



A film Model for Gas Absorption with Chemical Reaction Accompanied by Heat Generation

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A Film Model for Gas Absorption with Chemical Reaction Accompanied by Heat Generation

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The rise of temperature at the gas-liquid interface due to heat generation and the relevant enhancement factor for the absorption rate are analysed for gas absorption accompanied by an instantaneous irreversible reaction and a first order irreversible reaction based on the film theory, allowing for the temperature dependence of the gas solubility, diffusivities of the relevant species and the reaction rate constant. Then, the analytical exact or approximate solutions for them are presented.

1. Introduction

In the physical absorption of highly soluble gas and chemical absorption, the temperature of the liquid phase, especially near the gas-liquid interface, rises due to the heat generation caused by the heat of solution and the heat of reaction. Consequently the physico-chemical properties, such as the gas solubility, diffusivity and reaction rate constant may vary essentially, affecting the gas absorption rate. The importance of such non-isothermal effects has been demonstrated for many systems¹⁻¹²). Thus, these effects on the absorption rate must be understood for reasonably designing industrial absorbers and gas-liquid reactors accompanied by a considerable evolution of heat.

In our previous papers^{13,14}), the penetration theory solutions for both the interface temperature rise and the enhancement factor to be applicable over a wide range of non-isothermal conditions, have been developed for the various absorption schemes, such as physical absorption, and absorption with an instantaneous irreversible reaction and a first order irreversible reaction, assuming the reasonable temperature dependence of the physico-chemical properties. Analytical results have been compared with those for the corresponding film theory solutions in view of analogy with some system behavior, but without referring to the film theory analysis in detail. In this paper, the film theory solutions for both reaction schemes are described as a supplement to the previous work¹⁴).

2. Assumptions

The temperature dependence of the physico-chemical properties, such as the gas solubility A_i , liquid phase diffusivities D_A and D_B of a solute gas and a reactant, respectively, and the reaction rate constant k may be reasonably represented over a wide range of temperature by the following expression¹⁴):

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$$Q = Q_0 (1 + \theta)^\epsilon \quad (Q = A_i, D_A, D_B \text{ and } k) \quad (1)$$

where

$$\theta = (T - T_0)/T_0, \quad \epsilon = E/RT_0 \quad (2)$$

Any other property than A_i , D_A , D_B and k is assumed constant, independently of temperature. Moreover, the same assumptions as in the previous paper¹⁴⁾ have been made in this analysis.

3. Instantaneous Irreversible Reaction

3.1. Rigorous solutions

Let us consider the case where the solute gas A dissolves into a liquid and then reacts irreversibly and instantaneously with the reactant B , which is already present in the liquid phase, according to the following reaction:



Basic differential equations and the relevant boundary conditions for the diffusions of species A and B , and of heat are given by:

For region I ($0 < x < x'$)

$$\frac{d}{dx} [(1 + \theta)^{\epsilon_{DA}} \frac{da}{dx}] = 0 \quad (3)$$

$$\frac{d^2\theta}{dx^2} = 0 \quad (4)$$

For region II ($x' < x < x_f$)

$$\frac{d}{dx} [(1 + \theta)^{\epsilon_{DB}} \frac{db}{dx}] = 0 \quad (5)$$

$$\frac{d^2\theta}{dx^2} = 0 \quad (6)$$

$$x = 0; a = (1 + \theta_i)^{\epsilon_S}, \theta = \theta_i,$$

$$-\lambda T_0 \frac{d\theta}{dx} = -D_{A0} A_{i0} (1 + \theta_i)^{\epsilon_{DA}} (-\Delta H_S) \frac{da}{dx} \quad (7)$$

$$x = x'; a = 0, b = 0, \theta = \theta',$$

$$-\lambda T_0 \left(\frac{d\theta}{dx} \right)_{II} = -\lambda T_0 \left(\frac{d\theta}{dx} \right)_{I} - D_{A0} A_{i0} (1 + \theta')^{\epsilon_{DA}} (-\Delta H_R) \frac{da}{dx},$$

