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Mass transfer with complex chemical reaction in gas–liquid systems—II: Effect of unequal diffusivities on consecutive reactions

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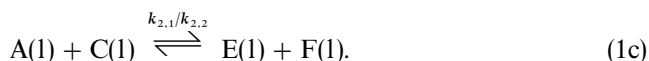
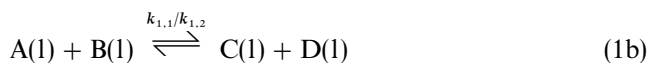
Abstract

A fundamental description of gas–liquid mass transfer with reversible consecutive reaction has been given. The Higbie penetration theory has been used and numerical simulations were carried out for isothermal absorption. Although the model can be adapted to reactions of general stoichiometric and kinetic orders, results have been provided for unit orders only. In Part I, results have been presented for the case of equal diffusivities of all the chemical species involved. In Part II, the effect of unequal diffusivity on the absorption rate and, hence, the overall enhancement factor in consecutive reaction systems has been presented in detail. Results presented here are dedicated to the case where both reaction steps are considered to be reversible. Finally, the model presented in this paper has been used to determine the selectivity towards the intermediate species using data previously reported in literature. The model system of chlorination of *p*-cresol in 1,2,4-dichlorobenzene has been used for this purpose. The strong influence of the mass transfer parameters on the selectivity of the intermediate has been shown. © 1998 Elsevier Science Ltd. All rights reserved.

Keywords: Gas absorption; Consecutive reactions; Modelling; Mass transfer

1. Introduction

The consecutive reaction stoichiometry considered is



Part I (Vas Bhat et al., 1998) of this work deals with consecutive systems with equal diffusivities of all components. It was shown that the overall enhancement factor was the summation of the enhancement factors for the individual reaction steps [reactions (1b) and (1c)]. In addition to the effect of reversibility on the gas absorption behaviour, an analysis of absorption into loaded solutions was also presented. Finally, an approximate

technique to evaluate the final enhancement factor was developed. The influence of various physical and/or chemical parameters were studied, namely, K_1 and K_2 which are the equilibrium constants of reactions (1b) and (1c) respectively and K_{R2} , defined as the ratio of the forward reaction rates of reactions (1c) to (1b) as indicated in Eq. (2a).

$$K_{R2} = \frac{k_{2,1}}{k_{1,1}}. \quad (2a)$$

Results have been presented as enhancement factors, E_A , defined as

$$E_A = \frac{N_A}{k_L(A_i - A_0)} \quad (2b)$$

and the Hatta number, Ha , defined as

$$Ha = \frac{\sqrt{k_{1,1}B_0D_A}}{k_L}. \quad (2c)$$

From Eq. (2c) it is clear that the definition of the Hatta number is based on the first reaction (1b). The Hatta numbers were varied by changing the liquid mass transfer coefficient, k_L , or the kinetic rate constant, $k_{1,1}$. The

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Table 1
Program input parameters

Variable	Value	Units
A_i	10	mol m^{-3}
B_T	40	mol m^{-3}
k_L	10^{-4} – 10^{-7}	m s^{-1}
$k_{1,1}$	0.25 – 2.6×10^5	$\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$
K_1	0.01–100	—
K_2	0.01–100	—
K_{R2}	10^{-5} – 10^2	—
α	10^{-3}	—
D_B	10^{-9}	$\text{m}^2 \text{s}^{-1}$

variables used in the simulations presented in this work are given in Table 1.

In order to maintain brevity, Part II deals with the effect of a change in diffusivity only for the case where both reactions (1b) and (1c) are reversible, as it is for this case that maximum deviations from the equal diffusivity situation are observed. Since this paper aims to understand the influence of species diffusivities on the overall mass transfer phenomenon, the diffusivity ratios have been varied between exaggerated extremes to magnify these effects. Consequently, these values of diffusion coefficients should not be expected to occur in real systems, though the effects that they produce may be observed in reality.

2. Influence of species diffusivity

Diffusivity of each chemical species has been varied individually. Results have been presented as a function of the diffusivity ratio of the species concerned,

defined as

$$r_i = \frac{D_i}{D_B} \quad (3)$$

where D_i is the diffusion coefficient of species 'i'.

2.1. Diffusivity of A

On account of the vast range of calculations possible, only some significant phenomena and/or non-trivial results have been elucidated here.

The effect of a change in the diffusivity of A on the mass transfer behaviour is shown in Fig. 1 where r_A is varied between two extreme ratios of 0.1–10 ($K_1 = 10$; $K_2 = 100$). In general, a higher enhancement is observed for a lower mobility of A. This stems from the fact that, a lower mobility of the gaseous species results in a greater concentration gradient near the gas–liquid interface and, consequently, a higher driving force. There is a two-step increase in the enhancement similar to that observed in the case of equal diffusivities. The intermediate asymptotic enhancement factor ($E_{\infty 1}$) can be calculated from standard methods such as the one presented by DeCoursey and Thring (1989).

2.1.1. Effect of K_1

The effect of K_1 on the mass transfer behaviour is observed in Fig. 2(a) and (b) for $r_A = 10$ and 0.1, respectively ($K_2 = 100$; $K_{R2} = 10^{-5}$). As is seen for reversible reactions with equal diffusivities, the values of the intermediate ($E_{\infty 1}$) and final enhancement factors (E_{∞}) increase with K_1 .

