

Application of film theory on the reactions of solid particles with liquids: Shrinking particles with changing liquid films



Tapio Salmi^{a,b,*}, Vincenzo Russo^{a,b}, Claudio Carletti^{a,b}, Teuvo Kilpiö^{a,b}, Riccardo Tesser^{a,b}, Dmitry Murzin^{a,b}, Tapio Westerlund^{a,b}, Henrik Grénman^{a,b}

^a Åbo Akademi, Chemical Engineering, FI-20500 Turku/Åbo, Finland

^b Università di Napoli Federico II, IT-80138, Napoli, Italy

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ABSTRACT

The reactivity of soluble solid particles with liquids was described with extended film theory: the solid material dissolves in the liquid phase and diffuses through the liquid film surrounding the particle. In both the liquid film and bulk liquid, chemical reactions take place. The solid particle shrinks due to the dissolution and consequent reactions and the film becomes thinner and thinner due to the decreasing particle size. A general mathematical model was developed for the solid particle, the liquid film and the liquid bulk phase. The dynamic models were based on mass balances for the solid, film and bulk liquid. The models consisting of coupled parabolic partial differential equations and ordinary differential equations were solved numerically by applying the method of lines. The gPROMS ModelBuilder was used in the computations of generic cases. The models predict the shift of the reaction domain being predominantly located in the liquid film towards the liquid bulk during the progress of the solid-liquid process. The roles of the liquid film and the liquid bulk phases were illustrated with contribution analysis.

1. Introduction

A lot has been written about the theory and practice of gas-liquid reactions since the milestone discoveries of the gas-liquid contact: film theory, penetration theory of Higbie and surface renewal theory of Danckwerts (see e.g. Higbie, 1935, Danckwerts, 1970, Levenspiel, 1990, Trambouze et al., 1988). The main idea of all these theories is that molecular diffusion affects the overall rates of the chemical reactions, which take place between dissolved gases and liquid-phase components. In the simplest approach, the film theory, it is presumed that a gaseous component dissolves in the liquid phase and start reacting in the liquid film surrounding the gas bubble. Depending on the relative rates of chemical reaction and diffusion, the reaction proceeds predominantly in the liquid film or in the liquid bulk. The faster the reaction is, the more dominant the film reaction becomes. The film thickness is usually assumed to remain constant throughout the process, because it is related to the mass transfer coefficient and the diffusion coefficient – a change in the film thickness is of course possible if the physical properties, such as density and viscosity, are changing during the reaction, either induced by chemical changes or changes in temperature and/or pressure.

The picture is dramatically altered if the gas is replaced by a solid

reactant, which first dissolves and then reacts with a liquid-phase component. The system is schematically illustrated in Fig. 1. If the liquid-phase turbulence is vigorous, i.e. a lot of energy is dissipated through stirring, the liquid film around the solid particle is diminished and the entire process progresses as a bulk-phase reaction. These conditions are achievable in laboratory-scale experiments, in which a high stirring efficiency is easily materialized. In industrial scale, however, it is not always possible to reach diffusion-free conditions in the treatment of solid materials with liquids, and film reactions commence to prevail. This is very probable for rapid reactions involving ions, such as various kinds of neutralization processes or the viscosity of the liquid is high.

Can these kinds of solid-liquid reactions be treated with the theories for gas-liquid contact? Principally yes, because the theories of liquid films and stagnant zones remain, but there is a significant difference: the film thickness can in many gas-liquid processes be assumed to remain constant, whereas the film thickness changes as the solid component reacts and the particles start to shrink. The general rule of thumb is that the film thickness (δ) around the solid particle is proportional to a power of the particle diameter (d) ($\delta=kd^\omega$, $\omega=1/3\dots 1$), as it has been reported by Green and Perry. As chemical reactions proceed, the reactant concentrations decrease and the solid particles

* Corresponding author at: Åbo Akademi, Chemical Engineering, FI-20500 Turku/Åbo, Finland.
E-mail address: tapio.salmi@abo.fi (T. Salmi).

