APPROXIMATE RELATIONS FOR CALCULATION OF ENHANCEMENT FACTOR IN GAS ABSORPTION WITH CHEMICAL REACTION

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Based on the film theory of mass transport, new approximate relations for reaction factor are developed for gas absorption accompanied by irreversible chemical reaction A (g) + zB (l) → → products. The relations are compared with exact numerical solutions obtained by the commonly used method of linearization (suggested by Van Krevelen and Hoftijzer and applied by Hikita and Asai) for several nonlinear reaction rate cases. The effect of mass transfer resistance in the gas phase is also considered and simple criteria for estimation of magnitude of the effect of chemical reaction on mass transport are given. It is shown, that the error of the new approximate method is several percent even in cases, where the error of the linearization method is high.

The problem of description of absorption with chemical reaction very often forms a part of complex process, where the effect of chemical reaction on the rate of absorption is just a one step in the mutually interconnected system of chemical and physical processes. If the reaction rates in chemisorption are described by nonlinear reaction rate expressions, then either computer time consuming numerical techniques are required to obtain accurate values of the reaction factor or proper approximate methods has to be used. Practical aspects of modelling of the complex systems also require, that the description of the partial processes are simple and modest in computer time requirements. These requirements are fulfilled by the further given approximate relations for reaction factor.

Approximate Relations for Reaction Factor

Reaction factor compares the rate of chemisorption with the rate of physical absorption occurring under the same conditions.

As the results of calculation of the reaction factor based on the film and penetration theories do not differ significantly from one another from a practical point of view[1,2], we shall use the simpler film theory under the following assumptions: the components in the liquid phase are nonvolatile (more general case is studied by Rod[3]); the concentrations of reactants and products at the end of the film are equal to the values in the bulk of liquid.

As we shall deal here also with the case of gas phase resistance and the literature on the subject usually neglects it, we shall start with the more detailed derivation of the reaction factor than it would be otherwise necessary.

Let us consider, that gas component A diffuses into the stagnant film of liquid B of the thickness s_0. If the concentration of the diffusing component is low and the flux density of the component B is zero, we can describe the flux density of the component A in the form:

$$J_{\mathrm{Az}} = -D_{\mathrm{A}}(\mathrm{d}C_{\mathrm{A}}/\mathrm{d}z)\,. \tag{1}$$

If the gas film resistance is neglected, we shall obtain on integrating Eq. (*1*) with the boundary conditions

$$z = 0: \quad C_{\mathrm{A}} = C_{\mathrm{Ab}} \tag{2}$$

$$z = s_0: \quad C_{\mathrm{A}} = C_{\mathrm{As}} \tag{3}$$

$$J_{\mathrm{Az}} = D_{\mathrm{A}}/s_0(C_{\mathrm{Ab}} - C_{\mathrm{As}}) \tag{4}$$

and the mass transfer coefficient k_{CA0} is then determined as

$$k_{\mathrm{CA0}} = D_{\mathrm{A}}/s_0\,. \tag{5}$$

If the gas phase resistance cannot be neglected, we shall integrate Eq. (*1*) with boundary conditions

$$z = 0: \quad -D_{\mathrm{A}}(\mathrm{d}C_{\mathrm{A}}/\mathrm{d}z) = k_{\mathrm{gCA}}(C_{\mathrm{Ag}} - C_{\mathrm{Agb}}) \tag{6}$$

and the condition (*3*). When the values of C_{Agb} are low, we can use the relation

$$C_{\mathrm{Ab}} = H_{\mathrm{A}}C_{\mathrm{Agb}} \tag{7}$$

and then we shall obtain the boundary condition (*6*) in the form:

$$z = 0: \quad -D_{\mathrm{A}}\,\mathrm{d}C_{\mathrm{A}}/\mathrm{d}z = (k_{\mathrm{gCA}}/H_{\mathrm{A}})(H_{\mathrm{A}}C_{\mathrm{Ag}} - C_{\mathrm{Ab}}) \tag{8}$$

or

$$C_{\mathrm{Ab}} = H_{\mathrm{A}}C_{\mathrm{Ag}} - (H_{\mathrm{A}}/k_{\mathrm{gCA}})\,J_{\mathrm{Azb}}\,. \tag{9}$$