However, in case of a low mobility of A [Fig. 2(b)], some peculiar, not a priori expected, effects are observed for the case of high K_1 values (typically $K_1 = 10$ –100). In

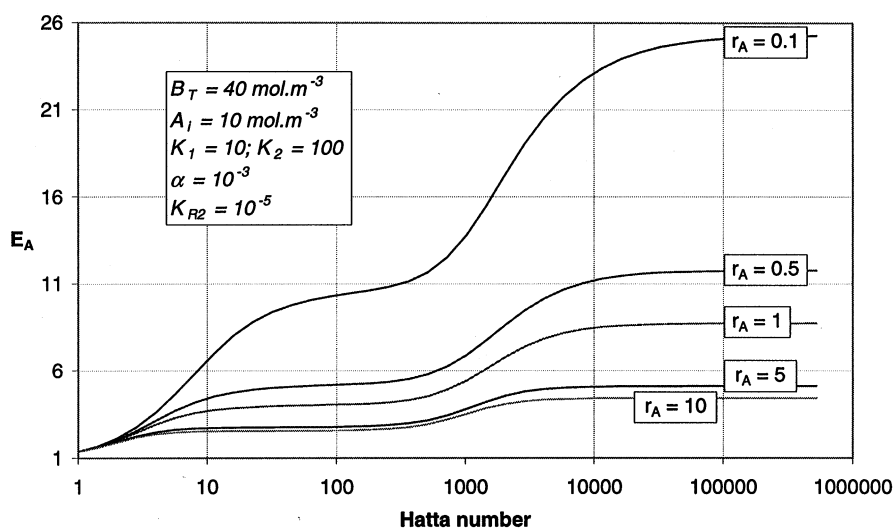


Fig. 1. Effect of diffusivity of A on enhancement.

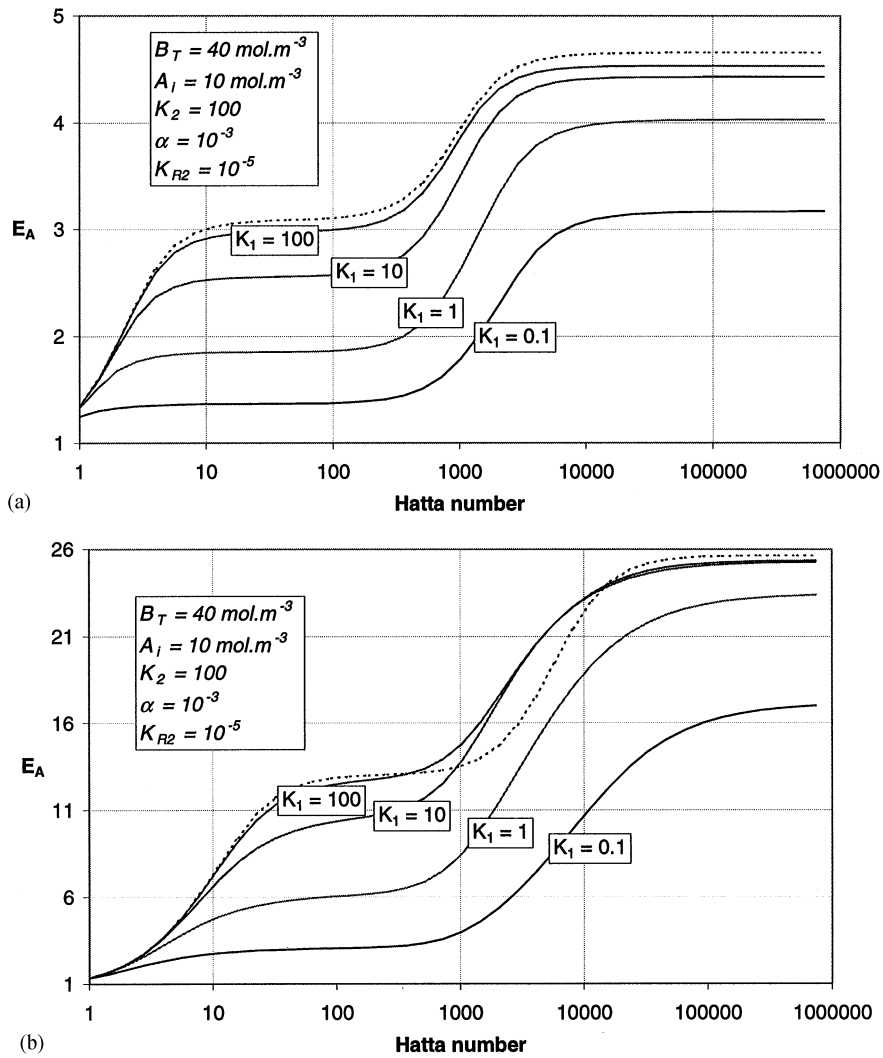


Fig. 2. (a) Effect of K_1 on enhancement for high mobility of A ($r_A = 10$). $K_2 = 100$; $K_{R2} = 10^{-5}$. Dashed line indicates case when both reactions are irreversible. (b) Effect of K_1 on enhancement for low mobility of A ($r_A = 0.1$). $K_2 = 100$; $K_{R2} = 10^{-5}$. Dashed line indicates case when both reactions are irreversible.

the region between $E_{\infty 1}$ and E_{∞} , the enhancement factor for the reversible case is higher than that for both irreversible reactions. This is explained by understanding the phenomena occurring within the penetration depth once the *kick-in point* has been crossed. Due to the relatively low diffusivity of A ($r_A = 0.1$), the reaction zone between A and B [due to the instantaneous reversible reaction 1(b)] is formed close to the interface. C and D formed at this zone can diffuse either towards the interface or to the liquid bulk. The fraction of C that moves towards the interface is in a position to react with A [via reaction 1(c)]. In contrast, the fraction of C that diffuses towards the liquid bulk can react with D via the backward reaction (1b) to give back A and B. Hence, the lower mobility of A is overcome by the transport of A towards the bulk in the form of more mobile components, C and D. In order to check this hypothesis, various simulations were carried out for different input parameters, the results of

which are presented in Table 2. These simulations are for a single Hatta number, in the transition region between $E_{\infty 1}$ and E_{∞} . The following points are of interest:

- If the hypothesis is correct, the additional enhancement should not be observed when reaction (1b) is irreversible. This is confirmed on comparing cases 1 and 2. Conversely, when reaction (1b) is reversible while reaction (1c) is kept irreversible (case 3) the enhancement rises again. This clearly indicates that the additional enhancement observed in this region is on account of the backward reaction of reaction (1b).
- According to the hypothesis, the additional enhancement of A is caused by its transfer into the penetration depth in the form of more mobile components, C and D. Changing the mobility of C would also affect the enhancement caused by reaction (1c). Instead, the mobility of D has been increased which results in higher