$$-D_{A0} A_{i0} (1 + \theta')^{\epsilon_{DA}} \frac{da}{dx} = \frac{D_{B0} B_0}{\nu} (1 + \theta')^{\epsilon_{DB}} \frac{db}{dx} \quad (8)$$

$$x = x_f; \quad b = 1, \theta = 0 \quad (9)$$

where

$$a = A/A_{i0}, \quad b = B/B_0 \quad (10)$$

Subscripts I and II refer to the values when x approaches x' from region I and from region II, respectively. In a few of the previous studies^{9,12}, the film thickness for mass transfer has been taken to be different from that for heat transfer in view of the boundary layer concept, but equal film thickness is assumed here for comparison of the present analytical results with the Danckwerts analysis¹⁵. The solutions of Eqs.(3) – (6) are given by:

For region I ($0 < x < x'$)

$$a = \frac{(1 + \theta_i)^{\epsilon_S} [\left\{ (1 + \theta_i - (\theta_i - \theta') \frac{x}{x'}) \right\}^{1 - \epsilon_{DA}} - (1 + \theta')^{1 - \epsilon_{DA}}]}{(1 + \theta_i)^{1 - \epsilon_{DA}} - (1 + \theta')^{1 - \epsilon_{DA}}} \quad (11)$$

$$\theta = (\theta' - \theta_i) \frac{x}{x'} + \theta_i \quad (12)$$

For region II ($x' < x < x_f$)

$$b = \frac{[1 + \theta' \frac{x_f - x}{x_f - x'}]^{1 - \epsilon_{DB}} - (1 + \theta')^{1 - \epsilon_{DB}}}{1 - (1 + \theta')^{1 - \epsilon_{DB}}} \quad (13)$$

$$\theta = \frac{\theta' (x_f - x)}{x_f - x'} \quad (14)$$

Applying boundary conditions, Eqs. (7) and (8), one obtains the following expressions representing the interface temperature rise θ_i , the location x' of the reaction plane and the temperature rise θ' at the reaction plane:

$$\begin{aligned} & (1 + \theta_i)^{1 - \epsilon_{DA}} + \frac{\psi}{Le} (1 + \theta_i)^{\epsilon_S} (\epsilon_{DA} - 1) \\ & = \left[1 - \frac{\psi r q (\epsilon_{DB} - 1) (P + 1)}{PLe} \right]^{(\epsilon_{DA} - 1) / (\epsilon_{DB} - 1)} \end{aligned} \quad (15)$$

$$\frac{x'}{x_f} = \frac{1}{1 + \frac{\theta'}{\theta' - \theta_i} \frac{r q}{(1 + \theta_i)^{\epsilon_S}} \frac{\epsilon_{DB} - 1}{\epsilon_{DA} - 1} \frac{(1 + \theta_i)^{1 - \epsilon_{DA}} - (1 + \theta')^{1 - \epsilon_{DA}}}{1 - (1 + \theta')^{1 - \epsilon_{DB}}} } \quad (16)$$

$$\theta' = \left[1 - \frac{\psi r q (\epsilon_{DB} - 1) (P + 1)}{PLe} \right]^{1 / (1 - \epsilon_{DB})} - 1 \quad (17)$$

where

$$Le = \alpha/D_{A0}, \quad P = \Delta H_S/\Delta H_R, \quad q = B_0/\nu A_{i0}, \quad r = D_{B0}/D_{A0},$$

$$\psi = \alpha A_{i0} (-\Delta H_S)/\lambda T_0 \quad (18)$$

The absorption rate of the solute gas A is:

$$N_A = -D_{A0} A_{i0} (1 + \theta_i)^{\epsilon_{DA}} \left(\frac{da}{dx} \right)_{x=0} \quad (19)$$

$$= \frac{D_{A0} A_{i0} (\epsilon_{DA} - 1) (\theta' - \theta_i) (1 + \theta_i)^{\epsilon_S}}{x' [(1 + \theta_i)^{1-\epsilon_{DA}} - (1 + \theta')^{1-\epsilon_{DA}}]} \quad (20)$$

