

MODEL DEVELOPMENT FOR DIFFUSION WITH INSTANTANEOUS CHEMICAL REACTIONS IN A SPHERICAL MULTICOMPONENT DROP

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Abstract—Diffusion accompanied by instantaneous chemical reactions in a multicomponent drop is modeled. The developed model is then simulated for the case of absorption of one solute from a continuous phase into the drop, followed by fast reactions with two different reactants existing in the drop. The results of the model are obtained by using Galerkin's finite element method and represented by unsteady concentration profiles of all components in the drop, the reaction front positions, and the cumulative mass flux and the enhancement factor of the diffusing solute. The effects of the system parameters, such as diffusivities of the solute and the reactants, the relative amount of the reactants in the drop, and the interfacial concentration of the solute, on the calculated quantities are evaluated.

Key words: Diffusion, Reaction Front, Moving Boundary, Drop, Fast Reaction

INTRODUCTION

Diffusion between drops or bubbles and surrounding fluid with an accompanying chemical reaction is important in a number of industrial gas-liquid and liquid-liquid contacting operations. The reaction may occur either in the continuous phase or in the dispersed phase, depending on the nature of the particular system. Theoretical analyses of diffusion with a chemical reaction to or from drops have been reported by several workers [Ruchenstein et al., 1971; Dang and Ruchenstein, 1973; Ramachandran et al., 1985; Kleninstreuer et al., 1985; Dutta et al., 1988].

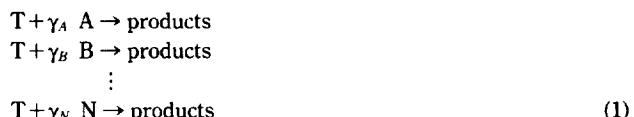
In many situations of practical interest, however, diffusion to a drop is associated with an instantaneous chemical reaction. This phenomenon proceeds through a moving boundary mechanism. The reaction between a solute diffusing into the drop from the surrounding continuous phase and a second reactant species present in the drop occurs at a reaction front that progressively moves away from the surface of the drop toward its center. As a result, the reaction front separates the drop into two regions, each containing only the solute or the reactant.

Despite its practical importance, the multicomponent system, which is common to general industrial processes, is not well understood. In an earlier paper, Noh et al. [1995] developed a mathematical model for multicomponent mass transfer accompanied by irreversible instantaneous chemical reactions with one reactant in a small drop. They simulated the model for the case where two solutes diffuse and react rapidly with a third reactant existing in the drop. The aim of the present paper is to develop a mathematical model to theoretically analyze the diffusion of one solute from the surrounding phase into a multicomponent drop accompanied by irreversible rapid chemical reactions in the drop. The developed model is then simulated for absorption of one solute and instantaneous chemical reactions of the solute with two chemical reactants present in the drop. The results of the analysis

are reported in terms of unsteady concentration profile of each species in the drop, the location of reaction front, and the cumulative mass flux and the enhancement factor of the solute for the various values of the system parameters.

MODEL DEVELOPMENT

Let us consider a non-circulating drop that contains n different reaction species, A, B, C, ..., N, and absorbs a solute, T, from the surrounding continuous phase. The initial concentrations of the reactants, C_{in} , are uniform in the drop. The bulk concentration of T in the continuous phase is constant and the corresponding equilibrium concentration at the drop surface is C_{Tc} . Due to the independent reactions of T with the reactants, there are n chemical reactions according to:



where γ_i 's are the ratios of stoichiometric coefficient of i to T. If the reactions are so fast that the overall rate is controlled by diffusion in the drop and mass transfer resistance in the continuous phase is negligible, the relevant governing equations in nondimensionless form are:

For region I ($\phi < \rho < 1$)

$$\frac{\partial^2 C_T^*}{\partial \rho^2} = \frac{\partial C_T^*}{\partial \tau}$$

For region II ($0 < \rho < \phi$)

$$D_{AT} \frac{\partial^2 C_A^*}{\partial \rho^2} = \frac{\partial C_A^*}{\partial \tau}$$

$$D_{BT} \frac{\partial^2 C_B^*}{\partial \rho^2} = \frac{\partial C_B^*}{\partial \tau}$$

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$$D_{NT} \frac{\partial^2 C_T^*}{\partial \rho^2} = \frac{\partial C_T^*}{\partial \tau} \quad (2)$$

$$\text{where } C_T^* = \rho \bar{C}_T = \rho \frac{C_T}{C_{T_0}}$$

$$C_A^* = \rho \bar{C}_A = \rho \frac{C_A}{C_{A_0}}$$

$$C_B^* = \rho \bar{C}_B = \rho \alpha_B \frac{C_B}{C_{B_0}}$$

$$C_N^* = \rho \bar{C}_N = \rho \alpha_N \frac{C_N}{C_{N_0}}$$

$$\tau = \frac{t D_T}{R^2}, \quad \alpha_i = \frac{C_{i_0}}{C_{A_0}}, \quad \rho = \frac{r}{R}, \quad \text{and} \quad D_{ij} = \frac{D_i}{D_j}$$

Here, C_i 's and D_i 's are concentration and diffusivity of i , respectively; r is radius coordinate of the system measured from the drop center; R is drop radius; $\phi \approx x/R$ is the location of the moving reaction front at any time τ ; and x is the distance from the drop center to the location of the reaction front at any time t .