Table 2

Effect of diffusivity of A on the enhancement factor: $K_1 = 10$; $K_2 = 100$; $K_{R2} = 10^{-5}$; $k_L = 9.77 \times 10^{-8} \text{ m s}^{-1}$; $Ha = 4096$

Case	r_A	r_C	r_D	$r_E = r_F$	(1b)	(1c)	E_A
1	0.1	1	1	1	Reversible	Reversible	20.53
2	0.1	1	1	1	Irreversible	Reversible	17.31
3	0.1	1	1	1	Reversible	Irreversible	20.98
4	0.1	1	1	1	Irreversible	Irreversible	17.53
5	0.1	1	10	1	Reversible	Reversible	21.13
6	0.1	1	10	1	Irreversible	Reversible	17.31
7	0.1	1	10	1	Reversible	Irreversible	21.55
8	0.1	1	10	1	Irreversible	Irreversible	17.53
9	0.1	0.1	0.1	1	Reversible	Reversible	16.34
10	0.1	0.1	0.1	1	Irreversible	Reversible	19.76
11	0.1	0.1	0.1	1	Reversible	Irreversible	16.75
12	0.1	0.1	0.1	1	Irreversible	Irreversible	20.65

enhancement factors (compare cases 1 and 5 and cases 3 and 7). This confirms the hypothesis that higher enhancement is obtained due to the transfer of A in the form of more mobile species.

- Finally, in order to show that this phenomenon is only true for low mobility of A, the diffusivities of C and D have also been reduced (cases 9–12). As can be expected, the enhancement factor is higher for the case when both reactions are irreversible and the hypothesis is no longer valid.

2.2. Diffusivity of C

Since C is both a reaction product as well as a reactant, a variation in its diffusivity is expected to have a significant effect on the mass transfer behaviour of the system. In order to distinguish between the various underlying phenomena, enhancement factors for two extreme cases of r_C (0.01 and 10) have been compared (Fig. 3). The simulations have been carried out for $K_1 = K_2 = 100$ and $K_{R2} = 10^{-5}$. Four distinct regions are observed (named positions I, II, III and IV). Dimensionless concentration profiles of all the chemical species over the penetration depth have been presented for each position. The corresponding values of simulation parameters at each of these positions are given along with the figures.

2.2.1. Position I

Since this position is before the *kick-in point* of reaction (1c), there is no production of E and F as can be seen in Fig. 4(a) and (b). From the figure it is clear that reaction (1b) is instantaneous, indicated by the formation of a reaction zone between A and B. Thus, near the interface, the concentration of A is governed by the equilibrium constant, K_1 . At higher r_C (Fig. 4b), C produced by reaction (1b) is transferred faster into the bulk on account of its greater mobility, thereby reducing the concentration of C near the interface. In order to maintain K_1 con-

stant, the concentration of A near the interface also falls. This increases the concentration gradient of A near the interface and, in turn, the enhancement. Conversely, for low mobility of C [Fig. 4(a)], C formed by reaction between A and B remains near the interface where it increases the concentration of A on account of the equilibrium constraint. This results in a lower enhancement in the absorption of A.

2.2.2. Position II

At lower r_C , the reduced mobility of C prevents it from diffusing into the liquid bulk, which causes the concentration of C near the interface to rise [Fig. 5(a)]. This means that reaction (1c) will 'kick-in' at correspondingly lower Hatta numbers as compared to the case with a higher r_C . This is clearly observed in Fig. 3 where at position II, reaction (1c) is already influencing the mass transfer for $r_C = 0.01$ while its effect is much less for $r_C = 10$. This is also observed from the concentration profiles of E (and F) in Fig. 5(a) and (b). For a low mobility of C ($r_C = 0.01$), C formed [via reaction (1b)] remains near the interface where it is available for reaction with A [via reaction 1(c)]. Due to the high concentration of C, the absorption rate of A is very high as well, leading to large enhancement. For a high mobility of C ($r_C = 10$), C can diffuse away from the interface so that its interfacial concentration is low (as compared to $r_C = 0.01$) and, hence, the absorption rate of A is also low.

2.2.3. Position III

On increasing the Hatta number from position II to position III (Fig. 3), there is an increase in enhancement due to the reaction between C and A via reaction (1c). For a low r_C , C is formed by reaction (1b) away from the interface. A fraction of this C formed diffuses towards the interface where it reacts with A. At lower Hatta numbers (closer to position II), the diffusion rate is sufficient to supply reaction (1c). As the Hatta number is increased