Defining the enhancement factor β as the absorption rate with heat effects relative to the isothermal physical absorption rate evaluated at the liquid bulk temperature, one obtains:

$$\beta = \frac{N_A}{D_{A0} A_{i0}/x_f} \quad (21)$$

$$= \frac{Le}{\psi} \left(\theta_i - \frac{\theta'}{P+1} \right) \quad (22)$$

Especially for $q = 0$, Eqs. (15) and (22) simplify to yield the solutions for physical absorption:

$$(1 + \theta_i)^{1-\epsilon_{DA}} + \frac{\psi}{Le} (1 + \theta_i)^{\epsilon_S} (\epsilon_{DA} - 1) = 1 \quad (23)$$

$$\beta = Le \theta_i / \psi \quad (24)$$

3.2. Results and discussion

Some of results calculated for instantaneous irreversible reaction are shown in Figs. 1–3. The broken lines for the interface temperature rise represent the solutions based on the ordinary Danckwerts model (ODM)¹⁵⁾, in which the physical properties are evaluated at liquid bulk temperature;

$$\theta_{OD,i} = \frac{\psi}{Le} \left[1 + \left(1 + \frac{1}{P} \right) r q \right] \quad (25)$$

while the broken lines for the enhancement factor present the isothermal enhancement factor given by:¹⁶⁾

$$\beta_{IS} = 1 + r q \quad (26)$$

In Fig. 2, the θ_i -lines for $-\epsilon_S = \epsilon_{DA} = 5$ and $-\epsilon_S = \epsilon_{DA} = 30$, which fall between the lines for $\epsilon_S = -5$ and $\epsilon_{DA} = 30$ and for $\epsilon_S = -30$ and $\epsilon_{DA} = 5$, have been omitted for clarity. As seen in Figs. 1 and 2, the interface temperature rise θ_i and the relevant en-

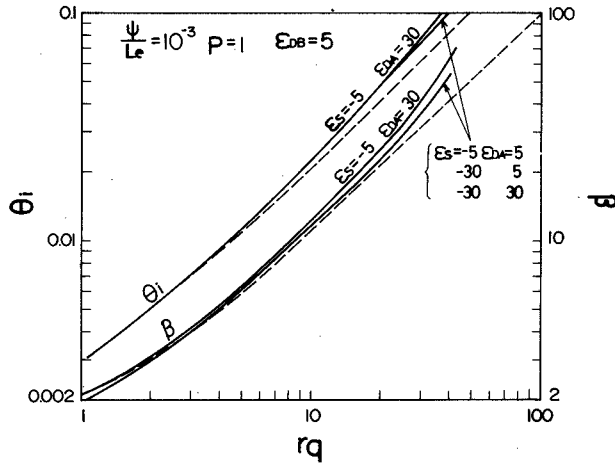


Fig. 1 Interface temperature rise θ_i and enhancement factor β for the instantaneous irreversible reaction.
— Rigorous solutions, Eqs. (15), (17) and (22).
---- ODM solutions, Eq. (25) for θ_i , and isothermal enhancement factor, Eq. (26) for β .

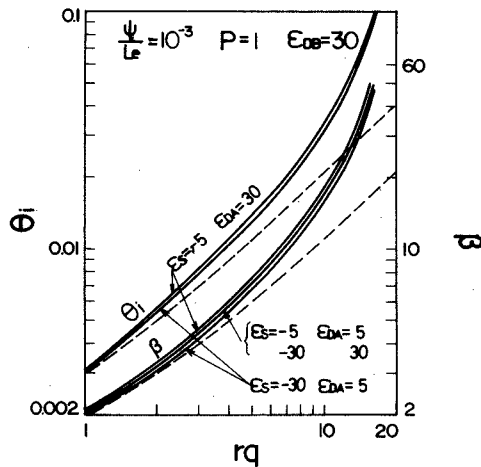


Fig. 2 Interface temperature rise θ_i and enhancement factor β for the instantaneous irreversible reaction.
Lines same as in Fig. 1.