On combining Eqs (*1*), (*3*), (*8*) and (*9*) we shall obtain

$$J_{\mathrm{Azb}} = \frac{D_{\mathrm{A}}}{D_{\mathrm{A}}H_{\mathrm{A}}/k_{\mathrm{gCA}} + s_0}(H_{\mathrm{A}}C_{\mathrm{Ag}} - C_{\mathrm{As}}) \tag{10}$$

and hence the overall mass transport coefficient can be defined as

$$k_{\mathrm{CA0}} = \frac{D_{\mathrm{A}}}{(D_{\mathrm{A}}H_{\mathrm{A}}/k_{\mathrm{gCA}}) + s_0} \, . \tag{11}$$

Let us deal now with the case, where into the stagnant film of the liquid *B* the gas phase component *A* is absorbed, which reacts with *B* irreversibly. We shall assume, that the component *B* is in abundance, and the concentration of the diffusing components is low. The mass balance of *A* within the film for *n*-th order reaction is then in the form

$$D_{\mathrm{A}}(\mathrm{d}^2 C_{\mathrm{A}}/\mathrm{d}z^2) = kC_{\mathrm{A}}^{n} \tag{12}$$

with boundary conditions (stagnant film in the contact with the turbulent liquid) *(2)* and *(8)* and *(3)*. We shall assume, that the film thickness is the same as in physical absorption.

We shall introduce the dimensionless criterion *M*, proposed by Hikita and Asai[4], together with some other dimensionless variables and rewrite Eq. *(12)* into the dimensionless form. No gas phase resistance:

$$M = \frac{2}{n+1} \cdot \frac{k\, C_{\mathrm{Ab}}^{n-1}}{D_{\mathrm{A}}} \cdot s_0^2 \, ; \tag{13}$$

Gas-phase resistance considered:

$$M = \frac{2}{n+1} \cdot \frac{k(C_{\mathrm{Ag}}H_{\mathrm{A}})^{n-1}\, s_0^2}{D_{\mathrm{A}}} \, ; \tag{14}$$

$$X_{\mathrm{A}} = C_{\mathrm{A}}/C_{\mathrm{B}}, \text{ or in the case of gas phase resistance } X_{\mathrm{A}} = C_{\mathrm{A}}/C_{\mathrm{Ag}}H_{\mathrm{A}} \, ; \tag{15}$$

$$Z = z/s_0 \, ; \quad \mathrm{Sh} = \frac{k_{\mathrm{gCA}} s_0}{D_{\mathrm{A}}H_{\mathrm{A}}} \, ; \qquad (16)/(17)$$

Eq. *(12)* is then in the form

$$\mathrm{d}^2 X_{\mathrm{A}}/\mathrm{d}z^2 = M[(n+1)/2]X_{\mathrm{A}}^{n} \, , \tag{18}$$

with boundary conditions

$$Z = 0: \quad X_{\mathrm{A}} = 1 \, , \tag{19}$$

or in the case of gas phase resistance

$$\mathrm{d}X_{\mathrm{A}}/\mathrm{d}Z = \mathrm{Sh}(X_{\mathrm{Ab}} - 1) \, , \tag{20}$$

$$Z = 1: \quad X_{\mathrm{A}} = X_{\mathrm{As}} \, . \tag{21}$$

The above shown relations are valid for nonnegative reaction order *n*. The further proposed approximate solution can be used also for negative order of reaction, however, another definition of the criterion M has to be used.

The reaction factor E describing the ratio of the rate of chemisorption to that of physical absorption can be determined from the relations:
no gas phase resistance

$$E = \left.\frac{dX_A}{dZ}\right|_{z=0} \Big/ (X_{Ab} - 1) \tag{22}$$

gas phase resistance

$$E = (1 + 1/\mathrm{Sh}) \left.\frac{dX_A}{dZ}\right|_{z=0} \Big/ (X_{As} - 1)\,. \tag{23}$$

Linearization Method of Hikita and Asai

The approximate methods of calculation of the reaction factor are usually based on the work of van Krevelen and Hoftijzer[5], which deals with the calculation of the reaction factor for irreversible bimolecular reaction. Hikita and Asai[4] used the method for calculation of the reaction factor for irreversible reaction of any nonnegative reaction order. Onda and coworkers[6] then used the results of Hikita and Asai[4] to derive the relation for calculation of the reaction factor also in the case of reversible, consecutive and parallel reactions.