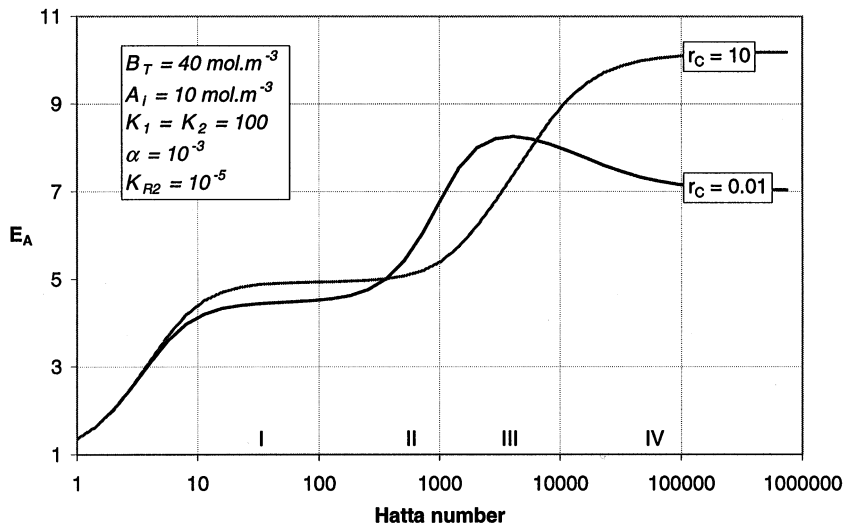
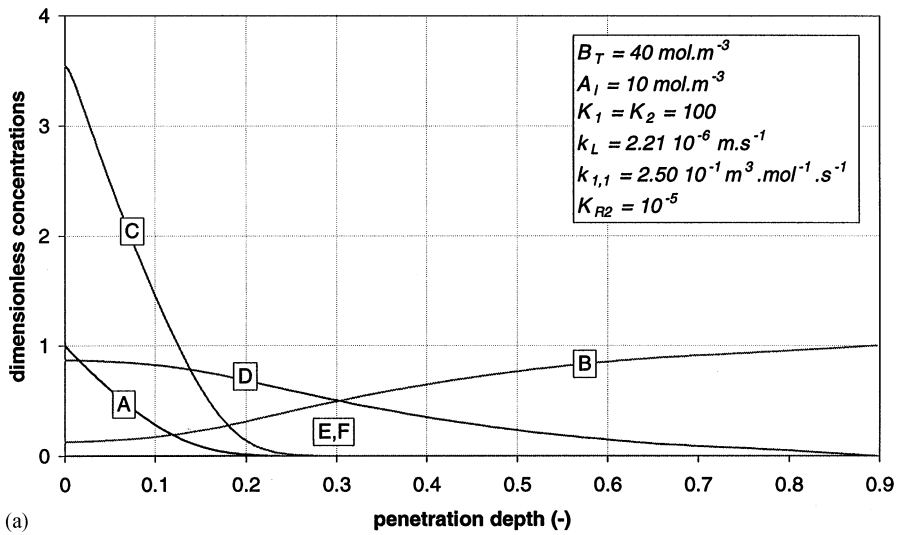
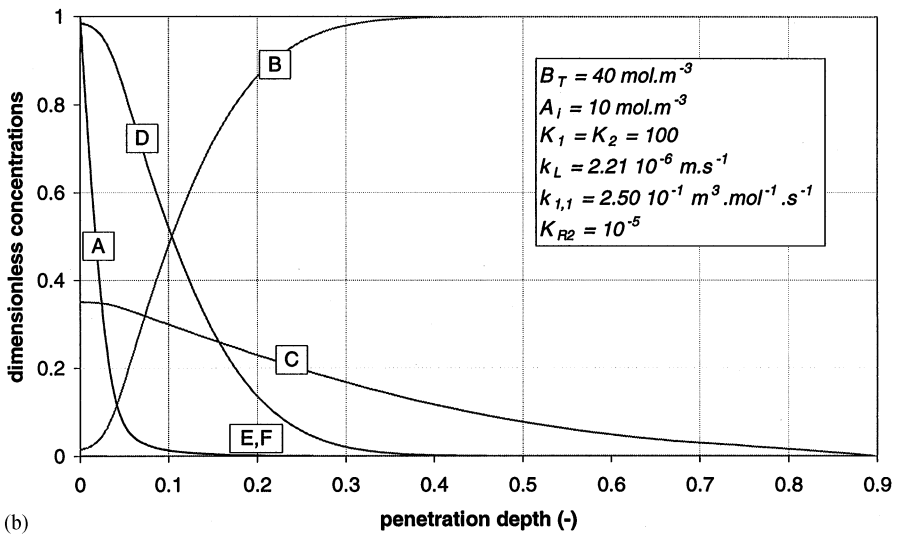


Fig. 3. Effect of diffusivity of C on enhancement. $K_1 = K_2 = 100$; $K_{R2} = 10^{-5}$.



(a)



(b)

Fig. 4. (a) Concentration profiles at position I: $r_C = 0.01$. Profiles at end of the contact time. $Ha = 45.2$; $E_A = 4.47$. (b) Concentration profiles at position I: $r_C = 10$. Profiles at end of the contact time. $Ha = 45.2$; $E_A = 4.91$.

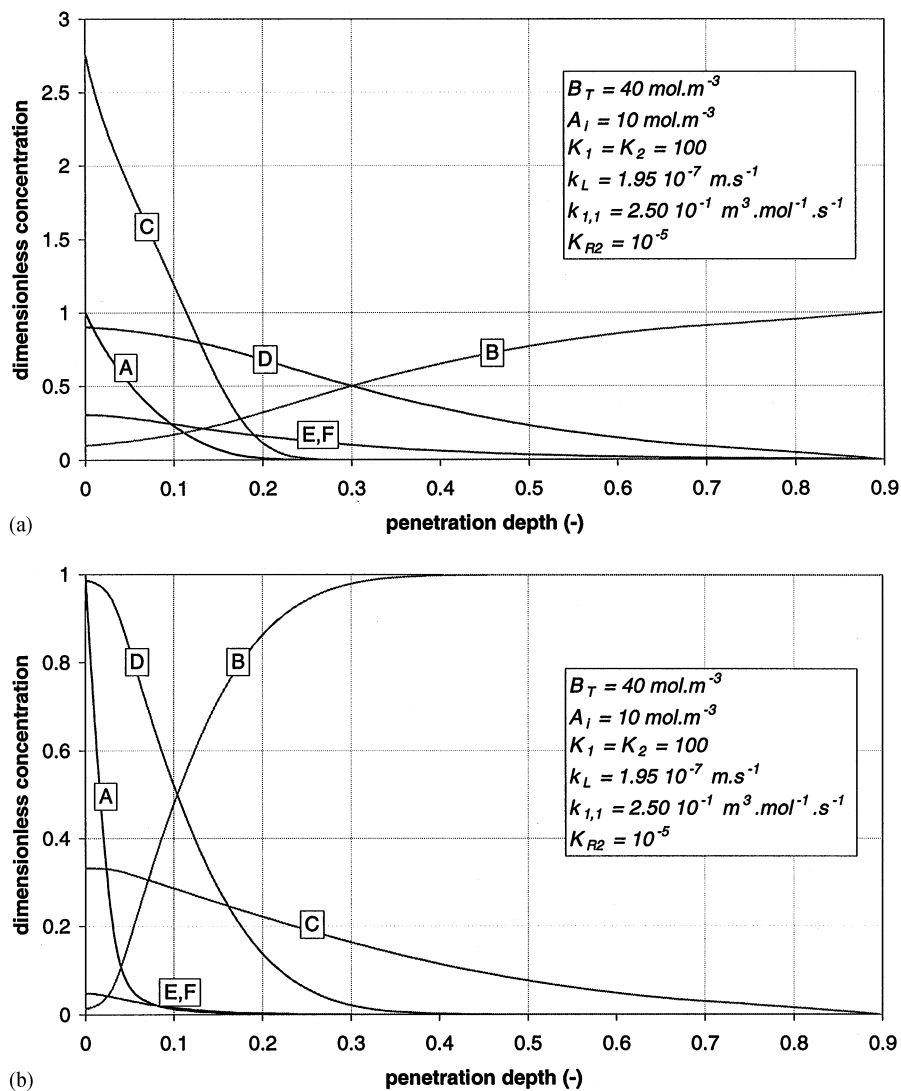


Fig. 5. (a) Concentration profiles at position II: $r_c = 0.01$. Profiles at end of the contact time. $Ha = 512$; $E_A = 5.42$. (b) Concentration profiles at position II: $r_c = 10$. Profiles at end of the contact time. $Ha = 512$; $E_A = 5.07$.

