

CALCULATION OF SIMULTANEOUS ABSORPTION OF TWO GASES REACTING WITH THE ABSORBENT

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Relations are derived based on the two-film theory enabling the rate of absorption to be calculated of two gases undergoing simultaneously an irreversible chemical reaction. The case considered here is that one of the reactions with the active component of the absorbent is instantaneous and the other is a second-order reaction occurring completely within the liquid film.

Simultaneous absorption of two gases reacting with an active component of the absorption solution is a very frequent case in industrial practice. Present state of the art regarding simultaneous absorption and relations for the absorption rates are summarized in the paper of Ramachandran and Sharma¹. An important type of such absorptions is that when one of the reactions is practically instantaneous.

Validity of published approximate solutions^{1,2} is typically confined to certain concentration regions or regimes characterizing the absorption while criteria for differentiation between individual regimes are not quite unambiguous. In reactor design where continuous wide ranging changes of concentrations are common this approach mandates application of different expressions to individual sections of the absorber along its height. This results in a discontinuous course of the computed concentration course within the reactor which is, of course, at variance with the physical nature of the process. Moreover, determination of absorption rates in the transition regions between individual regimes suffers from a considerable degree of uncertainty.

The object of this work is to provide a unified set of expressions valid in the entire range of concentration conditions and enabling calculation of the absorption rates of two components A and B reacting with the active component C according to the following schemes



The derivation starts from the two-film theory assuming that both reactions are irreversible while the first one (I) is instantaneous and the second one (II) is a second-order and fast enough to occur completely within the liquid film.

THEORETICAL

Depending on position of the reaction plane for the reaction (I), two regimes may be distinguished. A regime 1, when the reaction plane is identical with the interface ($\lambda = 0$), and a regime 2 when the reaction plane appears within the liquid film. ($0 < \lambda < \delta$). Concentration profiles of the reacting species for both of these regimes are depicted in Fig. 1. Under the regime 1 the rate of absorption of the species A is determined solely by diffusion within the gas film while the partial pressure of A and its concentration at the interface are zero. Interfacial concentration of C is finite and depends primarily on the bulk concentration of this species. A transition between the regime 1 and 2 may occur if the concentration of C at the interface vanishes at zero concentration of A. This state is usually termed the critical regime. Under the regime 2 c_A^* takes finite values and the reaction plane splits the diffusional film into two parts: Within $0 < x < \lambda$ only the species A and B diffuse away from the interface toward the reaction plane while within, $\lambda < x < \delta$ (i.e. within the reaction zone for the reaction (II)) a counter-current diffusion of the species B and C accompanied by the chemical reaction (II) takes place.

From the viewpoint of the two film theory, diffusion within the reaction zone may be described by the following differential equations

$$D_B d^2 c_B / dx^2 = k_R c_B c_C, \quad (1)$$

$$D_C d^2 c_C / dx^2 = z_B k_R c_B c_C \quad (2)$$

with the boundary conditions

$$x = \lambda, \quad c_B = c_B^+, \quad dc_C/dx = -J_C/D_C = z_A J_A/D_C; \quad (3)$$

$$x = \delta, \quad c_B = 0, \quad c_C = c_C^0. \quad (4)$$

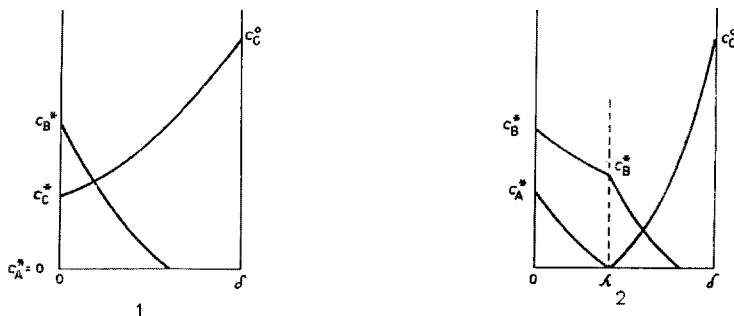


FIG. 1

Concentration Profiles of Reacting Species

Regime 1: Reaction plane at the interface; regime 2: Reaction plane within the film.

Mass flux of the species B through the reaction plane is given by

$$J_B = -D_B(dc_B/dx)_{x=\lambda} . \quad (5)$$

Introducing the following dimensionless parameters

$$M = k_R c_C^0 (\delta - \lambda)^2 / D_B , \quad (6)$$

$$Q = D_C c_C^0 / z_B D_B c_B^+ , \quad (7)$$

$$X = z_B J_B / (z_A J_A + z_B J_B) , \quad (8)$$

$$\Phi = J_B (\delta - \lambda) / D_B c_B^+ \quad (9)$$

and with the aid of the following dimensionless coordinates

$$b = c_B / c_B^+ , \quad (10)$$

$$c = D_C c_C / z_B D_B c_B^+ , \quad (11)$$

$$z = (x - \lambda) / (\delta - \lambda) . \quad (12)$$

the differential equations (1) and (2) may be arranged to give

$$d^2 b / dz^2 = M b c / Q , \quad (13)$$

$$d^2 c / dz^2 = d^2 c / dz^2 . \quad (14)$$

Integration of Eq. (14) for the transformed boundary conditions yields a relation between concentrations of the reacting species which can be expressed as

$$c = b + Q - (\Phi/x)(1 - z) . \quad (15)$$

Substituting on the right hand side of Eq. (13) from Eq. (15) leads to the following nonlinear differential equation

$$\frac{d^2 b}{dz^2} = \frac{M}{Q} b \left[b + Q - \frac{\Phi}{x} (1 - z) \right] . \quad (16)$$

