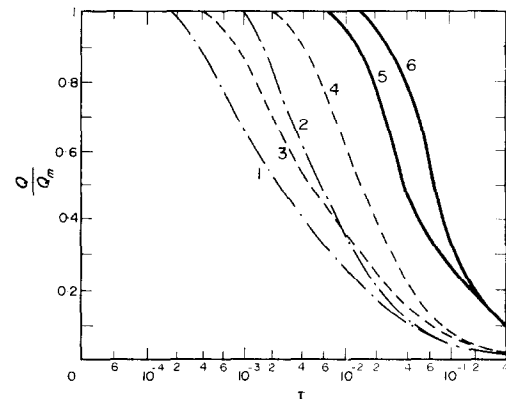


FIG. 7.  $Q/Q_m$  vs  $\tau$  at  $\beta = 0.005$ . - - - - - ,  $m = 1$ ; 1,  $n = 0.5$ ; 2,  $n = 5$ . - - - - - ,  $m = 2$ ; 3,  $n = 0.5$ ; 4,  $n = 5$ . - - - - - ,  $m = 10$ ; 5,  $n = 0.5$ ; 6,  $n = 5$ .

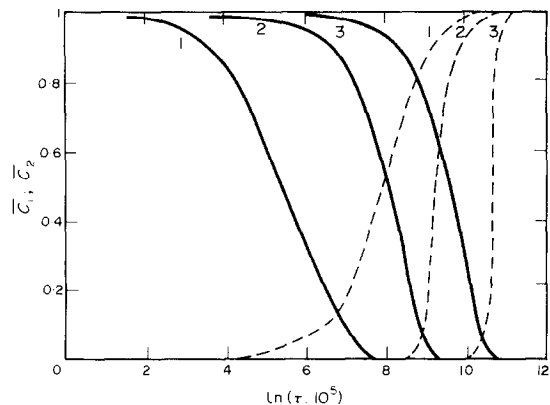


FIG. 5.  $\bar{C}_1$  and  $\bar{C}_2$  vs  $\tau$  at  $\beta = 0.05$ ;  $n = 5$  and  $m = 1$ ; 2; 10. —,  $\bar{C}_2$ ; - - - - - ,  $\bar{C}_1$ . 1,  $m = 1$ ; 2,  $m = 2$ ; 3,  $m = 10$ .

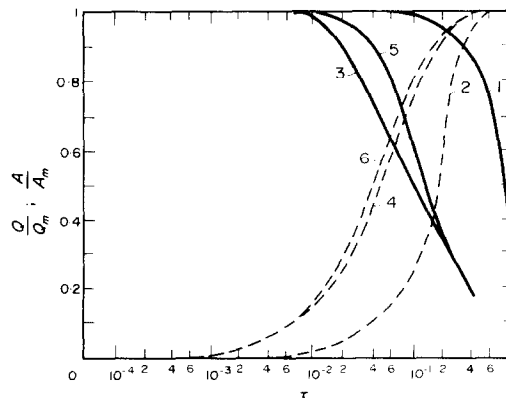


FIG. 8.  $Q/Q_m$  and  $A/A_m$  vs  $\tau$  at  $\beta = 0.05$ . —,  $Q/Q_m$ ; - - - - - ,  $A/A_m$ ; 1, 2,  $n = 0.5$ ;  $m = 10$ ; 3, 4,  $n = 0.5$ ;  $m = 1$ ; 5, 6,  $n = 5$ ;  $m = 1$ .

where  $A_0$  is the degree of saturation without chemical reaction. As is shown in [14], this relationship is valid for a fast chemical reaction situation provided diffusivities of reactants are equal to each other ( $n = 1$ ). As follows from this plot, the values of  $K \approx 10^4 - 10^5$  practically correspond to fast reaction conditions.

Figure 2 depicts  $A$  vs  $\tau$  as well. Here solid lines are

built for  $Pe = 40$  and dotted ones, for  $Pe \rightarrow \infty$ . This graph illustrates an effect of  $m$  and  $Pe$  on a transfer process. Since curves 3, 5 and 6 are built for  $n = 1$  and  $K = 10^5$ , they may be approximately described by formula (21). In this case, the value of  $A_0$  is determined by curve 1 at  $K = 0$ . Curve 4 may be predicted in the same way for which  $A_0$  may be defined by curve 2.

Enhancement of mass-transfer rate with increasing parameter  $n$  is shown in Fig. 3 where  $n$  varies from 1 to 10. At  $n = 10$   $A$  reaches its maximum with  $\tau \approx 0.04$  whereas for  $n = 1$  an appropriate value of  $\tau$  approximately equals 0.15.