further (closer to position III), the diffusion of C towards the interface becomes limiting, thereby reducing the concentration of C near the interface [Fig. 6(a)]. With a reduction in the concentration of C near the interface, the influence of reaction (1c) on enhancement also reduces. Another factor opposing the absorption of A into the liquid is the high concentration of E (and F) present near the interface. This (along with the low concentration of C) forces the concentration of A to rise in the vicinity of the interface on account of the equilibrium constraint of reaction (1c). At position III the effect of increasing enhancement due to the forward reaction, (1c) equals in magnitude to the reduction in enhancement due to the equilibrium constraint, K_2 . As a result, a maximum in the enhancement curve is achieved.

This maximum in enhancement is not observed for a high mobility of C ($r_c = 10$; Fig. 3). Here, the rate of

diffusion of C towards the interface is sufficiently high to supply reaction (1c) even beyond position III. The concentration of C near the interface is higher than for the case of $r_c = 0.01$ [Fig. 6(a) and (b)]. Consequently, reaction (1c) is able to influence enhancement beyond position III as can be seen in Fig. 3. In addition, the high concentrations of E (and F) near the interface do not increase the concentration of A close to the interface as the concentration of C is high enough to maintain the equilibrium condition of reaction (1c). Therefore, this opposing effect to enhancement (as seen in the case of a low mobility of C) is considerably weaker for a high r_c .

2.2.4. Position IV

Here both reactions (1b) and (1c) are instantaneous with respect to mass transfer as can be observed from Fig. 7(a) and (b). Thus, the equilibrium constants, K_1 and

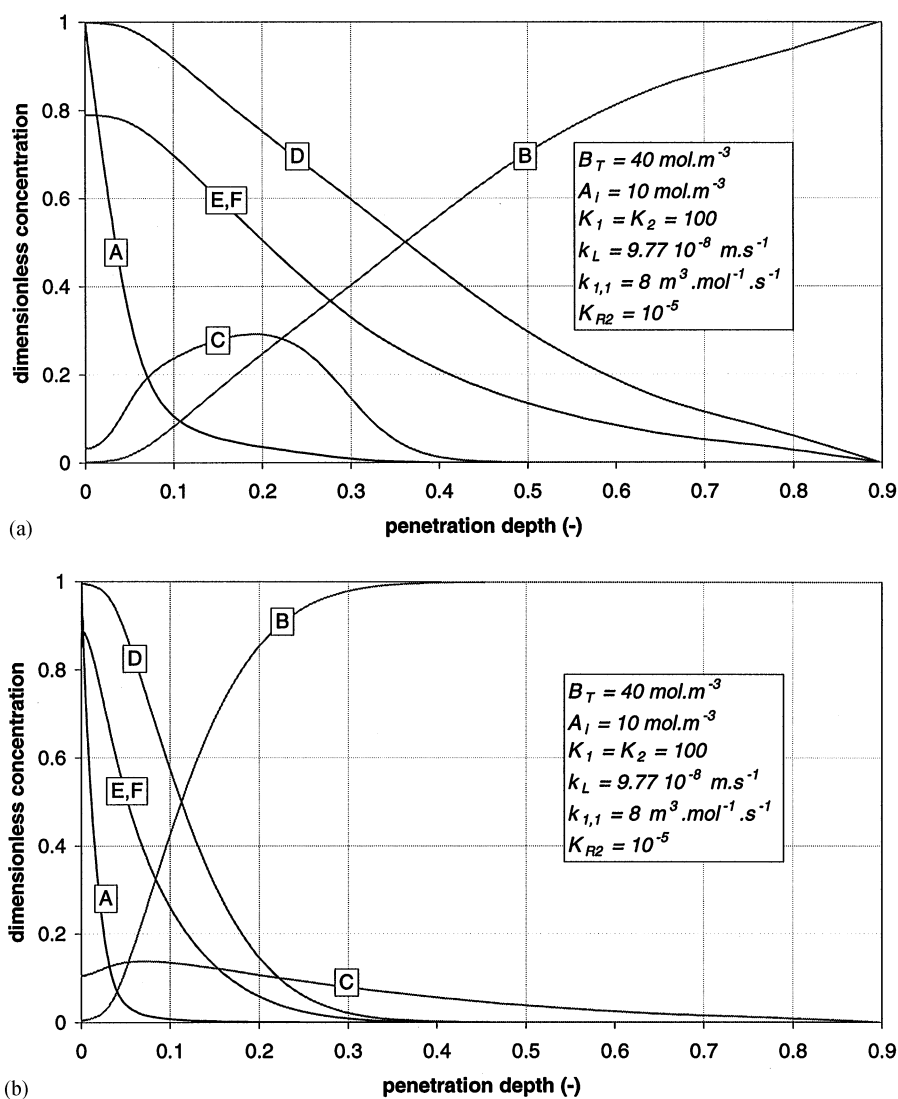


Fig. 6. (a) Concentration profiles at position III: $r_C = 0.01$. Profiles at end of the contact time. $Ha = 5790$; $E_A = 8.19$. (b) Concentration profiles at position III: $r_C = 10$. Profiles at end of the contact time. $Ha = 5790$; $E_A = 7.99$.

