



The obtainment of particle shape factor by the combination of experimental data and fluid–particle reaction model



Jiapeng Fu, Na Li ^{*}, Lian Li, Rui Luo, Qulan Zhou

State Key Laboratory of Multiphase in Power Engineering, Xi'an Jiaotong University, Xi'an 710049, China

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ABSTRACT

A new approach to calculate the shape factor of the solid particle(s) was introduced using the experimental data and fluid–particle reaction model. In fluid–particle reactions, the solid particle reactants have complex shapes, rather than standard sphere in theory. In order to evaluate the influence of particle shape changes during the reaction process, we established a fluid–particle reaction model incorporating a parameter called the shape factor. Combining the model and experimental data by mathematical method, we can obtain the shape factor and the comprehensive reaction coefficient. The results show that the shape factor is larger than 1 in the early stage, then begins to decline rapidly and gradually comes near to constant 1. It agrees well with the experimental observation, indicating that the shapes of limestone particles are changing from irregular shapes to sphere during the reaction progress. The fluid–particle reaction model with the shape factor can describe the reaction well, which demonstrates the validity of our work. Using this method, the particle shape factor and the comprehensive reaction coefficient of any fluid–particle reaction can be acquired, which has great value on the precise prediction and control of fluid–particle reaction.

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1. Introduction

The systems involving fluid–particle interaction are widely used in industrial processes. As a form of multiphase reaction, fluid–particle reactions take place in a variety of engineering processes. Applications are found in the fields of extractive metallurgy [1], control of sulfate pollutants using wet flue gas desulfurization (WFGD) [2,3], and catalyst manufacture. Researchers have launched plenty of theoretical and modeling research on the mechanism of fluid–particle reactions [1,4–11]. Many scholars demonstrated that the exclusion of particle size distribution from the reaction models could cause serious errors, and tried to join in the traditional model of particle size distribution model [8,12–16]. However, only a little work [17,18] has been published on the particle shape changing progress of the solid reactants, which is an important factor that determines the behavior of particulate systems [19].

Since in the majority of industrial applications particles are present in a range of sizes and shapes, a better characterization and understanding of particles shapes in fluid–particle reactions are essential for prediction and design of the system. The irregular shapes of solid particles are difficult to measure in experiment. Bouwman et al. [20] mentioned that particle's shape can be well described by using only one or two shape factors. Many scholars [21–30] had developed many different shape factors from the image analysis to describe the particle shapes. One common feature of most shape factors is their dependence on the

image analysis to estimate the basic dimensions of the particle, notably for the perimeter. Recently, 3D images of the particles have been obtained for determination of the real particle shape and sphericity, which have already been reported by some authors using different methods [19,31–35]. The measurement of 3D particle shape is still restricted in application for the difficulties in obtaining the spatial surface data for large number of particles.

In this paper, we proposed a particle shape factor and incorporated it into the fluid–particle reaction model in order to evaluate the influence of solid shape in the fluid–particle reaction. After considering the shape factor, the fluid–particle reaction model is improved and can describe the reaction process more precisely. The quantitative data of the particle shape factor and the reaction parameters can be used on the precise prediction and control of fluid–particle reaction.

2. Experimental

The experiment of hydrochloride acid dissolving limestone has been done on a static reaction system, as shown in Fig. 1. In the experiment, the hydrochloride acid of a constant pH at a certain temperature was prepared in the reactor. The combination of pH meter, electromagnetic value and automatic titrator was used to guarantee the experimental system maintains at a constant pH value, meanwhile, thermometer and thermostatic water bath ensured a constant temperature during the whole reaction progress. In order to study the shape changes during the reaction, we took out some solutions (less than 0.1%) and observed the particle shape with an optical microscope at different time. The

^{*} Corresponding author. Tel.: +86 18202988666.
E-mail address: lyna@mail.xjtu.edu.cn (N. Li).