The following initial and boundary conditions may be prescribed.

$$\begin{aligned} \text{At } \tau=0: \quad C_T^* &= 0, \quad C_A^* = \rho, \quad C_B^* = \alpha_B \rho, \dots, \quad C_N^* = \alpha_N \rho \quad \text{for } 0 < \rho < 1 \\ \text{At } \rho=1: \quad C_T^* &= 1 \quad \text{for } \tau > 0 \\ \text{At } \rho=0: \quad C_A^* = C_B^* = \dots = C_N^* &= 0 \quad \text{for } \tau > 0 \\ \text{At } \rho=\phi: \quad C_T^* = C_A^* = C_B^* = \dots = C_N^* &= 0 \quad \text{for } \tau > 0 \end{aligned} \quad (3)$$

The following compatibility condition relating the fluxes of T and the reactants in the drop at $\rho=\phi$ should be satisfied:

$$-N_T = \frac{N_A}{\gamma_A} + \frac{N_B}{\gamma_B} + \dots + \frac{N_N}{\gamma_N}$$

that is,

$$\begin{aligned} -\frac{\partial C_T^*}{\partial \rho} &= D_{AT} \beta_A \frac{\partial C_A^*}{\partial \rho} + D_{BT} \beta_B \frac{\partial C_B^*}{\partial \rho} \\ &+ \dots + D_{NT} \beta_N \frac{\partial C_N^*}{\partial \rho} \end{aligned} \quad (4)$$

$$\text{where } \beta_k = \frac{C_{k_0}}{\alpha_k \gamma_k C_{T_0}} = \frac{C_{k_0}}{C_{T_0} \gamma_k} \quad (k = A, B, \dots, N)$$

No analytical method to solve the above set of equations exists, and a direct numerical approach becomes complicated because the reaction front position, ϕ , is not known in advance. Therefore, it is desired that the reaction front is immobilized through an appropriate coordinate transformation. Accordingly, if the following new variables are introduced,

$$\omega_l = \frac{\rho - \phi}{1 - \phi} \quad \text{for } \phi \leq \rho \leq 1 \quad (5)$$

$$\omega_H = \frac{\phi - \rho}{\phi} \quad \text{for } 0 \leq \rho \leq \phi \quad (6)$$

Eqs. (2) to (4) reduce to:

$$\frac{1}{(1-\phi)^2} \frac{\partial^2 C_T^*}{\partial \omega_l^2} + \frac{1-\omega_l}{1-\phi} \frac{d\phi}{d\tau} \frac{\partial C_T^*}{\partial \omega_l} = \frac{\partial C_T^*}{\partial \tau}$$

$$\frac{D_{AT}}{\phi^2} \frac{\partial^2 C_A^*}{\partial \omega_l^2} - \frac{1-\omega_H}{\phi} \frac{d\phi}{d\tau} \frac{\partial C_A^*}{\partial \omega_H} = \frac{\partial C_A^*}{\partial \tau}$$

$$\frac{D_{BT}}{\phi^2} \frac{\partial^2 C_B^*}{\partial \omega_l^2} - \frac{1-\omega_H}{\phi} \frac{d\phi}{d\tau} \frac{\partial C_B^*}{\partial \omega_H} = \frac{\partial C_B^*}{\partial \tau}$$

⋮

$$\frac{D_{NT}}{\phi^2} \frac{\partial^2 C_N^*}{\partial \omega_l^2} - \frac{1-\omega_H}{\phi} \frac{d\phi}{d\tau} \frac{\partial C_N^*}{\partial \omega_H} = \frac{\partial C_N^*}{\partial \tau} \quad (7)$$

$$\begin{aligned} \text{At } \tau=0: \quad C_T^* &= 0, \quad C_A^* = 1 - \omega_H, \quad C_B^* = \alpha_B(1 - \omega_H), \dots, \\ C_N^* &= \alpha_N(1 - \omega_H) \quad \text{for } \omega_l \text{ and } \omega_H > 0 \end{aligned}$$

$$\text{At } \omega_l=1: \quad C_T^* = 1 \quad \text{for } \tau > 0$$

$$\text{At } \omega_H=1: \quad C_A^* = C_B^* = \dots = C_N^* = 0 \quad \text{for } \tau > 0$$

$$\text{At } \omega_l=\omega_H=0: \quad C_T^* = C_A^* = C_B^* = \dots = C_N^* = 0 \quad \text{for } \tau > 0 \quad (8)$$

and

$$\begin{aligned} \frac{\partial C_T^*}{\partial \omega_l} &= \left[\frac{1-\phi}{\phi} \left\{ \beta_A D_{AT} \frac{\partial C_A^*}{\partial \omega_l} + \beta_B D_{BT} \frac{\partial C_B^*}{\partial \omega_l} \right. \right. \\ &\quad \left. \left. + \dots + \beta_N D_{NT} \frac{\partial C_N^*}{\partial \omega_l} \right\} \right] \end{aligned} \quad (9)$$