K_2 , determine the concentrations of all components. For a case of lower mobility of C [$r_C = 0.01$; Fig. 7(a)], concentration of C near the interface is very low due to the transport limitation of C towards the interface. This combined with the high concentration of E (and F) near the interface forces the concentration of A to rise in the vicinity of the interface, which opposes the absorption of A and reduces the enhancement factor. In order to verify this hypothesis, simulations with identical process parameters and with reaction (1c) maintained irreversible were carried out (Fig. 8). The enhancement factor, in this case, does not reduce beyond position III, confirming that the reduction in the case of lower mobility is caused by the equilibrium constraint of reaction (1c).

This effect is not observed for higher mobilities [$r_C = 10$; Fig. 7(b)], as the concentration of C near the interface is higher (than $r_C = 0.01$). This prevents an in-

crease in the concentration of A near the interface even though the concentration of reaction products E (and F) may be high. Consequently, the infinite enhancement reached with high r_C is greater than that with a lower r_C .

3. Influence of mass transfer factors on selectivity

A number of examples of gas absorption with consecutive reaction are found in the organic process industry, namely the halogenation, alkylation and oxidation of aromatic compounds. In all these cases, the selectivity towards a particular product is desired. It has been shown earlier (van de Vusse, 1966a, b; Hashimoto et al., 1968) that the mass transfer factors, such as k_L , can significantly influence selectivity in systems involving consecutive reactions. For a review of previous research

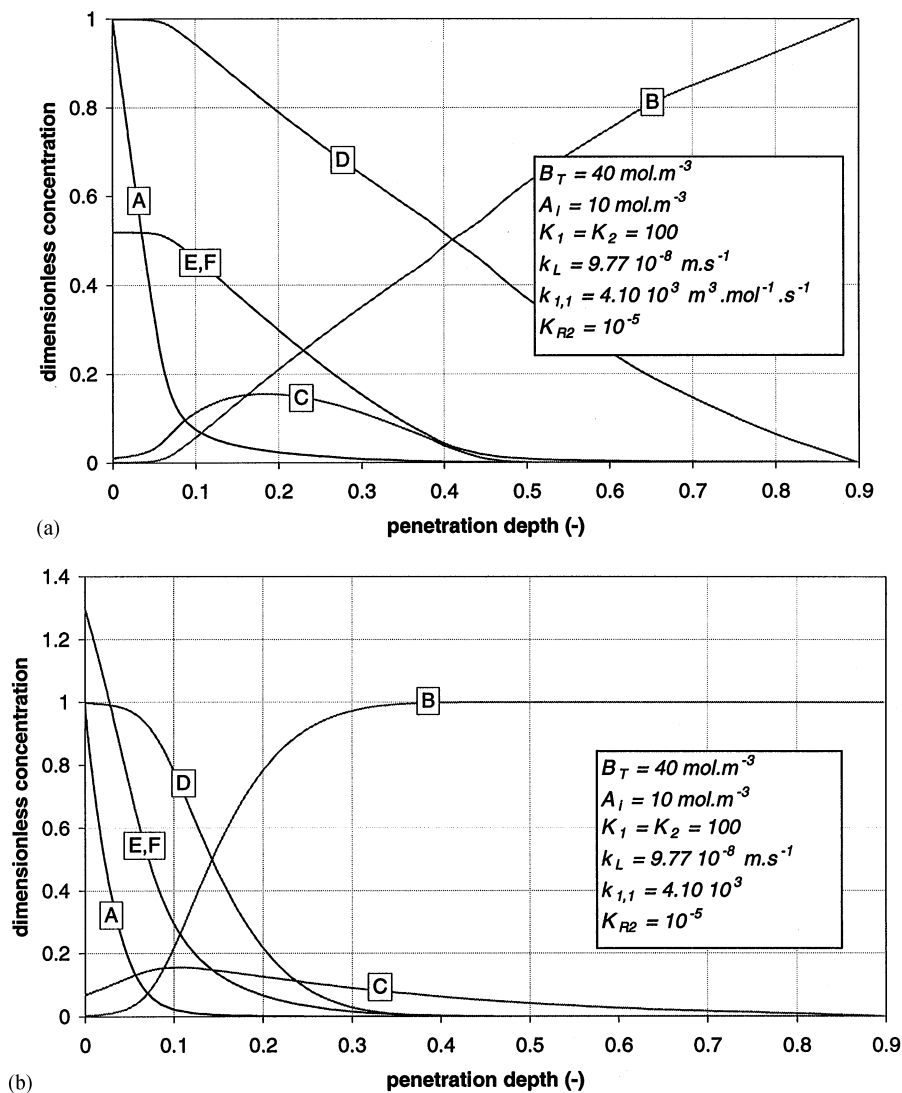
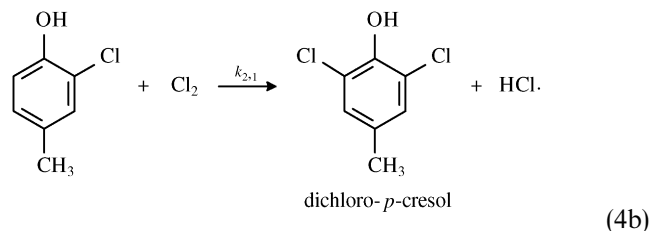
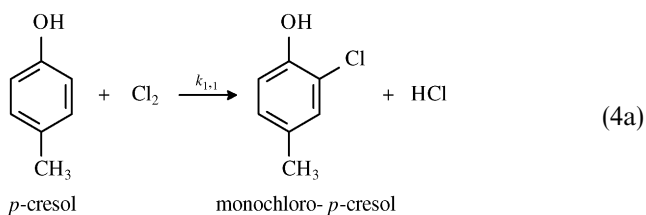


Fig. 7. (a) Concentration profiles at position IV: $r_c = 0.01$. Profiles at end of the contact time. $Ha = 1.31 \times 10^5$; $E_A = 7.12$. (b) Concentration profiles at position IV: $r_c = 10$. Profiles at end of the contact time. $Ha = 1.31 \times 10^5$; $E_A = 10.13$.

determining selectivity in consecutive reaction systems, the reader is referred to Darde et al. (1983). In order to validate the theoretical predictions of selectivity, experiments with different model reaction systems have been carried out in the past. van de Vusse (1966) used the chlorination of *n*-decane. However, in order to limit the number of by-products, the chlorination of *p*-cresol was subsequently used (Teramoto et al., 1970; Pangarkar and Sharma, 1974; Darde et al., 1984).