In the next figures the problem is analysed of mass transfer involving a fast chemical reaction. Here parameter  $\beta$  is of importance. By its magnitude one may judge, which of phases controls a transfer process. As is shown in [15], at  $\beta < 0.001$  the resistance of a dispersed phase is limiting and at  $\beta > 0.1$ , that of a continuous phase. Values of  $0.001 < \beta < 0.1$  correspond to the case of comparable phase resistances. Note that for any  $\beta$  a growth of  $m$  and  $n$  contributes to enhancement of a velocity of chemisorbent transferred to a drop surface and, moreover, that of  $m$  increases chemical capacity that results in  $\tau_1$  growth which determines an initial time interval where a reaction proceeds on a drop surface.  $\tau_1$  considerably depends on  $\beta$ ; at great  $\beta$ ,  $\tau_1$  is particularly great that is clear both from  $Q/Q_m$  and  $A/A_m$  dependences in Fig. 8 and from plots of mean concentrations in Figs. 4 and 5 where motion of reaction front is determined in terms of  $C_1$  inside a drop. During time interval  $\tau_1$ , when reaction occurs on a drop surface, extractant is not transferred into a drop and concentration  $C_1 = 0$ .

In Table 1  $A/(1+m)$  for  $\beta = 0.005$ ,  $m = n = 1$  is compared to  $A_0$  values for mass transfer involving no chemical reaction at the same value of  $\beta$ . As is seen from Table 1, the predicted values are in good agreement with those given by formula (21).

Table 1. Mean concentrations and extraction degree values at  $\beta = 0.005$ ,  $m = n = 1$

$\tau$	$\bar{C}_1$	$\bar{C}_2$	$A = \bar{C}_1 + m(1 - \bar{C}_2)$	$\frac{A}{1+m}$	$A_0$
0.0001	0	0.970	0.030	0.015	0.011
0.0004	0.003	0.890	0.113	0.057	0.057
0.0009	0.019	0.812	0.207	0.104	0.103
0.0025	0.061	0.671	0.390	0.195	0.198
0.0049	0.111	0.534	0.577	0.289	0.288
0.0080	0.158	0.424	0.734	0.367	0.372
0.0100	0.187	0.364	0.823	0.412	0.413
0.0200	0.295	0.175	1.120	0.560	0.562
0.0400	0.493	0.010	1.483	0.742	0.745
0.0625	0.724	0	1.724	0.862	0.856
0.1000	0.881	0	1.881	0.945	0.948
0.2000	0.984	0	1.984	0.992	0.998

Evaluate, at which  $Pe$ ,  $K$  and  $Re$  values the solutions obtained are applicable. For  $Pe$ , the above solutions may be applied provided that the Kronig and Brinck equations [11] are used for describing a transfer mechanism inside a drop. As is shown in [15], these equations may be used at  $Pe > 100$ .

Estimate the value of  $K$  at which the thickness of reaction front may be assumed much less than a drop radius. Determine a characteristic time of a chemical reaction as that during which extractant concentration decreases  $l$  times at  $m = 1$ . Here at  $t = 0$ ,  $C_1 = C_2 = C_{10}$  is assumed over the whole drop volume. Then  $t_x \approx$

$(l-1)/KC_{10}$ . A characteristic time of diffusion with liquid circulating in a drop is  $t_d = 0.022R^2/D_1$ . At  $t_x \ll t_d$  it is found that  $K \gg 100$ .

In the present paper the solutions to internal problems of mass transfer complicated by a chemical reaction are obtained for  $Re < 1$ . However, in some cases these may also be employed for  $Re > 1$ . Thus, for instance, for spherical drops at  $\mu < 2$  [15], the liquid flow pattern slightly changes with  $Re$  growth, and the solutions for  $Re < 1$  (and consequently, the solutions presented here for mass transfer with a chemical reaction) may be used at  $Re \approx 100$ .

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APPENDIX

1. On Numerical Solution of the Mass-Transfer Problem At Finite  $K$  and  $Pe$  Values

To find a numerical solution of the problem, use is made of one of the variants of the alternating-direction method [17]. A difference scheme is written as

$$\frac{C_{si,k}^{j+\frac{1}{2}} - C_{si,k}^j}{\tau_0} + Pe' \left( V_{ri,k} - \alpha_1 \frac{2}{r_i} \right) \frac{\delta C_{si,k}^{j+\frac{1}{2}}}{\delta r} = \alpha_1 \frac{\delta^2 C_{si,k}^{j+\frac{1}{2}}}{\delta r^2} - \alpha_2 \frac{K}{2} C_{1i,k}^j C_{2i,k}^j \quad (s = 1, 2) \quad (22)$$