An approximate solution to Eq. (16) may be obtained by the collocation method. The concentration profiles are approximated by the function

$$b = \sinh [G(1 - z)] / \sinh G , \quad (17)$$

obtained as a solution of a linearized form of Eq. (16), namely

$$d^2b/dz^2 = G^2b \quad (18)$$

for the given boundary conditions. The value of the parameter G is taken so as to make the function in Eq. (17) satisfy Eq. (16) for a selected value of the variable $z = z_{\text{col}}$.

The reaction factor Φ for the given approximation is given by the expression

$$\Phi = - \left(\frac{db}{dz} \right)_{z=0} = \frac{G}{\tanh G}. \quad (19)$$

On taking the collocation point as $z_{\text{col}} = 1$ one obtains, after combining Eqs (16) and (17), for G the value $M^{1/2}$. This leads generally always to too high a value for Φ corresponding to a pseudo first-order reaction. Taking $z_{\text{col}} = 0$ gives for G the expression $[(M/Q)(1 + Q - \Phi/x)]^{1/2}$. Substitution of this result into Eq. (19) gives lower values of the reaction factor in comparison with a numerical solution of Eq. (16). The numerical solution have shown that the best fit is obtained by taking

$$z_{\text{col}} = 1/[2(M + 1)^{1/2}]. \quad (20)$$

Using Eqs (16), (17) and (20) gives for G the following expression

$$G = \left[\frac{M}{Q} \left(\frac{\sinh \{G[1 - 1/(2(M + 1)^{1/2})]\}}{\sinh G} + Q - \frac{\Phi}{x} \left(1 - \frac{1}{2(M + 1)^{1/2}} \right) \right) \right]^{1/2} \quad (21)$$

which, in conjunction with Eq. (19), permits the value of the reaction factor to be determined for a given set of the parameters M , Q and X .

For the reaction regime 1 we have $\lambda = 0$ and $c_{\text{B}}^+ = c_{\text{B}}^*$, while the concentration c_{C}^* remains within 0 and c_{C}^0 . With increasing value of c_{C}^0 the value of Q increases (Eq. (7)) and for the asymptotic case $Q \rightarrow \infty$ the expressions (19) and (21) reduce to the exact solution for a pseudo first-order reaction, *i.e.* $\Phi = \sqrt{M}/\tanh \sqrt{M}$.

Decreasing value of c_{C}^0 causes the concentration c_{C}^* to drop up to the zero value for the critical regime. In this extreme case the approximate methods of calculation of the reaction factor exhibit maximum deviations from numerical solutions of Eq. (16).

For the reaction regime 2 we have $\lambda > 0$ and $c_{\text{C}}^+ = 0$. Eq. (15) indicates that under the conditions prevailing at the reaction plane ($z = 0$, $b = 1$, $c = 0$) we may also write that

$$\Phi = (1 + Q)X. \quad (22)$$

For determination of the position of the reaction plane, λ , and the concentration c_B^+ there are additional expressions available describing diffusional fluxes of the reaction components in the diffusion region

$$J_A = (D_A/\lambda) c_A^*, \quad (23)$$

$$J_B = (D_B/\lambda) (c_B^* - c_B^+). \quad (24)$$

In the asymptotic case $\lambda \rightarrow \delta$ the approximation takes the form of the accurate solution for the physical absorption. It is apparent that the maximum error in determining the mass fluxes under the regime 2 is committed if the reaction zone expands over the whole thickness of the film, *i.e.* again for the case of the critical regime ($\lambda = 0$).

For this reason we have tested the accuracy of the proposed approximate solution under the critical regime conditions because the error of the calculated absorption rates from other conditions will be smaller. For illustration Table I summarizes the reaction factors computed for selected combinations of the parameters covering the range of variables of practical importance. For comparison the table gives also the data computed from the equation proposed by Ramachandran and Sharma¹ for the regime 2. For the sake of obtaining an approximate solution to Eq. (16) the authors¹ assume a linear dependence of b on z . Under this assumption a simple relation for Φ in the critical regime results.*

$$\Phi = 1 + M/12. \quad (25)$$

Table I shows also for comparison the values of the the factor Φ computed from

$$\Phi = \frac{5}{2} + Q + \frac{30Q}{M} - \left[\left(\frac{3}{2} + Q + \frac{30Q}{M} \right)^2 - 5Q \right]^{1/2} \quad (26)$$

derived from a solution of Eq. (16) when the concentration profile of the component B had been approximated under the regime 2 by a parabola.