enhancement factor β depend greatly on ϵ_{DB} and to a little extent on ϵ_S and ϵ_{DA} . This behavior might be explained by the fact that the reaction plane approaches the gas-liquid interface with an increase of rq , so that the diffusion of the reactant B to the interface becomes rate-determining. Thus, the departures of the rigorous solutions for θ_i from the ODM solution and for β from the isothermal enhancement factor increase with an increase of ϵ_{DB} . The effects of P and ψ/Le on the interface temperature rise θ_i are always substantial, but their effects on the enhancement factor β depend on the ϵ_{DB} values and become large with an increase of ϵ_{DB} . The effect of P for $\epsilon_{DB} = 30$ is shown in Fig. 3. It can be seen that the rigorous solutions for θ_i and β approach the ODM solution and isothermal enhancement factor, respectively with an increase of P .

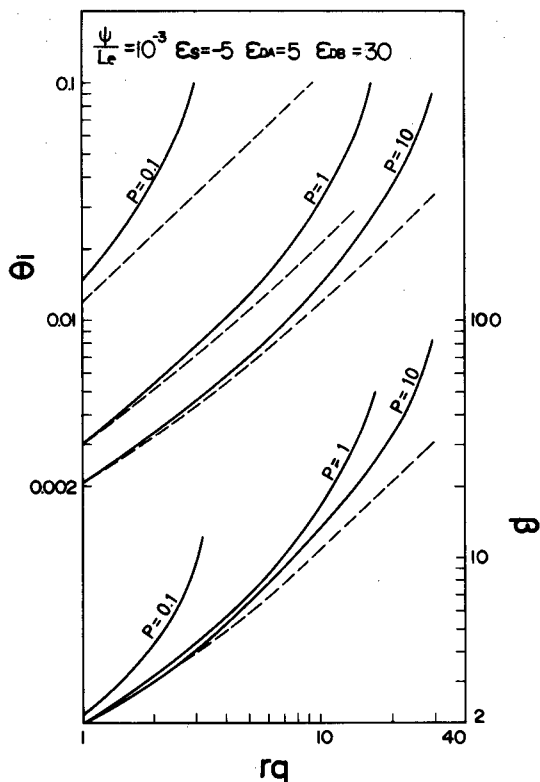


Fig. 3 Interface temperature rise θ_i and enhancement factor β for the instantaneous irreversible reaction.
Lines same as in Fig. 1.

4. First Order Irreversible Reaction

4.1. Approximate solutions

Let us consider the case in which the dissolved gas A reacts irreversibly according to the following reaction scheme:



This reaction is assumed to be first order with respect to the solute gas A , although the extension to a m -th order reaction might be done straightforwardly using the Hikita-Asai approximation¹⁷⁾.

The appropriate differential equations are:

$$D_{A0} \frac{d}{dx} \left[(1 + \theta)^{\epsilon_{DA}} \frac{da}{dx} \right] = k_0 (1 + \theta)^{\epsilon_R} a \quad (27)$$

$$\lambda T_0 \frac{d^2 \theta}{dx^2} = -k_0 A_{i0} (1 + \theta)^{\epsilon_R} (-\Delta H_R) a \quad (28)$$

with the boundary conditions

$$x = 0; a = (1 + \theta_i)^{\epsilon_S}, \theta = \theta_i$$

$$-\lambda T_0 \frac{d\theta}{dx} = -D_{A0} A_{i0} (1 + \theta_i)^{\epsilon_{DA}} (-\Delta H_S) \frac{da}{dx} \quad (29)$$

$$x = x_f; a = 0, \theta = 0 \quad (30)$$

The two sides of Eq.(27) are now multiplied by $-\Delta H_R A_{i0}$ and then added respectively to those of Eq.(28) to eliminate the reaction term.

