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Modelling solid-solid reactions: Contact-point approach

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Highlights

- In solid-solid reaction contact between particles occurs at specific locations.
- These reactions are diffusion controlled.
- Shape of contact point is not so important if area of contact is same.

1. Introduction

Models of solid-solid reactions generally follow two approaches- 1) The particle-continuum approach that derives from the gas-solid literature; Ginstling-Brounshtein (GB), Ishida-Wen (IW). This assumes one reactant particle to be completely surrounded by other reactant particles. 2) Contact point based approach with Hao-Tanaka (HT)[1] and Dalvi-Suresh (DS)[2] model being prominent examples. This kind of approach considers, the two reactant particles are in contact at specific locations called contact points. The latter approach is more realistic, however tends to approach the former when the contact points between the reacting particles (N_{AB}) are large in number. In this work, we model the contact point situation and solve it rigorously on a finite element platform (COMSOL), for different values of the parameters such as Thiele modulus (ϕ^2), molar capacity ratio (K), number of contact points (N_{AB}), etc. The study helps map the regions of parametric space in which different approximate models apply.

2. Numerical model

The system of under consideration is that of an assembly of spherical particles of A and B. The reaction between them, $aA + bB \longrightarrow pP$, takes place in the particles of A with B diffusing into A. The normalized equations for the concentrations of A and B within a particle of A are respectively.

$$\frac{\partial C_A^*}{\partial \tau} = -\frac{\phi^2}{K} C_A^* C_B^*$$

$$\frac{\partial C_B^*}{\partial \tau} = \left[\frac{1}{\eta^2} \frac{\partial}{\partial \eta} \left(\eta^2 \frac{\partial C_B^*}{\partial \eta} \right) + \frac{1}{\eta^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial C_B^*}{\partial \theta} \right) + \frac{1}{\eta^2 \sin\theta} \frac{\partial^2 C_B^*}{\partial \varphi^2} \right] - \phi^2 C_A^* C_B^*.$$

Initial conditions: At τ=0, C^*_B=0; C^*_A =1.

Boundary conditions: η=0, $\frac{\partial C_B^*}{\partial \eta} = 0$ (for all Θ and φ); η=1, C^*_B=1 (at contact points).

Here, $\phi^2 = \frac{k_p C_{A0} b r_{A0}}{D}, K = \frac{b C_{A0}}{a C_{B0}}, \eta = \frac{r}{r_{A0}}, C_B^* = \frac{C_B}{C_{B0}}, C_A^* = \frac{C_A}{C_{A0}}, \tau = \frac{tD}{r_{A0}^2}$. This model is simulated in COMSOL Multiphysics software by using 'Transport of diluted species' physics in 'Chemical Species transport' with time dependent study.

3. Results and discussion

The effect of parameters such as thiele modulus (ϕ^2), K, N_{AB} are discussed here. The contact point framework requires an initial area of contact between the particles for the diffusion-reaction process to start, and two different approaches are possible: in one, taken in the HT model, the contact region is assumed to be a disc-

like volume, while in the other, used in the DS model, the contact region is assumed to be spherical. A comparison of these two approaches shows that they are equivalent, as long as the thickness of the disc in the first and the radius of the contact region in the second are so chosen that the area is the same as shown in Figure 1 (a). The effect of thiele modulus (ϕ^2) is shown in Figure 1(b), which shows that as ϕ^2 increases, the thickness of the reaction zone decreases. Also, the reaction zone propagates inwards with time with a constant thickness in every case. For large ϕ^2 (say >100^2), the reaction is essentially at a front; for this case (and also for a large K), Figure 2 shows the results for N_{AB} =1, 8 and 100. DS model is an approximate version that approximates the diffusion to be purely radially outward from the contact points. Figure 2 shows this approximation to be valid for the parameter values considered. The good comparison has been seen to hold over the entire range of N_{AB} (1 to 100).

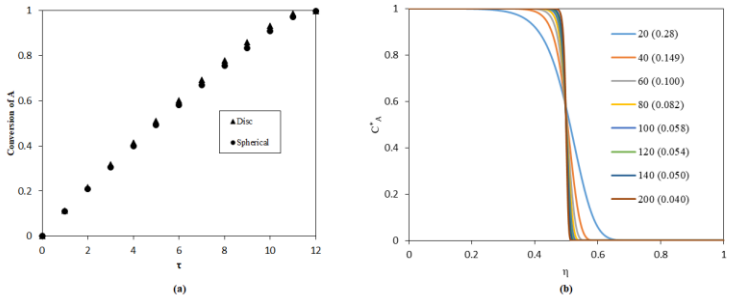

Figure 1. (a) Comparison between conversion time behaviors for disc type and spherical type contact point with same contact area (ϕ=100, K=100, N_{AB}=1). (b) Concentration profiles of A at different values of ϕ. *The bracket value given in legend is reaction zone thickness corresponding to ϕ.

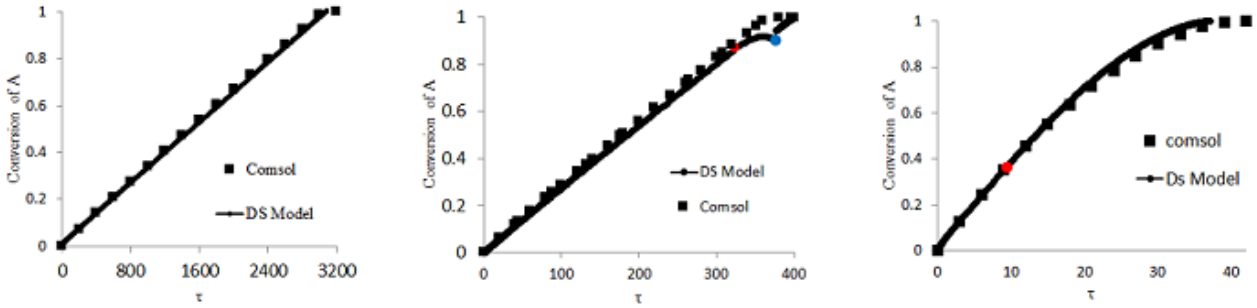

Figure 2. Conversion time plots compared with DS model for high ϕ^2(100^2) and K=(100) for N_{AB}=1, 8, 100 respectively.

4. Conclusions

The value of thiele modulus for solid-solid reactions is usually quite high, and hence such reactions are diffusion controlled. As ϕ^2 value increases reaction zone thickness decreases, with the reaction shifting from volume reaction towards reaction-at-a-front. In the contact point framework, it is shown that the shape of contact between two particles does not matter as long as its contact surface area is same. Also the present model shows good agreement with the Dalvi-Suresh model for the whole range of contact points from low to high.

References

[1] Y. J. Hao, T. Tanaka, Int. Chem. Eng. 30 (1990) 244-253.
[2] V. Dalvi, A. K. Suresh, AIChE J. 57 (2011) 1329-1338.

Keywords
Solid-solid reaction; COMSOL; Dalvi-Suresh; Contact point.