Table I indicates that Eq. (25) approaches the accurate solution only in region of low values of the parameter M while for higher values of M the deviation is unacceptable. The deviations of our solution given by Eqs (19) and (21) as well as the deviation of Eq. (26) are all within the limits of the accuracy tolerated in chemical engineering calculations. However, Eqs (19) and (21) are more general in that that unlike Eq. (26) are applicable in the entire concentration region.

* In ref.¹ the factor D_C/D_B in Eq. (37) is missing.

Calculation of the absorption rates. Eqs (7), (9), (23) and (24) contain unknown concentrations at the interface as well as those at the reaction plane. On eliminating these quantities with the aid of equations expressing mass fluxes in terms of the gas-side driving force as

$$J_A = k_{GA}(p_A - c_A^*/H_A), \quad (27)$$

$$J_B = k_{GB}(p_B - c_B^*/H_B), \quad (28)$$

we obtain

$$J_A = \frac{k_{GA}p_A}{1 + \lambda k_{GA}/D_A H_A}, \quad (29)$$

$$J_B = \frac{k_{GB}p_B}{1 + [\lambda(\Phi - 1) + \delta] k_{GB}/\Phi D_B H_B}, \quad (30)$$

$$Q = \frac{D_C c_C^0}{z_B D_B [p_B H_B - J_B (H_B/k_{GB} + \lambda/D_B)]}. \quad (31)$$

Eqs (6), (8), (9), (21), (29–31) constitute a complete set of equations for the calculation of the absorption rates under the regime 1 when $\lambda = 0$. In case of the regime 2 this set must be supplemented by Eq. (22). Formally both regimes may

TABLE I
Comparison of Approximate Values of Φ with Numerically Obtained Results

Q	X	M	Φ exact	Φ					
				Eq. (26)	deviation %	Eq. (25)	deviation %	Eq. (19), (21)	deviation %
0.5	0.8	3.781	1.200	1.213	1.1	1.315	9.6	1.196	-0.4
0.5	0.7	0.663	1.050	1.051	0.1	1.055	0.5	1.071	2.0
1.0	0.6	3.107	1.200	1.207	0.6	1.259	4.9	1.203	0.2
1.0	0.8	18.648	1.600	1.662	3.8	2.554	59.6	1.567	-2.1
5.0	0.3	16.663	1.800	1.829	1.6	2.389	32.7	1.723	-4.2
5.0	0.5	104.581	3.000	2.774	-7.5	9.715	223.8	2.885	-3.8
10.0	0.1	1.269	1.100	1.101	0.1	1.106	0.5	1.128	2.5
10.0	0.3	114.743	3.300	2.899	-12.1	10.562	220.0	3.147	-4.6
50.0	0.04	22.059	2.040	2.051	0.5	2.838	39.1	1.930	-5.4
50.0	0.02	0.242	1.020	1.020	0.0	1.020	0.0	1.035	1.5

be described by Eqs (6), (8), (9), (21), (29–31) in conjunction with

$$[(1 + Q)X - \Phi] \lambda = 0 \quad (32)$$

and the condition

$$\lambda \geq 0. \quad (33)$$

The equations formulated as above do not call for any special criteria to distinguish the two regimes.

DISCUSSION

The proposed set of equations describes the rate of absorption in the entire concentration range by a unified approach and provides a continuous change of the rate of absorption on transition between individual absorption regimes. This was not possible with the so far available methods. The formulation of the expressions facilitates programming of the calculation of the rate of absorption on a computer as it permits utilizations of standard subroutines for solving sets of nonlinear equations. The approximate solution proper provides a realistic estimate of the reaction factor in a wide range of operating conditions encountered in practical applications and, moreover, with an error acceptable for engineering calculations.

LIST OF SYMBOLS

b	dimensionless concentration of species B, Eq. (10)
c	dimensionless concentration of C, Eq. (11)
c_i	concentration of i in liquid
c_i^*	equilibrium concentration of i in liquid
c_i^+	concentration of i at the reaction plane
c_i^0	concentration of i in bulk phase
D_i	diffusion coefficient of i in liquid
G	parameter, Eq. (21)
$H_i = c_i^*/p_i$	Henry's constant
J_i	mass flux of i
k_R	reaction rate constant
k_{Gi}	mass transfer coefficient of i in gas film
M	parameter, Eq. (6)
p_i	partial pressure of i in gas
Q	parameter, Eq. (7)
x	coordinate of distance within liquid film
X	parameter, Eq. (8)
z	dimensionless concentration in liquid film, Eq. (12)
z_i	stoichiometric coefficient of i
δ	thickness of liquid film
Φ	reaction factor, Eq. (9)
λ	distance of reaction plane

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