This yields the following equation:

$$\frac{d}{dx} [D_{A0} A_{i0} (1 + \theta)^{\epsilon_{DA}} (-\Delta H_R) \frac{da}{dx} + \lambda T_0 \frac{d\theta}{dx}] = 0 \quad (31)$$

Integrating Eq.(31) twice with respect to x under the boundary conditions, Eqs.(29) and (30), and using the expression for the absorption rate N_A , Eq.(19) results in:

$$D_{A0} A_{i0} (-\Delta H_R) (1 + \theta_i)^{\epsilon_S} + \frac{\lambda T_0}{1 - \epsilon_{DA}} [(1 + \theta_i)^{1 - \epsilon_{DA}} - 1]$$

$$= -N_A (\Delta H_R + \Delta H_S) \int_0^{x_f} \frac{dx}{(1 + \theta)^{\epsilon_{DA}}} \quad (32)$$

The right hand side of this equation is not yet ready for evaluation, since the functional relation between θ and x is unknown. The approximate solution, which may be regarded as a substantially rigorous solution, can be obtained on the assumption that θ varies linearly with respect to x , as described in the previous paper¹⁴). The temperature profile in the liquid film for this model can be written as:

$$\theta = \theta_i \left(1 - \frac{x}{x_f}\right) \quad (33)$$

The substitution of Eq.(33) in Eq.(32) and subsequent integration lead to the following expression for the enhancement factor, which is defined by Eq.(21):

$$\beta = \frac{\theta_i [(\epsilon_{DA} - 1)(1 + \theta_i)^{\epsilon_S} + L e P \{1 - (1 + \theta_i)^{1 - \epsilon_{DA}}\}] / \psi}{(P + 1) [1 - (1 + \theta_i)^{1 - \epsilon_{DA}}]} \quad (34)$$

On the other hand, the substitution of Eq.(33) in Eq.(27) and integration with the relevant boundary conditions provide the concentration of the dissolved gas A in terms of the modified Bessel function of the first kind:

$$a = (1 + \theta_i)^{(2\epsilon_S + \epsilon_{DA} - 1)/2} \left[1 + \theta_i \left(1 - \frac{x}{x_f}\right)\right]^{(1 - \epsilon_{DA})/2}$$

$$\times \frac{I_p[\phi_2 \left\{ 1 + \theta_i \left(1 - \frac{x}{x_f} \right) \right\}^{\frac{\epsilon_R - \epsilon_{DA} + 2}{2}}] I_{-p}(\phi_2) - I_p(\phi_2) I_{-p}[\phi_2 \left\{ 1 + \theta_i \left(1 - \frac{x}{x_f} \right) \right\}^{\frac{\epsilon_R - \epsilon_{DA} + 2}{2}}]}{I_p(\phi_1) I_{-p}(\phi_2) - I_p(\phi_2) I_{-p}(\phi_1)} \quad (35)$$

where

$$p = \frac{|\epsilon_{DA} - 1|}{\epsilon_R - \epsilon_{DA} + 2}, \quad \gamma = x_f \sqrt{\frac{k_0}{D_{A0}}}$$

$$\phi_1 = \frac{2\gamma(1 + \theta_i)(\epsilon_R - \epsilon_{DA} + 2)^2}{(\epsilon_R - \epsilon_{DA} + 2)\theta_i}, \quad \phi_2 = \frac{2\gamma}{(\epsilon_R - \epsilon_{DA} + 2)\theta_i} \quad (36)$$

Using the definitions of N_A and β , from Eqs.(19) and (21), respectively, an additional expression, which should be solved in conjunction with Eq. (34) to obtain the simultaneous solutions for θ_i and β , becomes:

For $\epsilon_{DA} \leq 1$

$$\beta = (1 + \theta_i)^{\epsilon_{eff}} \gamma \frac{I_{p-1}(\phi_1) I_{-p}(\phi_2) - I_{1-p}(\phi_1) I_p(\phi_2)}{I_p(\phi_1) I_{-p}(\phi_2) - I_{-p}(\phi_1) I_p(\phi_2)} \quad (37)$$

For $\epsilon_{DA} > 1$

$$\beta = (1 + \theta_i)^{\epsilon_{eff}} \gamma \frac{I_{p+1}(\phi_1) I_{-p}(\phi_2) - I_{-(p+1)}(\phi_1) I_p(\phi_2)}{I_p(\phi_1) I_{-p}(\phi_2) - I_{-p}(\phi_1) I_p(\phi_2)} \quad (38)$$

where

$$\epsilon_{eff} = \epsilon_S + \frac{1}{2}(\epsilon_{DA} + \epsilon_R) \quad (39)$$