All the above linearization approximation techniques assumed reaction order to be equal to one ($n = 1$) with all other reaction rate parameters set to constant values within the film. The approximate values of the reaction factor E differ at most 6 per cent from exact values for second and third order reactions and no gas phase resistance. However, the difference for other reaction orders and the cases, where gas phase resistance is considered is higher, as it will be illustrated further on. These differences thus substantiate the introduction of new approximate method of calculation of the reaction factor.

The relation for the reaction factor obtained through linearization follows from the solution of Eq. (*18*) with boundary conditions (*19*) and (*21*) ($n = 1$):

$$E_{HA} = \frac{\sqrt{(M)}(1 - X_{As}\,\mathrm{sech}\,\sqrt{M})}{(1 - X_{As})\tanh\sqrt{M}}\,. \tag{24}$$

The relation (*24*) differs from the relation given by Hikita and Asai[4], as the authors[4] used the simplifying assumption, that the concentration of the component A at the end of the film for the physical absorption is equal to zero.

If finite rate of mass transfer in gas phase is considered, then we shall obtain in the same manner on solving Eq. (*18*) with boundary conditions (*20*) and (*21*):

$$E_{HA} = \frac{(\mathrm{Sh} + 1)\sqrt{M}}{1 - X_{As}} \cdot \frac{1 - X_{As}\,\mathrm{sech}\,\sqrt{M}}{\sqrt{M} + \mathrm{Sh}\tanh\sqrt{M}}\,. \tag{25}$$

Approximate Method Based on Perturbation Solutions

Differential equation (*18*) can be written in the form

$$\frac{\mathrm{d}^2 X_A}{\mathrm{d}Z^2} = \varepsilon f(X_A)\,, \tag{26}$$

where parameter $\varepsilon \in (0, \infty)$. For the values of the parameter $\varepsilon \ll 1$ regular perturbation solutions can be constructed, and for $\varepsilon \gg 1$ singular perturbation methods can be used for construction of the solution[7,8]. For intermediate values of $\varepsilon \sim 0(1)$, approximating function is used for description of the dependence of solution of Eq. (*26*) (*i.e.* Eq. (*18*)) on parameter ε. All solutions can be obtained for different forms of reaction rate functions $f(X_A)$. Here we shall present as an example in explicit form the solutions for n-th order irreversible reaction, where $\varepsilon = M$ and $f(X_A) = [n + 1)/2]\, X_A^n$. Only first order perturbation terms will be given, as the accuracy so obtained is considered satisfactory. Higher order perturbation solutions are given elsewhere[7].

Regular perturbation solution. a) If boundary condition (*19*) is considered, then regular perturbation solution up to the first order terms can be obtained in the form

$$E_{RA} = 1 + [M((n + 1)/2)\, P/(1 - X_{As})] \tag{27}$$

where

$$P = -\frac{(n + 2)(X_{As} - 1) + 1 - X_{As}}{(X_{As} - 1)^2 (n + 1)(n + 2)}\,. \tag{28}$$

b) If boundary condition (*20*) is considered, then enhancement (reaction) factor can be calculated as

$$E_{RA} = 1 + \frac{\mathrm{Sh} + 1}{\mathrm{Sh}} \cdot \frac{M(n + 1)/2)\, P}{1 - X_{As}}\,, \tag{29}$$

where

$$P = -\frac{\mathrm{Sh}[P_1^{n+2} - X_{As}^{n+2} + P_1^{n+1} P_2 (n + 2)]}{P_2^2 (n + 1)(n + 2)(1 + \mathrm{Sh})} \tag{30}$$