Eq. (7) with the corresponding boundary conditions, Eq. (8), and the compatibility condition, Eq. (9), is solved numerically using the usual Galerkin's formula applied over a fixed number of linear finite elements for the two regions, ω_l and ω_H , in the drop. Each dimensionless time step requires an iterative technique because of nonlinear involvement of ϕ in the governing equations. The detailed computational steps are given in the earlier paper [Noh et al., 1995].

RESULTS AND DISCUSSION

The developed model is simulated for the case of absorption of one solute, T , from a continuous phase into a two-component drop and irreversible instantaneous chemical reactions of the solute with two reactants, A and B , existing in the drop according to the following equations:

$$\begin{aligned} T + \gamma_A A &\rightarrow \text{products} \\ T + \gamma_B B &\rightarrow \text{products} \end{aligned} \quad (10)$$

The computational results for the case are obtained using Galerkin's finite element method and reported in terms of unsteady concentration profiles of all components in the drop, the locations of the reaction front, and the cumulative mass flux and the enhancement factor. The mass flux and the enhancement factor of the diffusing solute, T , may be calculated easily from the solution for concentration distribution as follows [Hines and Maddox, 1985]:

$$Q_T = \int_0^\tau \left(\frac{\partial C_T}{\partial \rho} \right)_{\rho=1, \text{chem}} d\tau \quad (11)$$

$$\begin{aligned} E_T &= \frac{\int_0^\tau \left(\frac{\partial C_T}{\partial \rho} \right)_{\rho=1, \text{chem}} d\tau}{\int_0^\tau \left(\frac{\partial C_T}{\partial \rho} \right)_{\rho=1, \text{phys}} d\tau} \\ &= \frac{3Q_T}{1 - \frac{6}{\pi} \sum_{n=1}^{\infty} \frac{1}{n^2} e^{-\pi^2 n^2 \tau}} \end{aligned} \quad (12)$$

It may be noted that the numerical integration can not be extended to $\tau=0$ and hence evaluation of time integrals, Eqs. (11) and (12), may contain a small error. This error, however, could be reduced by choosing a sufficiently small length of integral for τ near $\tau=0$.

Discussed are the effects of the system parameters-namely, the initial concentration ratio of A to T weighed by the stoichiometric coefficient in the reactions (β), the diffusivity ratio of B to A (D_{BA})