$$\frac{C_{si,k}^{j+1} - C_{si,k}^{j+\frac{1}{2}}}{\tau_0} + \left( \frac{Pe' V_{\theta i,k}}{r_i} - \alpha_1 \frac{\cotan \theta_k}{r_i^2} \right) \frac{\delta C_{si,k}^{j+1}}{\delta \theta} = \frac{\alpha_1}{r_i^2} \frac{\delta^2 C_{si,k}^{j+1}}{\delta \theta^2} - \alpha_2 \frac{k}{2} C_{1i,k}^j C_{2i,k}^j \quad (s = 1, 2) \quad (23)$$

$$\alpha_1 = \begin{cases} 1, & s = 1 \\ n, & s = 2 \end{cases} \quad \alpha_2 = \begin{cases} 1, & s = 1 \\ 1/m, & s = 2 \end{cases}$$

where  $\delta/\delta r$ ,  $\delta/\delta \theta$ ,  $\delta^2/\delta r^2$ ,  $\delta^2/\delta \theta^2$  are the three-point difference derivatives. The first-order derivatives are taken with weight, for example

$$\frac{\delta C_{i,k}}{\delta r} = \lambda \frac{C_{i,k+1} - C_{i,k}}{h_i} + (1-\lambda) \frac{C_{i,k} - C_{i-1,k}}{h_{i-1}} \quad 0 \leq \lambda \leq 1.$$

In the difference scheme besides integer steps with respect to  $r$  and  $\theta$

$$r_i = \sin\left(\frac{2i-1}{2N-1} \frac{\pi}{2}\right); \quad \theta_k = \frac{\pi(2k-1)}{M}; \quad i = 1, 2, \dots, N; \quad k = 1, 2, \dots, \mu;$$

fractional ones are also used

$$r_{i+\frac{1}{2}} = \sin\left(\frac{2i}{2N-1} \frac{\pi}{2}\right); \quad \theta_{k+\frac{1}{2}} = \frac{\pi k}{\mu}.$$

Weight values of  $\lambda$  and  $\mu$  for the first derivatives with respect to  $r$  and  $\theta$ , respectively, are chosen from the conditions:

$$\lambda = \begin{cases} 0, & V_{ri,k} \leq 0 \\ 1, & V_{ri,k} > 0 \end{cases} \quad \mu = \begin{cases} 0, & V_{\theta i,k} \leq 0 \\ 1, & V_{\theta i,k} > 0. \end{cases}$$

The limiting conditions at  $r = 0$ ;  $\theta = 0, \pi$  automatically hold due to a character of the scheme built [18]. Boundary conditions on a drop surface are directly approximated by:

$$C_{1N,\lambda}^{j+\frac{1}{2}} = 1; \quad C_{2N,\lambda}^{j+\frac{1}{2}} = C_{2N-1,\lambda}^{j+\frac{1}{2}}. \quad (24)$$

A system of equations (24)–(26) at each integer and fractional layers  $j, j + \frac{1}{2}$  represents a linear algebraic system with the number of unknown values corresponding to that

of the equations. For its solution a difference energy-type estimation is valid [19]

$$S_{up} \sum_{\Omega_n} h_i(\Delta \theta_i) r_i^2 \sin^2 \theta_k (C_{i,k}^m) + \tau_0 \sum_{k=0}^n h_i(\Delta \theta_i) \times \left[ \left( \frac{C_{i,r}^{k+\frac{1}{2}} - C_{i-1,r}^{k+\frac{1}{2}}}{h_i} \right) r_i^2 + \left( \frac{C_{i,t}^k - C_{i,t-1}^k}{\Delta \theta_i} \right)^2 \sin^2 \theta_i \right] \leq \mu' \quad (25)$$

where  $M^1$  is the constant defined by initial and boundary conditions;  $\Omega_n$  is the set of grid nodes in a rectangle  $0 \leq \theta \leq \pi, 0 \leq r \leq 1$ .

Similar to [19] it may be shown that at  $h, \tau_0, (\Delta \theta_i) \rightarrow 0$  the solution for a grid reduced to the exact one in a norm defined by the L.H.S. of equation (27) and in this case the order of convergence equals  $(h^2 + \tau)$ .

Estimation (27) gives a single-valued solution of the appropriate algebraic systems. Each system may be written in the form of a tridiagonal matrix and for its solution the elimination method is used.