and

$$P_1 = (X_{As} + \mathrm{Sh})/(1 + \mathrm{Sh}) \tag{31}$$

$$P_2 = [\mathrm{Sh}(X_{As} - 1)]/(1 + \mathrm{Sh})\,. \tag{32}$$

Singular perturbation solution. First order singular perturbation solution can be obtained for boundary condition (*19*) in the form (agrees with the solution for fast reaction)

$$E_{SA} = (M)^{1/2} (1 - X_{As}^{n+1})^{1/2}/(1 - X_{As}) \tag{33}$$

and for boundary condition (*20*) as

$$E_{SA} = (1 - X_{Ab}) (1 + \mathrm{Sh})/(1 - X_{As}) . \tag{34}$$

Where the value of X_{Ab} can be obtained on solving nonlinear equation

$$\mathrm{Sh}(X_{Ab} - 1) + (M)^{1/2} (X_{Ab}^{n+1} - X_{As}^{n+1})^{1/2} = 0 \tag{35}$$

by proper numerical method (*e.g.* Newton method).

If continuous dependence of the enhancement factor E on the parameter M is constructed, then we can proceed in reverse order and evaluate this dependence without use of any iterative numerical solution. For chosen value of E and value of Sherwood number Sh we can calculate X_{Ab} from relation (*36*)

$$X_{Ab} = 1 - \frac{E(1 - X_{As})}{1 + \mathrm{Sh}} \tag{36}$$

and then the corresponding value of M from (*37*)

$$M = \frac{\mathrm{Sh}^2(1 - X_{Ab})^2}{X_{Ab}^{n+1} - X_{As}^{n+1}} . \tag{37}$$

Approximating Function

On the basis of knowledge of functional forms of the solution for low and high values of the parameter $\varepsilon = M$ we can construct approximating function describing the dependence of reaction factor E for intermediate values of the parameter M, if the dependence of solution on the parameter is monotonic and smooth. Let regular perturbation solution is valid for values of $\sqrt{M} \in (0; M_1)$ and singular perturbation solution is valid for values of $\sqrt{M} \in (M_2; \infty)$.

For the cases, where gas phase resistance is not negligible, altogether eight different forms of the approximating functions were tested. They will be listed in the order used in the Tables, where the exact and approximate values are compared. In cases, where gas phase resistance is not considered, three approximating functions were tested: *1*) straight line, $\sim E_{PA}$, *2*) polynomial $\sim E_{1A}$, *3*) exponential $\sim E_{3A}$. These last three approximation functions appear to be the most convenient, both with respect to the simplicity of evaluation of parameters and comparably high accuracy. The following eight types of approximating functions were tested

a) Linear function

$$E_{PA} = A_1 \sqrt{M} + A_2 ; \qquad (38)$$

b) Approximating function with the same slopes as regular and singular solution connected through the inscribed $\sim E_{KA}$ (the results are not comparable with the complexity of the function).

c) Polynomial function E_{1A}

$$E_{1A} = A_3 + A_4 Z + A_5 Z^2 + A_6 Z^3 , \qquad (39)$$

where

$$Z = (\sqrt{M} - M_1)/(M_2 - M_1) ; \qquad (40)$$

d) Power law function

$$E_{2A} = A_{10} M^{A11/2} + A_{12}$$

e) Exponential function

$$E_{3A} = A_7 \exp(A_8 \sqrt{M}) + A_9 \qquad (41)$$

f) Function E_{4A}

$$E_{4A} = A_{13} \,.\, A_{14}^{\sqrt{M}} + A_{15}$$

g) Function E_{TA}

$$E_{TA} = A_{16} \tanh \sqrt{M} + A_{17}$$

h) Function E_{CA}

$$E_{CA} = A_{18} \coth \sqrt{M} + A_{19} .$$

Constants A_i in approximating function are evaluated from the known functional values of chemical factor and its derivatives with respect to $\sqrt{M}$ at the points $\sqrt{M} = M_1$ and $\sqrt{M} = M_2$.