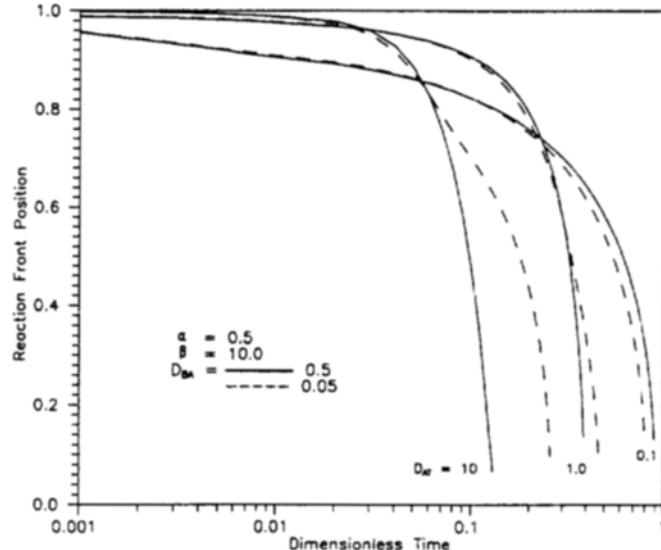
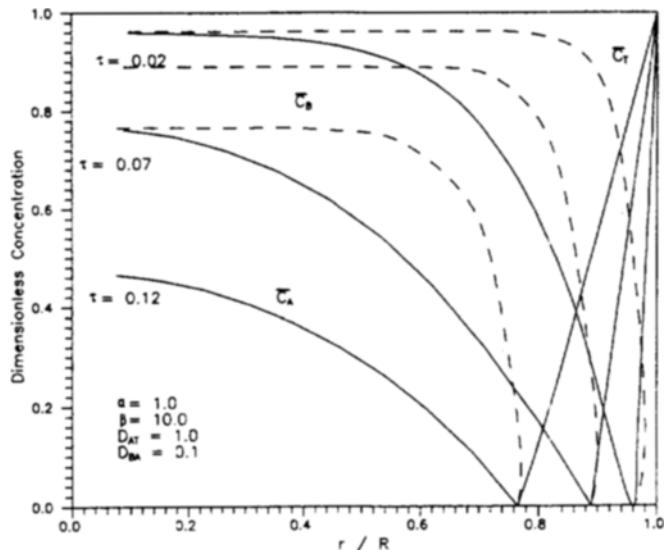
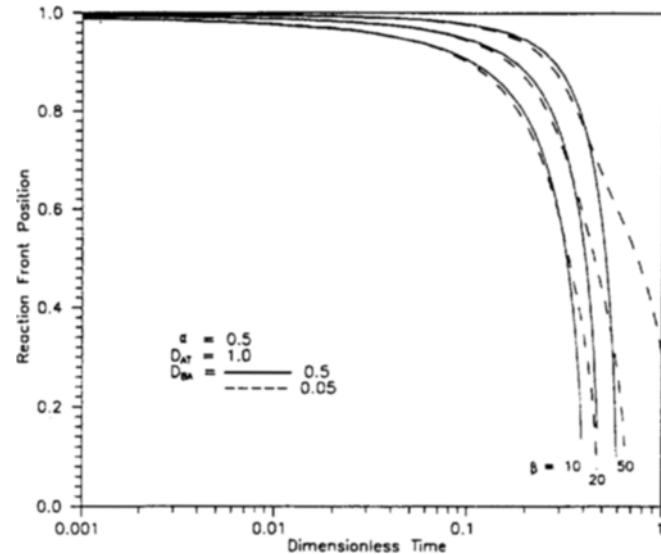
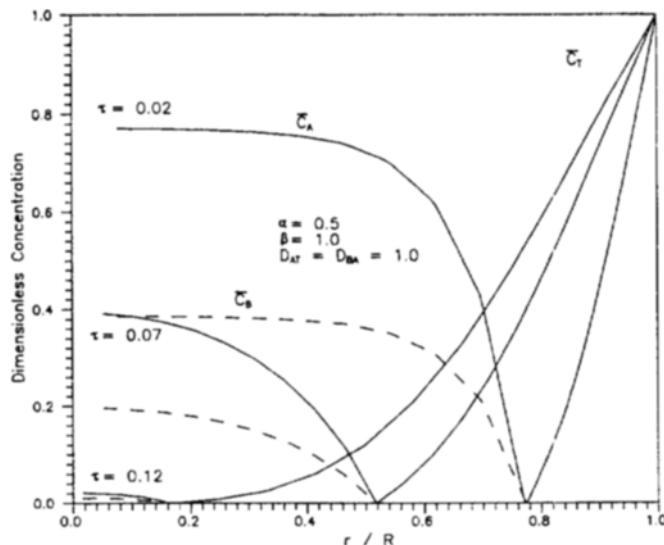


Fig. 2. Variation of concentration profiles (II).

Fig. 4. Progress of reaction front (II).

and of A to T (D_{AT}) on the computational results. β is denoted by a single parameter, β , because the ratios of stoichiometric coefficients of the two reactions are taken as unity for the simplicity of the calculation.

From general physical considerations, it is seemed that the location of the reaction front will be determined by two parameters: the diffusion rates and the amounts of the solute and the reactants. Larger concentrations of A and B will retard the movement of the reaction front. The effect of higher diffusivities of A and B will be similar. These physical interpretations are confirmed very well by the computational results of the present study.

The concentration profiles of all components in the drop are shown in Figs. 1 and 2 with different values of α , β , D_{BA} , and constant D_{AT} as functions of time and radius. Fig. 1 indicates that when the diffusivities of all components are the same, T reacts with A and B simultaneously, regardless of the initial amount of A and B in the drop. In Fig. 2, it is shown that if B diffuses

slower than A, the concentration of B remains almost constant before the reaction front, followed by a rapid approach to zero around the reaction front. This confirms that T mainly reacts with the faster diffusing A as the reaction proceeds, even though the same amount of A and B exists in the drop.

Figs. 3 and 4 show the progress of the reaction front with constant value of α . As can be seen in Fig. 3, larger β at constant D_{AT} results in the slower movement of the reaction front. For constant β , as the diffusivity of A becomes larger, the initial movement of the reaction front becomes slower but advances so fast at later time (Fig. 4). Slower diffusing B compared to A has an accelerating effect on the movement of the reaction front at early time and an decelerating effect at later time. This decelerating effect becomes obvious at large values of β (Fig. 3) and D_{AT} (Fig. 4). This confirms that when $D_{BA} < 1$, most of A is consumed at initial time and T reacts only with the slow diffusing B at later time. However, for the slow diffusing A compared to T ($D_{AT} = 0.1$),