Nomenclature

A	surface area, m^2
a	surface area-to-volume ratio, m^2/m^3
a', b'	coefficients in the correlation for Sherwood number, dimensionless
ADn	dimensionless parameter ($n=1-4$), dimensionless
c	concentration, mol/m^3
D	diffusion coefficient, m^2/s
d	particle diameter ($=2R$), m
G	mass flow-to-reactor cross-section, $kg/(m^2 s)$
k	reaction rate constant, $m^3/(mol s)$
k_L	mass transfer coefficient, m/s
M	molar mass, kg/mol
N	diffusion flux, $mol/(m^2 s)$
n	amount of substance, mol
R	particle radius, m
R, R'	reaction rates, $mol/(m^3 s)$
r, r'	generation rate, $mol/(m^3 s)$
r	radial coordinate, m
S	number of chemical reactions, dimensionless
s	shape factor, dimensionless
T	temperature, K
t	time, s
V	volume, m^3
x	dimensionless film coordinate, dimensionless
y	dimensionless concentration, dimensionless

Greek letters

α	dimensionless number, dimensionless
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α', β'	exponent in the correlation for Sherwood number parameter in rate equation, dimensionless
δ	film thickness, m
ε	dissipated energy, W/kg
θ	dimensionless time, dimensionless
κ	contribution, mol/s
λ	normalized contribution, dimensionless
ν	stoichiometric coefficient, dimensionless
ν	kinematic viscosity, m^2/s
ρ	density, kg/m^3
τ	characteristic reaction time, s

Dimensionless numbers

Re	Reynolds number, dimensionless
Sc	Schmidt number, dimensionless
Sh	Sherwood number, dimensionless

Subscripts and superscripts

B	bulk phase
F	film
i	liquid-phase and general component index
j	solid-phase component index
k	reaction rate index
L	liquid phase
P	particle
0	initial quantity
*	saturated state

diminish in size. These phenomena shift the process from film reaction to bulk-phase reaction as the reaction proceeds: the film becomes thinner and the reaction rates decline.

The goal of current work is to apply the film theory to reactive solids immersed in liquids, in such a way that realistic geometric forms of solids are considered and the film thickness is updated during the progress of the reaction. The theory is illustrated with numerical simulations of generic cases and parametric study.

2. Modelling principles

2.1. Basic assumptions

The modelling is based on the following hypotheses. A solid material is dispersed in a liquid, where it dissolves and reacts with components in the liquid phase. Because 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. As the reaction progresses, it usually also becomes slower. When this effect is coupled to the decrease of the film thickness, the focus of the chemical transformation is shifted from the liquid film towards the liquid bulk. For the sake of simplicity, to illustrate the basic features of the model, equal particle sizes and isothermal conditions are assumed. Of course, a further improvement of the model would include both the particle size distribution and the heat balances equations. Ideal mixing is assumed. If mixing intensity is local, the model requires to be applied using local conditions. Thus no concentration gradients appear in the liquid bulk. The entire model is dynamic, time dependent. The model can easily be generalized to other kinds of chemical reactors, and particle size distributions can be included in the model.

The reaction system is described by the standard stoichiometric approach,

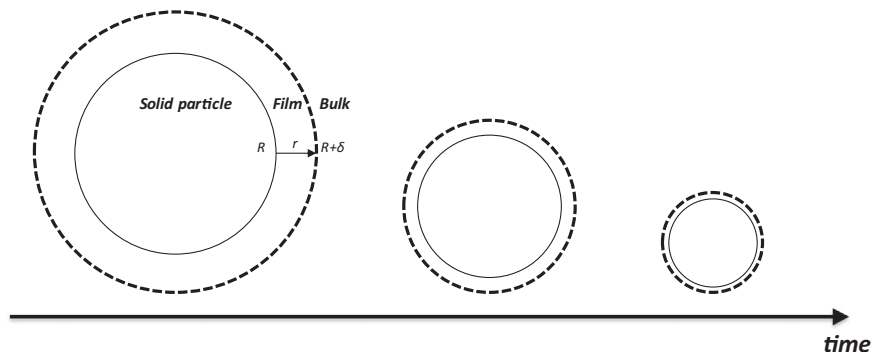


Fig. 1. Solid-liquid reaction system: evolution with time of a shrinking solid particle with a surrounding film.

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