If we shall denote

$$E_1 = E(M_1) ; \quad E_2 = E(M_2) \qquad (42)$$

$$E'_1 = \frac{\mathrm{d}E}{\mathrm{d}\sqrt{M}} \bigg| \sqrt{M} = M_1 \quad E'_2 = \frac{\mathrm{d}E}{\mathrm{d}\sqrt{M}} \bigg| \sqrt{M} = M_2$$

then

$$A_1 = (E_2 - E_1)/(M_2 - M_1) , \qquad (43)$$

$$\begin{aligned} A_2 &= E_1 - A_1 M_1 \,, \\ A_3 &= E_1 \,, \\ A_4 &= E'_1(M_2 - M_1) \,, \\ A_5 &= 3(E_2 - E_1) - (M_2 - M_1)(2E'_1 + E'_2) \,, \\ A_6 &= 2(E_1 - E_2) + (M_2 - M_1)(E'_1 + E'_2) \end{aligned} \tag{44}$$

and

$$\begin{aligned} A_8 &= (\ln E'_1 - \ln E'_2)/(M_1 - M_2) \,, \\ A_7 &= (E_1 - E_2)/[\exp(A_8 M_1) - \exp(A_8 M_2)] \,. \end{aligned} \tag{45}$$

Hence if functional forms of regular and singular perturbation solutions are known and the values of M_1 and M_2 are chosen, then parameters of approximating functions can be easily evaluated. The values of M_1 and M_2 can be obtained apriori from the estimates of the errors of approximation of individual perturbation solutions and checked against exact numerical solution. This was done for the power – law kinetics with the values of the order of reaction chosen as $n = 3$; 2·5; 2; 1·5; 1; 0·5 and the values of dimensionless concentrations at the film end $X_{As} = 0{\cdot}01$; 0·05; 0·1. It is found, that best values are $M_1 = 0{\cdot}6$ and $M_2 = 2{\cdot}5$.

The approximating functions will reasonably well describe the course of dependence $E = E(\sqrt{M})$ in situations, where this dependence is sufficiently smooth and does not have extrema within the interval $\sqrt{M} \in (M_1, M_2)$. These requirements are satisfied for the forms of reaction rate functions studied.

Numerical Solution

Differential equation (*18*) with boundary conditions (*19*), (*20*) and (*21*) forms boundary value problem. To solve it for specified values of M, n and Sh we have to use some iterative numerical procedure, how it was done *e.g.* by Onda and coworkers[6], which can be connected with relatively high computer time requirements. However, if we wish to determine continuous dependence of the enhancement factor on the parameter M, we can for boundary conditions (*19*) and (*21*) transform the original problem in such a way, that it can be solved as initial value problem. The procedure is well known from the solution of other engineering problems[9]. Let us introduce new coordinate variable

$$U = \sqrt{M} \cdot Z \tag{46}$$

and rewrite Eq. (*18*) into the form

$$\mathrm{d}^2 X_A / \mathrm{d}U^2 = [(n + 1)/2] \, X_A^n \tag{47}$$

with boundary conditions

$$U = 0 \qquad X_{\mathrm{A}} = 1 \tag{48}$$

$$U = \sqrt{M} \quad X_{\mathrm{A}} = X_{\mathrm{As}}\,. \tag{49}$$

If we choose the value of the derivative at the point $(\mathrm{d}X_{\mathrm{A}}/\mathrm{d}U)|_{U=\sqrt{M}}$ and integrate until the boundary condition (*48*) is satisfied then the length of integration interval gives the value of $\sqrt{M}$ and reaction factor can be calculated as

$$E = -\left.\frac{\mathrm{d}X_{\mathrm{A}}}{\mathrm{d}U}\right|_{\mathrm{U}=0} \frac{\sqrt{M}}{1 - X_{\mathrm{As}}}\,. \tag{50}$$

Hence no iteration procedure is required and every iteration gives one point on the dependence $E = E(\sqrt{M})$. For boundary conditions (*20*) and (*21*) we have used iterative procedure, as the above method is not usefully applicable here[7].

Comparison of Exact and Approximate Solutions

Approximate solution obtained from the above relations will be compared with exact solutions both in graphical and tabular form.