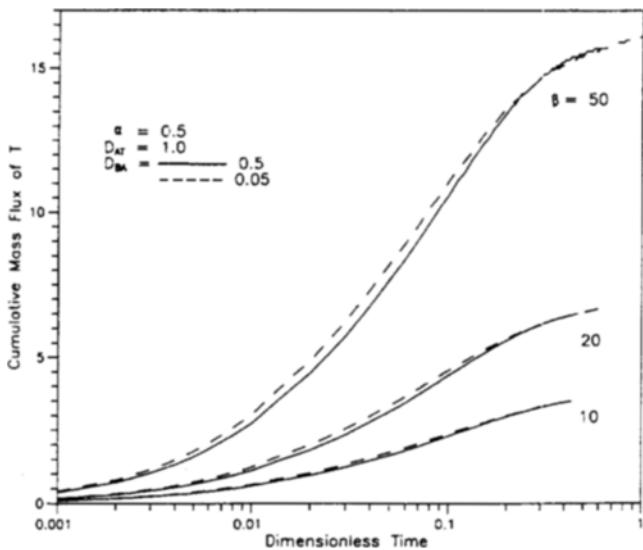


Fig. 5. Variation of cumulative mass flux of T (I).

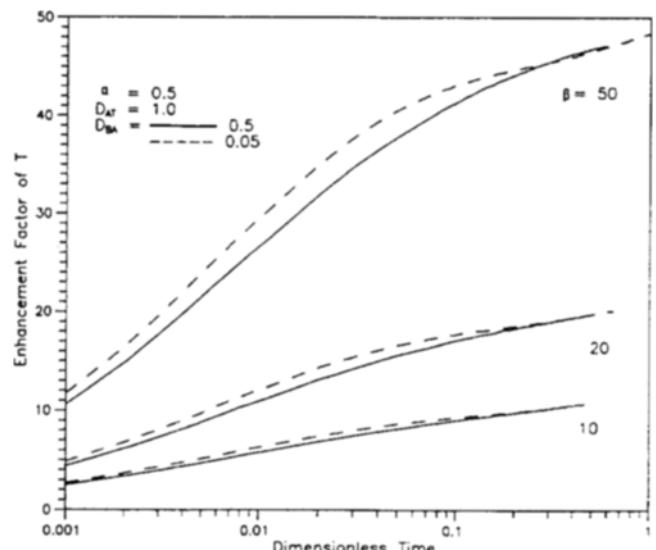


Fig. 7. Variation of enhancement factor of T (I).

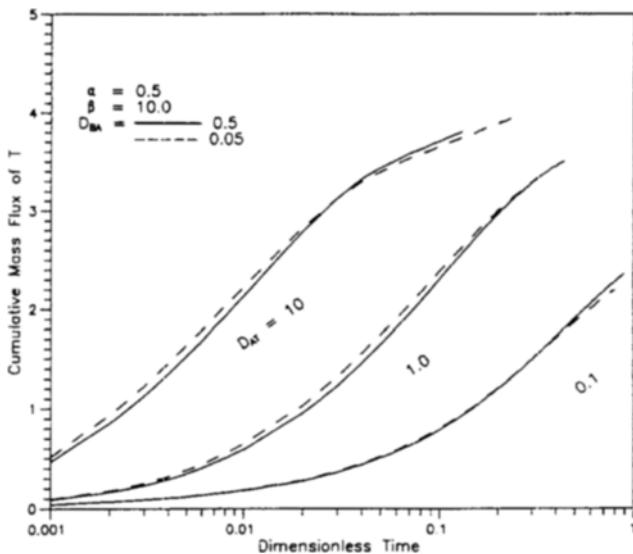


Fig. 6. Variation of cumulative mass flux of T (II).

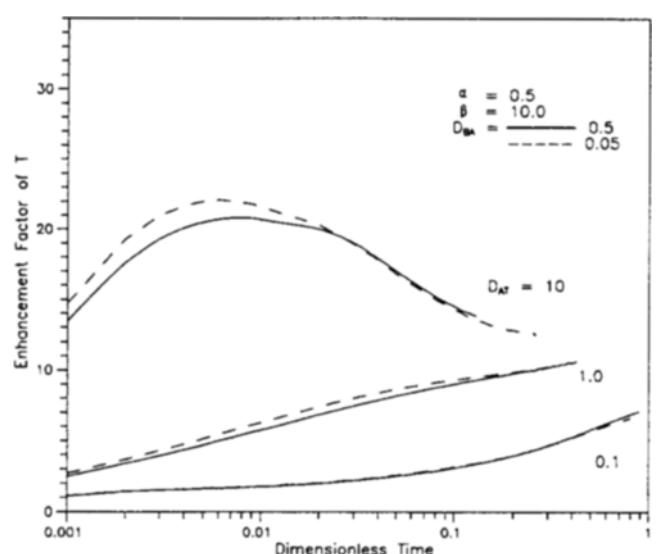


Fig. 8. Variation of enhancement factor of T (II).

the movement of the reaction front becomes fast as D_{BA} decreases (Fig. 4).