The flux model described in this paper has been used to determine differential selectivity for the chlorination of *p*-cresol in 1,2,4-trichlorobenzene. The reaction scheme considered is given by reaction (4a) and (4b). The production of the intermediate product, monochloro-*p*-cresol (MCPC) should be maximised, whereas that of the undesired dichloro-*p*-cresol (DCPC) should be as low as possible. The input data for the same has been taken from Pangarkar and Sharma (1974), see Table 3. Since no

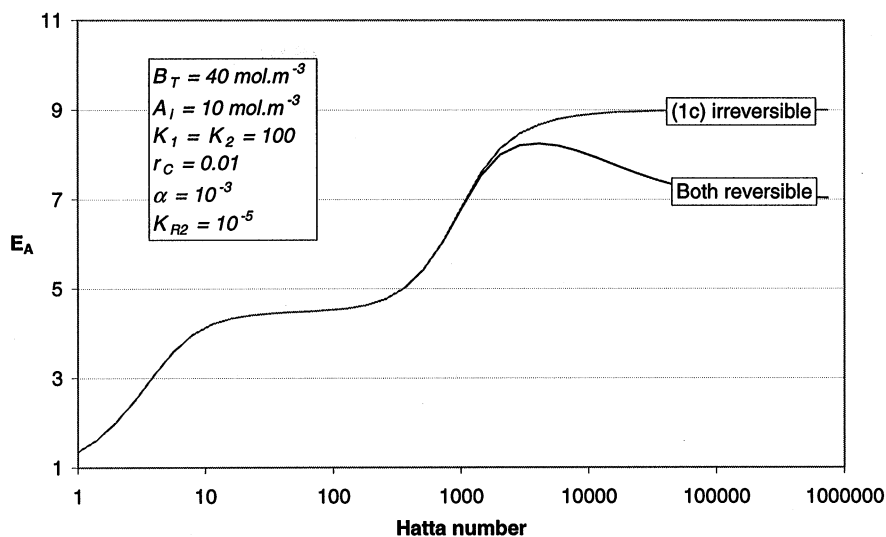


Fig. 8. Effect of irreversibility of reaction (1c) on enhancement for low mobility of C.

Table 3
Input parameters for chlorination of *p*-cresol in 1,2,4-trichlorobenzene (simulation results presented in Fig. 9)

Parameter	Value	Units
T	373.15	K
$[Cl_2]_i$	270	$mol\ m^{-3}$
$[p\text{-cresol}]_0$	4000	$mol\ m^{-3}$
$k_{1,1}$	0.19	$m^3\ mol^{-1}\ s^{-1}$
$k_{2,1}$	0.015	$m^3\ mol^{-1}\ s^{-1}$
D_{Cl_2}	5.4×10^{-9}	$m^2\ s^{-1}$
$D_{p\text{-cresol}}$	3.9×10^{-9}	$m^2\ s^{-1}$
D_{MCPC}	3.3×10^{-9}	$m^2\ s^{-1}$
k_L	$10^{-7}\text{--}10^{-1}$	$m\ s^{-1}$

(Taken from Pangarkar and Sharma, 1974).
Liquid phase assumed to be unloaded.

information of equilibrium constants for the system is available, both reactions are assumed to be irreversible. By varying the mass transfer coefficient, k_L , the Hatta number has been changed over a wide range ($0.01 < Ha < 10^4$) which covers all regimes of mass transfer. The fully developed concentration profiles (at the end of the Higbie contact time) of *p*-cresol, MCPC and DCPC, were numerically integrated over the penetration depth to obtain the average concentration of each species. The Simpson's 1/3rd rule was used for this purpose. These values were used to determine the differential selectivity, σ , and the overall conversion of *p*-cresol, ζ , defined as:

$$\sigma = \frac{[MCPC]}{[DCPC]} \quad (5a)$$

$$\zeta(\%) = \left(1 - \frac{[p\text{-cresol}]_{\text{avg}}}{[p\text{-cresol}]_0} \right) \quad (5b)$$

where the square parenthesis indicate concentrations. It is important to note that the parameters, σ and ζ , are

based on concentrations within the liquid package and within a single contact time.

The variation of σ and ζ with the Hatta number has been presented in Fig. 9. A significant influence of the mass transfer parameters on selectivity is observed. This has been reported earlier, among others, by van de Vusse (1966a, b), Teramoto et al. (1970) and Pangarkar and Sharma (1974). At high k_L values, corresponding to low Hatta numbers, the rate of mass transfer is much greater than the kinetic rate so that the overall absorption is determined by the rate of reaction (4a). As the Hatta number increases, the extent of reaction (4b) increases as well, thereby increasing the formation of DCPC. This, in turn, steadily reduces the selectivity towards MCPC. However, the production of MCPC is attractive only at significant conversions of *p*-cresol. As expected, the conversion curve increases with Hatta number as it depends directly on the reaction between Cl_2 and *p*-cresol [reaction (4a)]. Thus, increasing the Hatta number increases the enhancement, that in turn influences conversion due to the greater availability of Cl_2 in the penetration depth. In actual operation a compromise will have to be met between maximising selectivity on the one hand and conversion on the other. It is interesting to note that the conversion curve does not form an intermediate plateau as is expected of consecutive reaction schemes. This is because at the process temperature (100°C), the value of K_{R2} is rather high ($\sim 8 \times 10^{-2}$) so that reaction (4b) *kicks-in* even before reaction (4a) has reached its infinite enhancement value.