In Fig. 1 are compared the exact values of enhancement factor with the approximate values obtained by the linearization method (Hikita and Asai[4]) and proposed method for half order reaction ($n = 0{\cdot}5$) and $X_{\mathrm{As}} = 0{\cdot}01$. It can be seen from

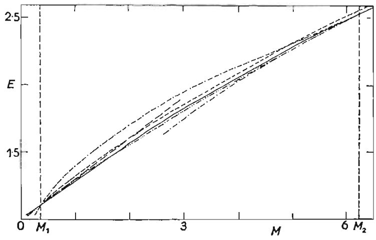

FIG. 1

Comparison of the Exact Values of the Enhancement Factor E (full line) with the Values Obtained from the Approximation Procedures

Half order reaction, $x_{\mathrm{AS}} = 0{\cdot}01$; ——— exact solution ($E$), — — — regular solution (E_{RA}), — · — singular solution (E_{SA}), -——— linearization solution (Hikita, E_{HA}), --·--· approximation function E_{PA}, -···-··· approximation functions $E_{1\mathrm{A}}$ and $E_{3\mathrm{A}}$.

the figure, that proposed approximation functions E_{1A}, E_{3A} are more accurate than that proposed by Hikita and Asai[4].

Similar comparison can be studied in detail for the third order reaction and the value of $X_{As} = 0{\cdot}1$ in Table I. The proposed approximation has relative error less than 3%, which is approximately half of the error of the Hikita and Asai approximation.

Effect of Gas Phase Resistance

In Table II a comparison between exact and approximate solution is shown for the second order reaction, where $X_{As} = 0{\cdot}05$ and Sh = 2. As can be seen from the Table, the linearization approximation fails to describe exact values of E, particularly at higher values of M. Similar conclusions can be drawn also for other reaction orders and values of the Sherwood number. The approximation method proposed in this paper gives values of the reaction factor, which differ from the exact values always less than 6%. On the contrary, the error of the approximate values obtained from the linearization procedure can be four times as high.

TABLE I

Comparison of Exact and Approximate Values of Reaction Factor

Third order reaction, $X_{As} = 0{\cdot}1$, $M_1 = 0{\cdot}6$, $M_2 = 2{\cdot}5$.

M	Exact solution	Solution by Hikita method	Regular perturbation solution	Singular perturbation solution	Polynom. approx. function E_{1A}	Exponent. approx. function E_{3A}	Valid
0·2235	1·024	1·013	1·024	—	—	—	regular solution valid
0·3228	1·049	1·040	1·050	—	—	—	
0·4386	1·090	1·074	1·092	—	—	—	
0·4978	1·114	1·095	1·119	—	—	—	
0·5748	1·151	1·126	1·159	—	1·159	1·159	
0·6787	1·207	1·173	1·221	—	1·213	1·218	approximation function valid
0·8265	1·298	1·254	1·328	0·318	1·311	1·309	
1·053	1·462	1·402	1·533	1·170	1·463	1·463	
1·445	1·794	1·714	2·002	1·606	1·761	1·768	
2·315	2·650	2·572	3·573	2·572	2·577	2·583	
3·874	4·320	4·291	—	4·304	4·566	4·420	singular solution valid
4·458	4·961	4·943	—	4·953	—	—	
5·344	5·941	5·932	—	5·938	—	—	
6·961	7·731	7·733	—	7·734	—	—	

TABLE II

Comparison of Exact and Approximate Values of Reaction Factor, Second Order Reaction, $X_{As} = 0{\cdot}05$, Sh = 2