The cumulative mass flux of T, obtained by integral of the concentration profile of T, is shown in Figs. 5 and 6. Fig. 5 shows that as β with constant D_{AT} increases, the amount of T absorbed increases as expected. The slower diffusing B causes slightly the larger amount of T absorbed at initial stage. Each curve appears to reach its own asymptotic value at final stage, being independent on D_{BA} . Fig. 6 shows the effect of D_{AT} with constant β . If the diffusivity of A becomes larger, a greater amount of T is absorbed at early time. For very slow movement of A compared to T ($D_{AT} = 0.1$), there is no significant effect of D_{BA} on the amount of T absorbed. At later time, all the cumulative mass flux curves must tend to the final limiting value. Obviously, the diffusivities of all components in the drop seem to have no effect on the limiting value.

Fig. 7 shows the effect of β on the enhancement factor of T with constant α and D_{AT} . Again, larger β and the slower movement

of B cause the larger enhancement factor of T at early stage. At final stage, the asymptotic value of the enhancement factor is reached, which is independent on D_{BA} . An interesting phenomenon is represented in Fig. 8, which shows the enhancement factor of T at different D_{AT} and constant β . Here it is seen that for larger value of D_{AT} , the enhancement factor shows a maximum, and then drops down to the limiting value. This is because most of A is consumed at early stage, followed by simple physical absorption at later stage. For small value of D_{AT} , the curve shows the constant enhancement factor for a while at early time. Thereafter, the value gradually increases and the limiting value is reached asymptotically. The diffusivity ratio $D_{AT} = 1.0$ demarcates the boundary between these two types of phenomena. The slower diffusing B compared to A causes the higher enhancement factor of T with larger D_{AT} at early stage, but, as expected, does not affect the final asymptotic value. This is because at initial time, T mainly reacts with A which exits more and diffuses faster than

B. At later time when most of A is consumed, the less amount of T is absorbed and reacts with the slow moving B. For very slow moving A ($D_{AT}=0.1$), this effect appears to be negligible. The effect of α , the initial amount of B relative to A, is not discussed because it is similar to that of D_{BA} .

CONCLUSIONS

Diffusion accompanied by irreversible instantaneous chemical reactions in a multicomponent drop was mathematically modeled and simulated for absorption of one solute and its reaction with two different reactants existing in the drop. In order to fix the reaction front, the radial coordinate system was transformed into a new one which contains the reaction front position. The developed model was solved using Galerkin's linear finite element method, and the calculated results were presented in terms of unsteady concentration profiles, the progress of the reaction front, and the cumulative mass flux and the enhancement factor of the solute with different system parameters. Parametric studies showed the influences of the diffusivity ratios and the relative amount of the reactants in the drop. The prediction of the model on the effects of those quantities is in agreement with the general physical considerations; (1) as the diffusivities of the reactants in the drop increase, the solute is absorbed rapidly from the surrounding fluid -approaching the final asymptotic value which is independent on the diffusion rates of the solute and the reactants; (2) with the larger amount of the reactants in the drop, the amount of the solute absorbed becomes larger.

NOMENCLATURE

A, B, N :	reactants existing in a drop
C_i	: concentration of i
\bar{C}_i	: dimensionless concentration of i
C_i^*	: transformed concentration of i
C_{Ti}	: concentration of T at drop surface
C_{io}	: initial concentration of i in a drop
D_{ij}	: diffusivity ratio, D_i/D_j
E_T	: enhancement factor of T
N_i	: mass flux of i
Q_T	: cumulative mass flux of T
r	: radius coordinate
R	: drop radius
x	: location of the reaction front
T	: diffusing solute from a surrounding phase to a drop

Greek Letters

α_i	$: C_{io}/C_{A0}$
β_k	$: C_{A0}/\gamma_k C_{Ti}$
γ_i	: ratio of stoichiometric coefficients of i to T
ρ	: dimensionless radial position, r/R
τ	: dimensionless time, tD_T/R^2
ϕ	: dimensionless position of reaction front, x/R
ω_i, ω_{ii}	: transformed coordinate variables