Here, ϵ_{eff} is the dimensionless effective activation energy of the isothermal limiting absorption rate with $\gamma \gg 1$.¹⁸⁾

$$N_{A,IS} = A_{i0} \sqrt{k_0 D_{A0}} \quad (40)$$

Next, we consider another approximate solution using the modified Danckwerts model (MDM) defined in our previous paper¹⁴⁾. In this model, the temperature-dependent properties are evaluated at the interface temperature θ_i . The MDM solutions for θ_i and β can be obtained from both the interface temperature rise on the basis of the ODM¹⁵⁾ and the isothermal enhancement factor¹⁸⁾

$$\theta_{OD,i} = \frac{\psi}{Le} \left[\left(1 + \frac{1}{P} \right) \gamma \coth(\gamma) - \frac{1}{P} \right] \quad (41)$$

$$\beta_{IS} = \gamma \coth(\gamma) \quad (42)$$

by substituting $Le (1 + \theta_{MD,i})^{-\epsilon_{DA}}$, $\beta_{MD} (1 + \theta_{MD,i})^{-(\epsilon_S + \epsilon_{DA})}$, $\gamma (1 + \theta_{MD,i})^{(\epsilon_R - \epsilon_{DA})/2}$ and $\psi (1 + \theta_{MD,i})^{\epsilon_S}$ for Le , β_{IS} , γ and ψ , respectively to finally yield:

$$\theta_{MD,i} = \frac{\psi}{Le} (1 + \theta_{MD,i})^{\epsilon_{DA} + \epsilon_S} \left[\left(1 + \frac{1}{P}\right) (1 + \theta_{MD,i})^{(\epsilon_R - \epsilon_{DA})/2} \right. \\ \left. \times \gamma \coth \left\{ \gamma (1 + \theta_{MD,i})^{(\epsilon_R - \epsilon_{DA})/2} \right\} - \frac{1}{P} \right] \quad (43)$$

$$\beta_{MD} = (1 + \theta_{MD,i})^{\epsilon_{eff}} \gamma \coth \left[\gamma (1 + \theta_{MD,i})^{(\epsilon_R - \epsilon_{DA})/2} \right] \quad (44)$$

4.2. Results and discussion

Some illustrative results are shown in Figs. 4 and 5. The calculations were performed for the following combinations of ϵ values:

$\epsilon_{eff} = 25$ ($\epsilon_S = -5, \epsilon_R = 30, \epsilon_{DA} = 30$), $\epsilon_{eff} = 10$ ($\epsilon_S = -10, \epsilon_R = 30, \epsilon_{DA} = 10$);
 $\epsilon_S = -10, \epsilon_R = 20, \epsilon_{DA} = 20$), $\epsilon_{eff} = 0$ ($\epsilon_S = -10, \epsilon_R = 15, \epsilon_{DA} = 5$; $\epsilon_S = -20,$
 $\epsilon_R = 30, \epsilon_{DA} = 10$; $\epsilon_S = -5, \epsilon_R = 5, \epsilon_{DA} = 5$; $\epsilon_S = -30, \epsilon_R = 30, \epsilon_{DA} = 30$),