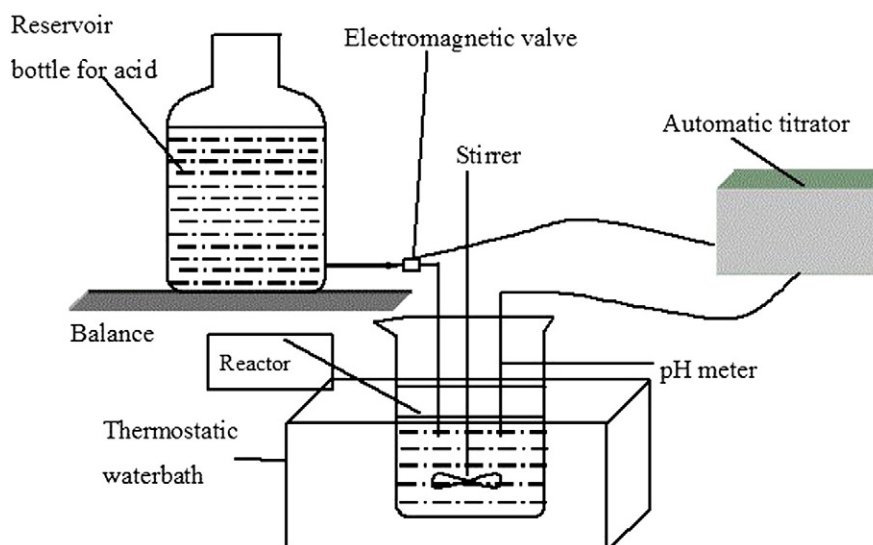


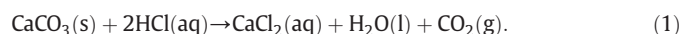
Fig. 1. Experimental system of hydrochloride acid dissolving limestone.

amount of dissolved solid particles was calculated by the consumption of hydrochloric acid solution, which was measured by an electronic balance during the reaction time. In the experiment, the temperature ranged from 50 °C to 80 °C, and pH values was from 4.6 to 6.2.

The raw limestone samples from different sources in China, as shown in Table 1, were ground and sieved to five samples by vibrating screen, and particle size distribution of each sample was measured by the laser particle size analyzer Spraytec 300, which is made by the Malvern Instruments, with the measure range from 0.5 μm to 2000 μm. Melvin Spraytec measures the spray particle size with laser diffraction technique. When the laser beam gets through the spray, the particle size measurement is completed by measuring the intensity of the scattered light.

3. Fluid–particle reaction model

Fluid–particle reaction is a typical reaction type, with a solid and a fluid reactant, generating solid and fluid products. The reaction of hydrochloride acid dissolving limestone particle is shown in Eq. (1):



Fundamental dynamic models are frequently used by engineers to develop new chemical processes and to predict the behavior of existing industrial processes. Among the major models that have been developed for non-catalytic fluid–particle reactions, the shrinking core model (SCM) is most widely used. The SCM [9,10,14] describes the reaction progress between fluid and mono-particle, and is applicable to an initially non-porous particle, which reacts with a reagent leaving a reacted layer around unreacted core or detached. Since the resultant CaCl_2 could be dissolved in the reagent, that is, detached from the reactant CaCO_3 particle surface during the reaction, the chemical reaction rate is determined by the diffusion capacity of the reactants (H^+) in

the fluid or the surface chemical reaction. Then the chemical reaction rate can be expressed as

$$q_m = A_0 \frac{C_f}{\frac{1}{k_f} + \frac{1}{k_r}} \quad (2)$$

where A_0 is the surface area of the particle; C_f is the reactant concentration in the fluid, mol m^{-3} ; k_f is the chemical comprehensive reaction coefficient on the surface, m s^{-1} ; and k_r is the mass transfer coefficient in the fluid film surrounding the solid particle. Usually, mass transfer coefficient is determined by the reaction condition, e.g., concentration, stirring, and temperature. If the reaction condition is fixed, k_f should be regarded as a constant. k_r is the chemical reaction rate of a particle on unit surface area, which is determined by the chemical reaction property. Under certain temperature, k_r could also be assumed to be constant.

On the other hand, the mass balance can be described in terms of the shrinking rate of the particle core as a function of the instantaneous fluid flux

$$q_m = -\frac{1}{b} \frac{d\left(\frac{4}{3}\pi R^3 \rho_s\right)}{dt} \quad (3)$$

where ρ_s is the mole concentration of the solid reactant, mol m^{-3} ; R is the radius of ideal solid particle, m ; and b is moles of the consumed solid per mole of reacted fluid. For the reaction of hydrochloride acid with limestone particle, b is 1/2.

In the SCM, the solid reactant is considered to be spherical, non-porous and initially surrounded by a fluid film, through which mass transfer occurs between the solid particle and the bulk of the fluid. Actually, the solid particles have complex shapes, and thus have different surface areas compared to standard spheres as assumed in theory.

Traditionally, particle shape is quantified by the use of shape factors, which are dimensionless numbers applies to all geometric shapes and independent of scale and particle's orientation. The most commonly used shape factor is the sphericity [24,31,36,37]. Referring to Wadell's definition of a particle's sphericity [31,37], we defined a shape factor to describe the deviation between the real solid particles and their corresponding sphere with equivalent radius.

$$\phi = \frac{A}{A_0} \quad (4)$$

Table 1
Characteristics of the limestone.

Limestone	CaCO ₃ (%)	MgCO ₃ (%)	Al ₂ O ₃ (%)	Fe ₂ O ₃ (%)	Acid insoluble (%)	ρ _m (mol/L)
Liquan	94.21	2.04	0.81	0.35	2.59	24.8
Jiaochang	92.50	4.26	0.08	0.28	2.88	25.1

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