REFERENCES

Dang, V. I. and Ruchenstein, E., "High Reynolds Numbers Unsteady Convective Mass Transfer from Fluid Spheres", *Int. J. Heat Mass Trans.*, **16**, 1371 (1973).
 Dutta, B., Middya, U. and Ray, P., "Mass Transfer with Instantaneous Chemical Reaction in a Rigid Drop", *AIChE J.*, **34**, 694 (1988).
 Hines, A. and Maddox, R., "Mass Transfer, Fundamentals and Applications", Prentice-Hall, New Jersey, 1985.
 Kleinstreuer, C., Ramachandran, S. and Altwicker, E., "Sulfur Dioxide-Absorption with Chemical Reaction in an Accelerating Stream of Drops", *Chem. Eng. J.*, **30**, 45 (1985).
 Noh, B. I., Yoon, T. K., Moon, B. H. and Kim, J. H., "Model Development for Multicomponent Mass Transfer with Rapid Chemical Reactions in a Small Drop", *The Korean Journal of Chemical Engineering*, **12**(1), 18 (1995).
 Ramachandran, S., Kleinstreuer, C. and Altwicker, R., "Coupled Two-Phase Mass Transfer to Spherical Drops-Trace Gas Absorption and Oxidation by a Single Drop", *The Canadian Journal of Chemical Engineering*, **63**, 911 (1985).
 Ruchenstein, E., Dang, V. and Gill, W., "Mass Transfer with Chemical Reaction from Spherical One or Two Component Bubbles or Drops", *Chem. Eng. Sci.*, **26**, 647 (1971).

neous Chemical Reaction in a Rigid Drop", *AIChE J.*, **34**, 694 (1988).

Hines, A. and Maddox, R., "Mass Transfer, Fundamentals and Applications", Prentice-Hall, New Jersey, 1985.
 Kleinstreuer, C., Ramachandran, S. and Altwicker, E., "Sulfur Dioxide-Absorption with Chemical Reaction in an Accelerating Stream of Drops", *Chem. Eng. J.*, **30**, 45 (1985).

Noh, B. I., Yoon, T. K., Moon, B. H. and Kim, J. H., "Model Development for Multicomponent Mass Transfer with Rapid Chemical Reactions in a Small Drop", *The Korean Journal of Chemical Engineering*, **12**(1), 18 (1995).

Ramachandran, S., Kleinstreuer, C. and Altwicker, R., "Coupled Two-Phase Mass Transfer to Spherical Drops-Trace Gas Absorption and Oxidation by a Single Drop", *The Canadian Journal of Chemical Engineering*, **63**, 911 (1985).

Ruchenstein, E., Dang, V. and Gill, W., "Mass Transfer with Chemical Reaction from Spherical One or Two Component Bubbles or Drops", *Chem. Eng. Sci.*, **26**, 647 (1971).

APPENDIX : DERIVATION OF THE GOVERNING EQUATIONS THROUGH THE COORDINATE TRANSFORMATION

1. Governing Equations

By introducing the following variables for the coordinate transformation,

$$\omega_I = \frac{\rho - \phi}{1 - \phi} \quad \text{for } \phi \leq \rho \leq 1 \quad (5)$$

$$\omega_{II} = \frac{\phi - \rho}{\phi} \quad \text{for } 0 \leq \rho \leq \phi \quad (6)$$

we have

$$\frac{\partial \omega_I}{\partial \rho} = \frac{1}{(1 - \phi)} \quad \frac{\partial \omega_I}{\partial \phi} = \frac{(\rho - 1)}{(1 - \phi)^2} \quad (A-1)$$

$$\frac{\partial \omega_{II}}{\partial \rho} = -\frac{1}{\phi} \quad \frac{\partial \omega_{II}}{\partial \phi} = \frac{\rho}{\phi^2} \quad (A-2)$$

1-1. For region I ($\phi < \rho < 1$)

$$\frac{\partial^2 C_T^*}{\partial \rho^2} = \frac{\partial C_T^*}{\partial \tau} \quad (2)$$

Hence, $C_T^* = f(\omega_I, \tau)$ and $\phi = f(\tau)$. Therefore, it follows that

$$\begin{aligned} dC_T^* &= \frac{\partial C_T^*}{\partial \tau} d\tau + \frac{\partial C_T^*}{\partial \omega_I} d\omega_I \\ &= \frac{\partial C_T^*}{\partial \tau} d\tau + \frac{\partial C_T^*}{\partial \omega_I} \frac{\partial \omega_I}{\partial \phi} \frac{\partial \phi}{\partial \tau} d\tau \end{aligned}$$

By dividing both sides by $d\tau$ and using Eqs. (5) and (A-1), we get

$$\begin{aligned} \frac{\partial C_T^*}{\partial \tau} &= \frac{\partial C_T^*}{\partial \tau} + \frac{(\rho - 1)}{(1 - \phi)^2} \frac{d\phi}{d\tau} \frac{\partial C_T^*}{\partial \omega_I} \\ &= \frac{\partial C_T^*}{\partial \tau} - \frac{(1 - \omega_I)}{(1 - \phi)} \frac{d\phi}{d\tau} \frac{\partial C_T^*}{\partial \omega_I} \end{aligned} \quad (A-3)$$

The lefthand side of Eq. (2) reduces to

$$\frac{\partial^2 C_T^*}{\partial \rho^2} = \frac{\partial}{\partial \rho} \left(\frac{\partial C_T^*}{\partial \rho} \right) = \frac{1}{(1 - \phi)^2} \frac{\partial^2 C_T^*}{\partial \omega_I^2} \quad (A-4)$$