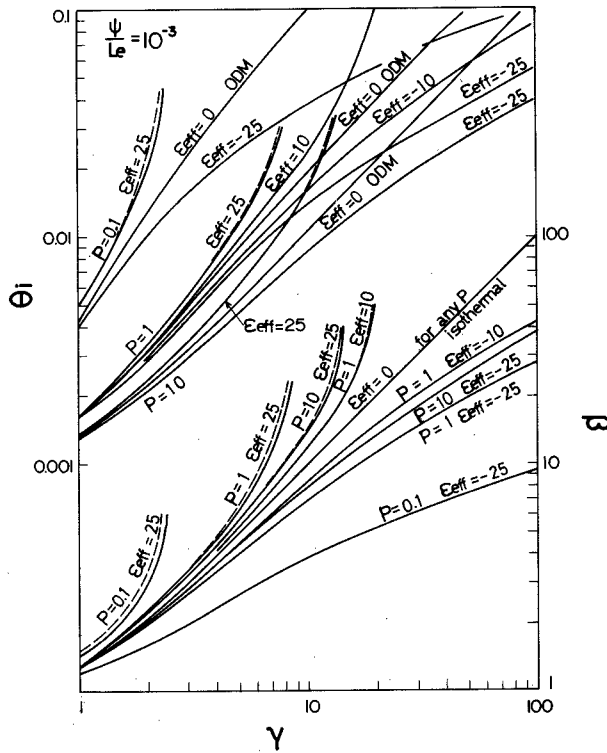


Fig. 4 Interface temperature rise θ_i and enhancement factor β for the first order irreversible reaction.
— Approximate solutions, Eqs. (34) and (38).
- - - MDM solutions, Eqs. (43) and (44).

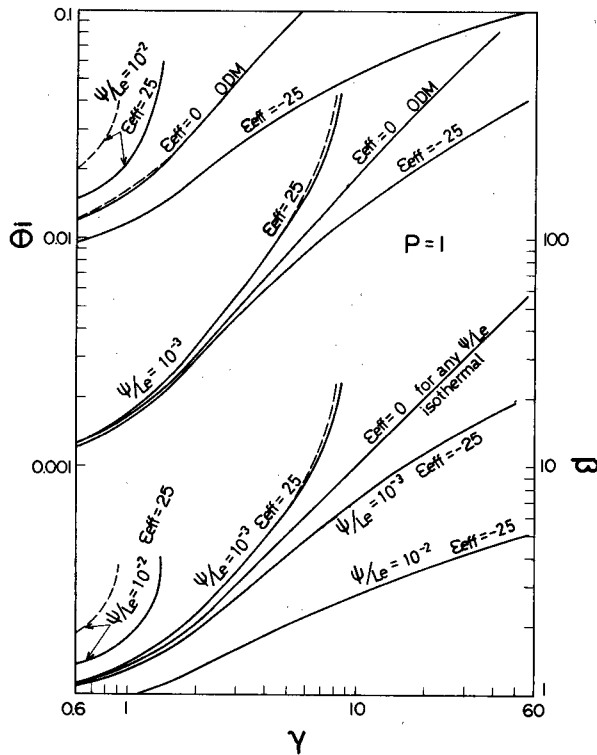


Fig. 5 Interface temperature rise θ_i and enhancement factor β for the first order irreversible reaction. Lines same as in Fig. 4.

$$\epsilon_{eff} = -10 (\epsilon_S = -20, \epsilon_R = 10, \epsilon_{DA} = 10; \epsilon_S = -20, \epsilon_R = 15, \epsilon_{DA} = 5), \text{ and} \\ \epsilon_{eff} = -25 (\epsilon_S = -30, \epsilon_R = 5, \epsilon_{DA} = 5)$$

The calculated results show no appreciable difference in both θ_i and β for any combination of ϵ values, as long as the ϵ_{eff} remains constant. Further, θ_i and β for $\epsilon_{eff} = 0$ agree well with the temperature rise based on the ODM, Eq. (41) and the isothermal enhancement factor, Eq. (42), respectively. It may be noted that θ_i always increases with a decrease of P and an increase of ψ/Le for given values of ϵ_{eff} , whereas the relevant enhancement factor β behaves in the same manner as θ_i only for $\epsilon_{eff} > 0$ and conversely for $\epsilon_{eff} < 0$. Such behavior of β might be explained by two counteracting effects due to temperature, the increase of diffusivity and reaction rate constant and the decrease of solubility, with temperature rise. The broken lines in these figures represent the MDM solutions, Eqs. (43) and (44). It may be seen that the MDM solutions, which are much easier to use, are also applicable with reasonable accuracy, except for the case of large values of ψ/Le ($= D_{A0} A_{i0} (-\Delta H_S) / \lambda T_0$), which represents a measure of heat generation rate concerned with the dissolution of gas relative to the rate of heat conduction.