4. Conclusions

A fundamental description of gas–liquid mass transfer for isothermal reversible consecutive reactions has been

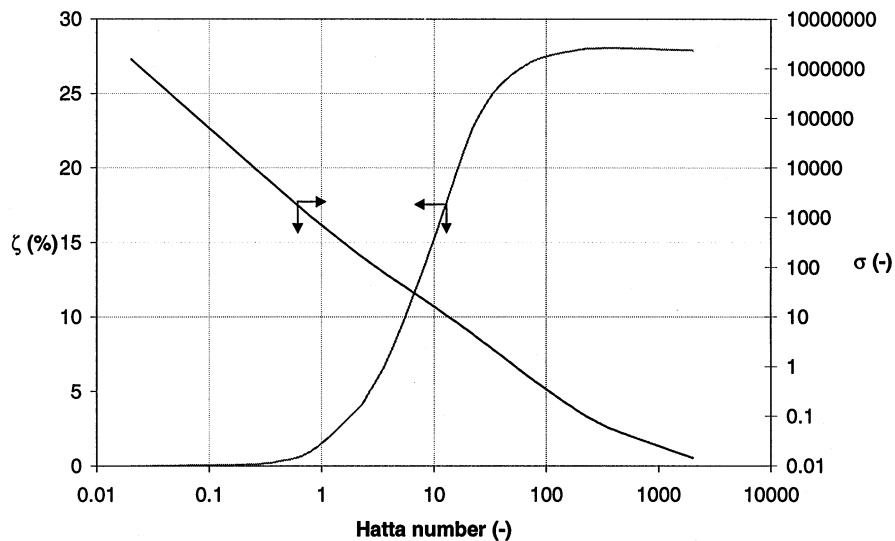


Fig. 9. Variation of selectivity, σ , and conversion, ζ , with Hatta number. Chlorination of *p*-cresol in 1,2,4-trichlorobenzene. Input data given in Table 3. Average concentrations determined at end of contact time.

Table 4
Selection of enhancement factors at different Hatta numbers (additional parameters given in Table 1 and the respective figures)

Figure	Ha	E_A		
		$r_A = 0.1$	$r_A = 5$	$r_A = 10$
1	4	3.60	2.48	2.37
	128	10.47	2.80	2.58
	1024	13.80	3.81	3.51
	741460	25.27	5.11	4.43
2(a) $r_A = 10$	4	$K_1 = 0.1$ 1.36	$K_1 = 10$ 2.37	$K_1 = 100$ 2.60
	128	1.38	2.58	3.00
	1024	1.79	3.51	3.87
	741460	3.17	4.43	4.53
2(b) $r_A = 0.1$	4	$K_1 = 0.1$ 2.32	$K_1 = 10$ 3.60	$K_1 = 100$ 3.66
	128	3.06	10.47	12.61
	1024	3.98	13.80	14.79
	741460	17.02	25.27	25.35

presented. Results for the case where both reactions are reversible have been presented for unequal diffusivities of the chemical species.

Of the various chemical species present, variations in the diffusivity of two of them show a significant effect on the overall mass transfer behaviour. These are essentially, the gas-phase component and the intermediate formed by the first reaction.

In the case of variation in the diffusivity of A, it has been shown that for low mobility, the enhancement for the case with both reactions reversible can be higher than that for the case with both reactions irreversible. This is explained by the fact that species A is transported within

the penetration depth in the form of other, more mobile, components.

In case of the intermediate, C, it is observed that the influence of the second reaction (1c) on the overall enhancement is observed at lower Hatta numbers for a lower mobility of C. Beyond the intermediate enhancement value, the overall enhancement is determined by two opposing factors. Forward reaction of reaction (1c) increases the enhancement. As the Hatta number is increased further, the backward reaction (1c) prevails which forces the enhancement to reduce. For low mobility of the intermediate, it has been shown that these opposing effects cause a maximum in the enhancement

curve before approaching the final infinite enhancement factor.

Finally, the model presented in this paper has been used to determine differential selectivity towards the intermediate in the consecutive reaction scheme. Experimental data presented previously by Pangarkar and Sharma (1974) for the chlorination of *p*-cresol have been used for this purpose. As has been reported earlier, a strong influence of mass transfer parameters on the selectivity of the intermediate was observed with selectivity reducing with an increase in Hatta number. In practice, however, a compromise needs to be reached between selectivity towards the intermediate on the one hand and conversion on the other. Due to lack of comprehensive data such as equilibrium constants, the full potential of the model could not be exploited.

The present model provides a rigorous mathematical analysis of the consecutive reaction system under conditions of unequal diffusivity. With a view of encouraging further numerical and/or approximate examination of this reaction scheme, a selection of results (obtained with this model) has been presented in Table 4.

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Notation

A	component A, concentration of component A, mol m^{-3}
A_T	total A in all forms ($= A_0 + D_0 + E_0$), dimensionless
B	component B, concentration of component B, mol m^{-3}
B_T	total B in all forms ($= B_0 + D_0$), dimensionless
C	component C, concentration of component C, mol m^{-3}
D	component D, concentration of component D, mol m^{-3}
D_{sub}	diffusivity, sub: component, $\text{m}^2 \text{s}^{-1}$
E	component E, concentration of component E, mol m^{-3}
E_A	enhancement factor, defined by reaction (2b), dimensionless
E_∞	final infinite enhancement factor, dimensionless
$E_{\infty 1}$	intermediate asymptotic enhancement factor, dimensionless
Ha	Hatta number, defined by reaction (2c), dimensionless

K_{sub}	equilibrium constant, sub: reaction number, dimensionless
K_{R2}	$k_{2,1}/k_{1,1}$, dimensionless
$k_{\text{sub}1, \text{sub}2}$	reaction rate constant sub1: reaction number, sub2: reaction direction, $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$
k_L	liquid-side mass transfer coefficient, m s^{-1}
N_A	gas flux, $\text{mol m}^{-2} \text{s}^{-1}$
r_{sub}	diffusivity ratio, defined by D_{sub}/D_B , sub: component, dimensionless

Greek letters

α	loading factor ($= A_T/B_T$), dimensionless
σ	differential selectivity, defined by Eq. (5a), dimensionless
ζ	conversion of <i>p</i> -cresol, defined by Eq. (5b), dimensionless

Subscripts

0	initial condition
G, g	gas phase
i	interface
L, l	liquid phase
red	reduced
T	total

Abbreviations

MCPC	monochloro- <i>p</i> -cresol
DCPC	dichloro- <i>p</i> -cresol

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