By substituting Eqs. (A-3) and (A-4) into Eq. (2), we get

$$\frac{1}{(1-\omega)^2} \frac{\partial^2 C_T^*}{\partial \omega_I^2} + \frac{(1-\omega_I)}{(1-\phi)} \frac{d\phi}{d\tau} \frac{\partial C_T^*}{\partial \omega_I} = \frac{\partial C_I^*}{\partial \tau} \quad (7)$$

1-2. For region II ($0 < \rho < \phi$)

$$D_{II} \frac{\partial^2 C_i^*}{\partial \rho^2} = -\frac{\partial C_i^*}{\partial \tau} \quad (i=A, B, \dots, N) \quad (2)$$

Similarly, we have the following:

$$\begin{aligned} C_I^* &= f(\omega_{II}, \tau) \text{ and } \phi = f(\tau) \\ dC_i^* &= \frac{\partial C_i^*}{\partial \tau} d\tau + \frac{\partial C_i^*}{\partial \omega_{II}} d\omega_{II} \\ &= \frac{\partial C_i^*}{\partial \tau} d\tau + \frac{\partial C_i^*}{\partial \omega_{II}} \frac{\partial \omega_{II}}{\partial \phi} \frac{d\phi}{d\tau} d\tau \\ \frac{dC_i^*}{d\tau} &= \frac{\partial C_i^*}{\partial \tau} + \frac{\rho}{\phi^2} \frac{d\phi}{d\tau} \frac{\partial C_i^*}{\partial \omega_{II}} \\ &= \frac{\partial C_i^*}{\partial \tau} + \frac{(1-\omega_{II})}{\phi} \frac{d\phi}{d\tau} \frac{\partial C_i^*}{\partial \omega_{II}} \\ D_{II} \frac{\partial^2 C_i^*}{\partial \rho^2} &= D_{II} \frac{1}{\phi^2} \frac{\partial^2 C_i^*}{\partial \omega_{II}^2} \end{aligned} \quad (A-5) \quad (A-6)$$

Substituting Eqs. (A-5) and (A-6) into Eq. (2) yields

$$\frac{D_{II}}{\phi^2} \frac{\partial^2 C_i^*}{\partial \omega_{II}^2} - \frac{(1-\omega_{II})}{\phi} \frac{d\phi}{d\tau} \frac{\partial C_i^*}{\partial \omega_{II}} = \frac{\partial C_i^*}{\partial \tau} \quad (7)$$

2. Initial and Boundary Conditions

Accordingly, Eq. (3) reduces to

$$\begin{aligned} \text{At } \tau=0; \quad C_T^* &= 0, \quad C_A^* = 1-\omega_{II}, \quad C_B^* = \alpha_B(1-\omega_{II}), \dots, \\ C_N^* &= \alpha_N(1-\omega_{II}) \text{ for } \omega_I \text{ and } \omega_{II} > 0 \end{aligned}$$

$$\text{At } \omega_I=1; \quad C_T^* = 1 \text{ for } \tau > 0$$

$$\text{At } \omega_{II}=1; \quad C_A^* = C_B^* = \dots = C_N^* = 0 \text{ for } \tau > 0$$

$$\text{At } \omega_I=\omega_{II}=0; \quad C_T^* = C_A^* = C_B^* = \dots = C_N^* = 0 \text{ for } \tau > 0 \quad (8)$$

3. Compatibility Condition

$$\begin{aligned} -\frac{\partial C_T^*}{\partial \rho} &= D_{AT} \beta_A \frac{\partial C_A^*}{\partial \rho} + D_{BT} \beta_B \frac{\partial C_B^*}{\partial \rho} \\ &\quad + \dots + D_{NT} \beta_N \frac{\partial C_N^*}{\partial \rho} \end{aligned} \quad (4)$$

Here, the partial derivatives of both sides reduce to

$$\frac{\partial C_T^*}{\partial \rho} = \frac{1}{(1-\phi)} \frac{\partial C_I^*}{\partial \omega_I} \quad (A-7)$$

$$\frac{\partial C_i^*}{\partial \rho} = -\frac{1}{\phi} \frac{\partial C_i^*}{\partial \omega_{II}} \quad (i=A, B, \dots, N) \quad (A-8)$$

Rearranging Eq. (4) using Eqs. (A-7) and (A-8) results in

$$\begin{aligned} \frac{\partial C_T^*}{\partial \omega_I} &= \left(\frac{1-\phi}{\phi} \right) \left\{ \beta_A D_{AT} \frac{\partial C_A^*}{\partial \omega_{II}} + \beta_B D_{BT} \frac{\partial C_B^*}{\partial \omega_{II}} \right. \\ &\quad \left. + \dots + \beta_N D_{NT} \frac{\partial C_N^*}{\partial \omega_{II}} \right\} \end{aligned} \quad (9)$$