Advanced model for shrinking solid particles under varying mixing conditions

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Highlights

- The reactions of dissolved non-ideal solids are of high importance in many industries
- A new theoretical approach was developed for shrinking solids, for which the solid component is dissolved in liquid and reacts in liquid film and liquid bulk
- The generalized model predicts how the reaction proceeds in the liquid film and in bulk liquid under varying mixing conditions

1 Introduction

Solid-liquid reactions are applied in wide range of industrial production, from mining to the production of fine chemicals, food ingredients and pharmaceuticals. A solid material is dispersed in a liquid, where it dissolves and reacts with components in the liquid phase. If the chemical reactions are presumed to be rapid, the reactions proceed partially in the liquid film surrounding the solid particles, partially in the liquid bulk phase. The solid particles diminish in size because of dissolution, which implies that the liquid film around the particles becomes thinner and thinner (Figure 1). In industrial scale, it is not always possible to reach diffusion-free conditions in the treatment of solid materials with liquids, and film reactions prevail. This is very probable for rapid reactions involving ions, such as various kinds of neutralization processes or in cases when the liquid viscosity is high. The goal of the current work is to apply the film theory to reactive solids immersed in liquids, in such a way that realistic geometric forms of solids (including surface defects) are considered and the film thickness is updated during the progress of the reaction.
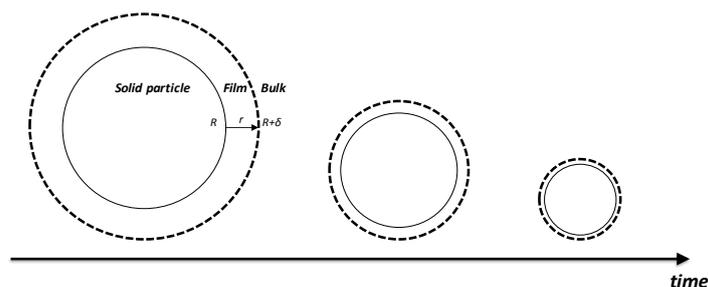
Figure 1. Solid-liquid reaction system: a shrinking solid particle with a surrounding film.

2 Modelling principles and results

A stirred batch reactor with dispersed particles is considered. The model is compressed to dimensionless equations as follows. The dimensionless mass balance equation for the components in the liquid bulk is

$$\frac{dy'_i}{d\theta} = r'_i \frac{\tau}{c_0} - \left(\frac{D_i a_0 \tau / R_0}{\delta / R_0} \right) \frac{n_j}{n_{0j}}^{s/(s+1)} \frac{dy_i}{dx} \tag{1}$$

where $D_i a_0 \tau / R_0$ is a dimensionless number. The gradient (dy_i/dx) is obtained from the film equation

$$\frac{dy_i}{d\theta} = \frac{D_i \tau}{R_0^2 (\delta / R_0)^2} \left(\frac{d^2 y_i}{dx^2} + \frac{s(\delta / R_0)}{R / R_0 + (\delta / R_0)x} \frac{dy_i}{dx} \right) + r_i \frac{\tau}{c_0} \tag{2}$$

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where $0 \le x \le 1$, $y_i = c_i/c_0$, $\theta = t/\tau$, τ=characteristic (arbitrary) time and $D_i\tau/R_0^2$ is a dimensionless number. R/R_0 (=particle radius/initial particle radius) is obtained from $R/R_0 = (n_j/n_{0j})^{1/(s+1)}$. The dimensionless film thickness (δ) is

$$\delta / R_0 = \left(\frac{n_j}{n_{0j}}\right)^{1/(s+1)} \left(1 + \alpha \left(\frac{n_j}{n_{0j}}\right)^{2/(3(s+1))}\right)^{-1} \tag{3}$$

where α is a dimensionless number, which is 0 for silent conditions and increases with increasing mixing rate. The model equations were solved numerically by gPROMS Model Builder v.4 software.

The considered example describes a system, in which a chemical reaction between a dissolving component (B) and a component in the liquid phase (A), reacting in both the film and the bulk phases, takes place. Saturation prevails in the liquid phase in the immediate vicinity of the solid-liquid interface. A parametric study was conducted by using the model, by checking the influence of several parameters on the concentration of each component in both the film and the bulk, moreover, on the particle radius conversion. The shape parameter (s) range was chosen to 2-4 to investigate realistic particle shapes with surface defects. Later, the model was applied to the dissolution of limestone in acidic medium.

Components A (liquid-phase reactant) and C (liquid-phase product) show similar profiles, but they are opposite in absolute values. Component B which is assumed to have an initial concentration in the film equal to zero, dissolves and reacts simultaneously, showing a decreasing profile from the particle surface to the film along the time. The effect of the stirring rate was investigated in different cases: stagnant system ($\alpha = 0$) and increasing stirring rate ($\alpha > 0$). Three different simulations have been performed, by varying parameter α. By increasing the stirring rate, i.e. the α-value, both an enhanced dissolution of B component and a faster diffusion of A in the film phase (Figure 2A) are observed, which leads to an enhanced formation of the product. The reaction is shifted from the film to the liquid bulk as the reaction progresses (Figure 2B).
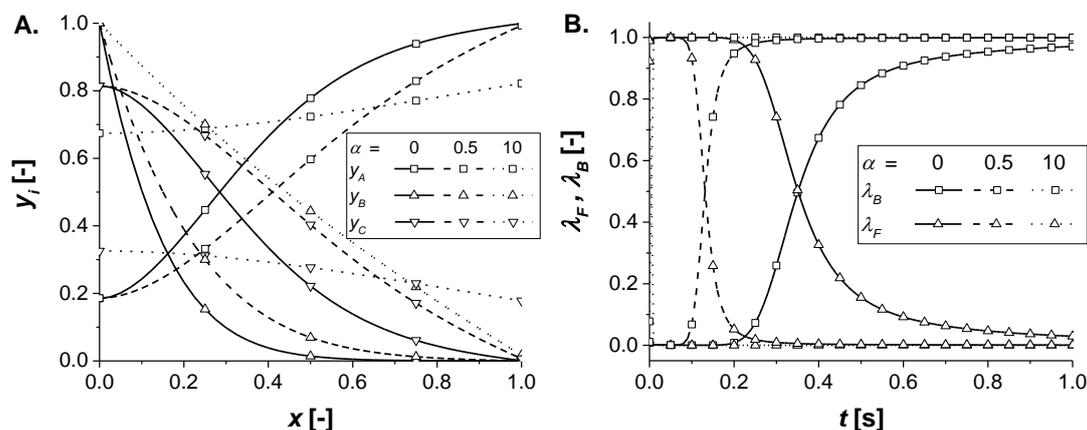
Figure 2. A. Dimensionless concentration profiles in the film phase; B. contribution analysis.

3. Conclusions

The presented shrinking particle model can be considered as an advancement in facing physical systems where reactive components dissolve in liquid phase (film or bulk) before undergoing chemical reactions. The mass balance equations were derived for solid particles dispersed in batch reactors and the performance of the model was demonstrated with numerical simulations. The model can be regarded as a general one and it can describe a wide range of reactive systems with dissolving solids and varying film thicknesses.