2. On Numerical Solution of the Problem of Mass Transfer with a Fast Reaction

To solve equations (11) and (12), a uniform difference scheme is built of the type

$$\left[ p_j \left( x_i + \frac{h_{i+1}}{2} \right) \frac{u_{i+1}^j - u_i^j}{h_{i+1}} - p_j \left( x_{i-1} + \frac{h_i}{2} \right) \frac{u_i^j - u_{i-1}^j}{h_i} \right] = \frac{q(x_i) u_i^j - u_{i-1}^{j-1}}{16 \tau_i}$$

where  $h_i = x_i - x_{i-1}$ ,  $x_i$  is the point of segment partition  $[0, 1]$

$$u = \begin{cases} C_1, & 0 \leq x \leq l \\ C_2, & l \leq x \leq 1 \end{cases}$$

$$p_j \left( x_i + \frac{h_{i+1}}{2} \right) = \begin{cases} np \left( x_i + \frac{h_{i+1}}{2} \right) & \text{provided } u_i^j \geq p \text{ and } u_{i+1}^j \geq 0 \\ p \left( x_i + \frac{h_{i+1}}{2} \right) & \text{provided } u_i^j < 0 \text{ and } u_{i+1}^j < 0 \\ np \left( x_i + \frac{h_{i+1}}{2} \right) \frac{|u^+| + |u^-|}{n|u^-| + |u^+|} & \text{provided } u_i^j \text{ and } u_{i+1}^j \text{ have different signs.} \end{cases}$$

Positive and negative values of  $u^j$  function at the point  $(x_i, \tau_j)$  or  $(x_{i+1}, \tau_j)$  are designated through  $u^+$  and  $u^-$ .

This scheme is non-linear. For its solution the conventional method of successive approximations is used: by  $u_i^{j+1}$  the coefficients  $p_j^0(x_i + (h_{i+1}/2))$  are obtained for the layer  $\tau_j$ ; then, the linear scheme obtained is solved by the elimination method that results in  $u_i^{j(1)}$ . These values are used to build values of  $p_j^{(1)}(x_i + (h_{i+1}/2))$  and so forth unless  $u_i^{j(k)}$  values for two neighbouring iterations become sufficiently close. It should be also noted that the system of linear algebraic equations appearing at each iteration comprises so many equations as the number of the unknown values. This is due to the fact that the scheme at the node  $x = 1$  is written in accordance with the method elaborated in [18]. Calculations were performed by using an alternating grid with spacing refining to zero

$$\left[ x_i = 1 - \cos\left(\frac{\pi i}{2n+1}\right) \right]$$

and variable time step being smaller at the initial section where great gradients of the desired values take place.

**TRANSFERT DE MASSE EN PRESENCE D'UNE TRANSFORMATION  
CHIMIQUE DANS UNE GOUTTE**

**Résumé**—L'expérience est effectuée sur une goutte sphérique en mouvement dans un milieu continu pour  $Re < 1$  en présence d'une réaction chimique irréversible du second ordre à l'intérieur de la goutte.

Des solutions des équations de transfert sont présentées à la fois pour des valeurs finies de la constante de vitesse de la réaction chimique avec une résistance limitative de la phase dispersée et pour une réaction rapide avec des résistances de phase comparables.

On présente les résultats numériques relatifs aux concentrations moyennes des réactants, aux degrés d'extraction en fonction du temps de contact des phases et des paramètres du problème.

**STOFFÜBERGANG BEI CHEMISCHER UMWANDLUNG EINER  
SUBSTANZ IN EINEM TROPFEN**

**Zusammenfassung**—Es wird eine irreversible chemische Reaktion zweiter Ordnung untersucht in einem kugeligen Tropfen, der sich mit  $Re < 1$  bewegt.

Lösungen der Übergangsgleichungen sind sowohl für endliche Werte der chemischen Reaktion angegeben als auch für schnelle Reaktionen mit vergleichbarem Phasenwiderstand.

Die numerischen Ergebnisse sind wiedergegeben für mittlere Konzentrationen der Reaktanten für den Extraktionsgrad und für die Strömung in Abhängigkeit einer dimensionslosen Phasenkontaktzeit und anderer Parameter.

**МАССОПЕРЕНОС, СОПРОВОЖДАЕМЫЙ ХИМИЧЕСКИМ ПРЕВРАЩЕНИЕМ  
Вещества в капле**

**Аннотация** — Исследуется массообмен между сферической каплей, движущейся при  $Re < 1$ , и сплошной средой в присутствии необратимой химической реакции второго порядка, протекающей внутри капли.

Изложены решения уравнений переноса как для конечных значений константы скорости химической реакции при лимитирующем сопротивлении диспергированной фазы, так и для быстро протекающей реакции при соизмеримых фазовых сопротивлениях.

Представлены результаты численных расчетов для средних концентраций реагирующих веществ, степени извлечения и потока в зависимости от безразмерного времени контакта фаз и параметров задачи.