The satisfactory agreement between these two solutions, suggests that the interface temperature rise and enhancement factor are insensitive to the assumption of the temperature profile in the liquid film. This is because the diffusion depth x_f of heat is much greater than that of the dissolved gas which is confined near the interface for

$\gamma \gg 1$. In fact, the MDM is not justified for the film theory solutions of physical absorption and of instantaneous irreversible chemical absorption, where either the dissolved gas A or reactant B exists throughout the liquid film with significant variation of temperature.

5. Conclusions

The following conclusions can be made from the present analysis:

1. The interface temperature rise θ_i and relevant enhancement factor β depend greatly on ϵ_{DB} and to a little extent on ϵ_S and ϵ_{DA} for an instantaneous irreversible reaction, while they depend on $\epsilon_S + (\epsilon_{DA} + \epsilon_R)/2 (= \epsilon_{eff})$, and not on the individual values of ϵ_S , ϵ_{DA} and ϵ_R for a first order irreversible reaction.
2. The interface temperature rise θ_i always increases with a decrease of $P (= \Delta H_S / \Delta H_R)$ and an increase of $\psi/Le (= D_{A0}A_{i0}(-\Delta H_S)/\lambda T_0)$ when other conditions remain unchanged, whereas the relevant enhancement factor β behaves in the same manner as θ_i for $\epsilon_{eff} > 0$ and conversely for $\epsilon_{eff} < 0$.
3. The modified Danckwerts model (MDM), in which the physicochemical properties are evaluated at the interface temperature, is effective for obtaining the approximate solutions of θ_i and β for a first (possibly m -th) order irreversible reaction, and not for an instantaneous irreversible reaction, in contrast with the penetration theory analysis where MDM is applicable for any reaction scheme¹⁴.

Nomenclature

A	: concentration of dissolved gas, mol/m ³
A_i	: physical solubility of gas, mol/m ³
a	: dimensionless concentration of dissolved gas, A/A_{i0} , —
B	: concentration of reactant, mol/m ³
b	: dimensionless concentration of reactant, B/B_0 , —
C_p	: specific heat of liquid, J/(kg·K)
D	: diffusivity, m ² /s
E	: activation energy, J/mol
k	: reaction rate constant, l/s
Le	: Lewis number, α/D_{A0} , —
N	: absorption rate, mol/(m ² ·s)
P	: $\Delta H_S/\Delta H_R$, —
p	: parameter defined by Eq. (36), —
Q	: temperature-dependent property (A_i, D_A, D_B and k)
q	: concentration ratio, $B_0/\nu A_{i0}$, —
R	: gas constant, J/(mol·K)
r	: diffusivity ratio, D_{B0}/D_{A0} , —
T	: thermodynamic temperature, K
x	: distance from interface into liquid, m
x_f	: effective film thickness, m

Green symbols

α	: thermal diffusivity, $\lambda/\rho C_p$, m ² /s
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- β : enhancement factor, —
 γ : dimensionless parameter, $x_f \sqrt{k_0/D_{A0}}$, —
 ΔH_R : enthalpy change due to reaction, J/mol
 ΔH_S : enthalpy change due to reaction, J/mol
 e : activation energy group, E/RT_0 , —
 θ : dimensionless temperature rise, $(T-T_0)/T_0$, —
 λ : thermal conductivity of liquid, W/(m·K)
 ν : number of moles of reactant B reacting with one mole of dissolved gas A , —
 ρ : liquid density, kg/m³
 ϕ_1, ϕ_2 : variables defined by Eq. (36), —
 ψ : $\alpha A_{i0} (-\Delta H_S)/\lambda T_0$, —

Subscripts

- A : dissolved gas
 B : reactant
 D : diffusion
 eff : effective value
 i : gas-liquid interface
 IS : isothermal condition
 MD : modified Danckwerts model
 OD : ordinary Danckwerts model
 R : reaction
 S : solution
 0 : liquid bulk condition

Superscript

- r : reaction plane

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