$\sqrt{M}$	E	E_{RA}	E_{SA}	E_{HA}	E_{PA}	E_{1A}	E_{2A}	E_{3A}	E_{4A}	E_{TA}	E_{CA}	Valid
0·1	1·004	1·002	—	1·002	0·956	—	—	—	—	—	—	regular
0·2	1·008	1·008	—	1·010	0·979	—	—	—	—	—	—	solution
0·3	1·017	1·017	—	1·022	1·001	—	—	—	—	—	—	valid
0·4	1·030	1·031	—	1·039	1·024	—	—	—	—	—	—	
0·5	1·046	1·048	—	1·059	1 047	—	—	—	—	—	—	
0·6	1·064	1·070	—	1·084	1·070	1·070	1·070	1·070	1·070	1·070	1·070	
0·8	1·108	1·124	—	1·143	1·115	1·111	1·098	1·100	1·100	1·221	1·297	approximation
1·0	1·160	1·134	0·932	1·211	1·161	1·145	1·130	1·132	1·132	1·337	1·419	function
1·5	1·289	1·436	1·176	1·401	1·274	1·211	1·226	1·223	1·223	1·509	1·552	valid
2·0	1·419	1·775	1·358	1·587	1·388	1·284	1·340	1·332	1·332	1·579	1·595	
2·5	1·542	2·21	1·500	1·751	1·502	1·405	1·471	1·461	1·461	1·606	1·610	
3·0	1·634	—	1·616	1·889	1·616	1·616	1·616	1·616	1·616	1·616	1·616	
4·0	1·800	—	1·793	2·102	—	—	—	—	—	—	—	singular
5·0	1·927	—	1·925	2·254	—	—	—	—	—	—	—	solution
7·0	2·111	—	2·110	2·456	—	—	—	—	—	—	—	valid
10·0	2·287	—	2·286	2·632	—	—	—	—	—	—	—	

This is illustrated also in the Fig. 2 where the approximate and the exact solutions are compared for half order reaction, $X_{AS} = 0{\cdot}01$ and Sh = 2. We can see, both from the tables and the figures, that the quality of approximation in the region $\sqrt{M} \in (M_1, M_2)$ is within the limits of the above given errors if we choose any of the approximate functions E_{PA}, E_{1A}, E_{3A}.

Estimation of the Effect of Chemical Reaction on the Rate of Transport

For small values of the parameter $\sqrt{M}$ regular perturbation solution is valid with error less than three per cent; hence this solution can be used for estimation of the values of the parameter $M, M = M_c$ where values of enhancement factor will differ from that in the case of physical absorption by more than Δ. Thus we shall obtain for power-law kinetics, if we set

$$\Delta = E - 1, \text{ that} \tag{51}$$

$$M_c = [2(1 - X_{As}) \,.\, \Delta]/(n + 1)\, P\,, \tag{52}$$

where P is given by Eq. (*28*). When also gas phase resistance is considered, we can obtain

$$M_c = 2\,\mathrm{Sh}(1 - X_{As}) \,.\, \Delta/(\mathrm{Sh} + 1)\,(n + 1)\, P \tag{53}$$

where P is given by relations (*30*), (*31*) and (*32*).

From the above relations we thus can easily evaluate for any type of reaction kinetics whether the effect of chemical reaction on the rate of transport has to be considered.

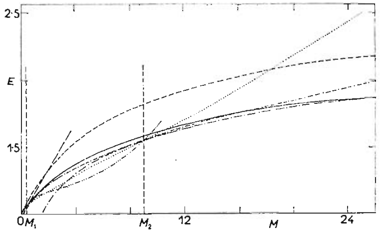

FIG. 2

Comparison of the Exact Values of the Enhancement Factor E (full line) with the Values Obtained from the Approximation Procedures

Half order reaction $X_{AS} = 0{\cdot}01$, Sh = 2; *cf.* Fig. 1 for legend.

LIST OF SYMBOLS

A	reaction component
B	reaction component
C_A	concentration A in the liquid phase
D	diffusion coefficient
E	enhancement (reaction) factor
H_A	equilibrium constant
J_A	flux density of the component A
k	reaction rate constant
k_{CA0}	mass transfer coefficient without chemical reaction
k_{gCA}	mass transfer coefficient in the gas phase
M	parameter — see Eqs (*13*), (*14*)
n	reaction order
P	parameter — see Eqs (*28*), (*30*)
Sh	Sherwood number
s_0	film thickness
U	transformed dimensionless coordinate
X_A	dimensionless concentration of component A
z	distance within the film
Z	independent variable
ε	perturbation parameter
Δ	the effect of chemical reaction on enhancement factor

Subscripts

b	surface condition
c	critical value of the parameter
g	gas phase
o	physical absorption
s	value at the end of the film

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