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Transformation of local bubble rise velocity measurements to global results: Shown by a Monte Carlo simulation of a fluidized bed

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ABSTRACT

To design bubbling fluidized bed reactors and study chemical reactions, the knowledge of hydrodynamic properties, such as bubble size, rise velocity and hold-up is of importance. Local measurements of those properties are valuable, but do not automatically reflect the properties of the full bed. In the manuscript a method based on Bayes' theorem is developed, which helps to transform local bubble rise velocity measurements into a global result. The transformation method was tested by means of a Monte Carlo simulation.

Introduction

Bubbling fluidized bed reactors are applied for gas–solid reactions with high requirements for heat and mass transfer. The measurement of the bubble rise velocity distribution (BRVD) within a bubbling fluidized bed reactor is important for the characterization of the reactor performance. It defines the residence time of the different gas bubbles, mixing behavior and is therefore a key parameter for the conversion of reactants. The BRVD within the complete reactor has to be known, to properly predict the chemical conversion, as under-estimated bubble size and velocity for instance can lead to un-predicted reactant bypass. Additionally, the BRVD is needed for the development and validation of detailed computer models for efficient scale-up of fluidized bed reactors (Rüdisüli et al., 2012b).

Different methods have been established to measure the BRVD, ranging from local and intrusive capacitance and optical probe measurements (Werther and Molerus, 1973; Cartellier, 1992) to three dimensional techniques such as tomography (Dyakowski, 1996; Rees et al., 2006; Holland et al., 2008; Mudde, 2011; Brouwer et al., 2012). Up to now, local capacitance and optical probe measurements remain the method of choice, because they are cheap and easy to apply.

However, the local measurements have to be back transformed into a global result to predict the correct bubble rise velocity (BRV) of the full bed, whereupon global means every bubble rising in the fluidized bed is considered. Otherwise, the global number weighted mean BRV of the bed is significantly overestimated by the local measurements, because large and therefore, according to different bubble rise velocity correlations, fast bubbles are more likely pierced by a local probe, compared to small and therefore slow bubbles, which is explained in details in the remainder of the paper.

In a previous work, (Rüdisüli et al., 2012a) analyzed the mean local chord-length, which is normally smaller than the bubble diameter. They demonstrated for different setups that the higher probability to pierce a large bubble approximately counterbalances the smaller chord-length. Which means, the locally measured mean chord-length matches approximately the mean bubble diameter of all bubbles present in the bed. However, for the mean BRV no counteracting effect occurs; and the mean BRV is overestimated due to different pierce probabilities. Both, the mean and the whole distribution are biased.

The objective of this paper is to pinpoint the error sources and to transform the local velocity measurements into a global result. To this end, Monte Carlo simulations on a bubbling fluidized bed are conducted, and a mathematical backward transformation

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based on Bayes' theorem is proposed to transform the local bubble rise velocity into a global one. Furthermore, a sensitivity study to investigate the influence of the assumptions made for the mathematical backward transformation is conducted.

Model and methodology

A Monte Carlo model was developed to compare the local mean BRV with the mean BRV present in the whole cylindrical fluidized bed. The model assumptions are that a homogeneous spatial distribution of spherical bubbles exists in the bed, and that the bubble size distribution of a real bed can be represented using a Gamma or Rayleigh distribution, as shown in (Clark et al., 1996; Gheorghiu et al., 2003). Three different means: the number, diameter and surface weighted mean are compared to the detected results of a perfectly working local, virtual probe. The virtual probe detects every bubble, its chord-length as well as the BRV at the tip. In the Monte Carlo model, first a bubble size distribution is defined using Eq. (1) (Gamma distribution) or Eq. (2) (Rayleigh distribution), where μ is the Rayleigh distribution parameter, q and λ are the shape parameter and scale factor of the Gamma distribution. A fixed number of bubbles is assigned to the distribution.

$$P(y|q,\lambda) = \frac{1}{\lambda^q \Gamma(q)} y^{q-1} \exp\left(-\frac{y}{\lambda}\right) \tag{1}$$

$$P(y|\mu) = \frac{y}{\mu^2} \exp\left(-\frac{y^2}{2\mu^2}\right) \tag{2}$$

Out of the respective distribution, the Monte Carlo model randomly selects a single bubble with defined size, to rise in a straight line in axial direction of the cylindrical fluidized bed. The starting point of this bubble is randomly selected on the cross sectional area, such that the complete bubble is within the reactor. No further wall effects are taken into account in the simulation. An example of such a bubble distribution in a similar simulation is given in (Rüdisüli et al., 2012a). The corresponding bubble rise velocity is assigned to the bubble diameter according to the correlation of Davidson and Harrison applicable for a single bubble:

$$u_B = 0.711 \cdot \sqrt{g \cdot d_B} \tag{3}$$

In the remainder of the paper, we will refer to the factor 0.711 as the "prefactor", the BRVs and diameters are called the simulated data. The virtual, local probe tip is placed in the centerline of the tubular reactor with 145 mm in diameter. The bubble rise velocity and chord-length detected at the tip of the probe is equal to the simulated bubble rise velocity and chord-length present at this point. No detection error is considered in the model, which means that the detected and simulated BRV is equal. The data of the virtual probe is in the following called the locally detected data.

In Fig. 1(a), an example of nine randomly simulated bubbles and the probe is shown (top-view). Apparently, only one out of nine bubbles (i.e., the largest bubble) is pierced by the probe. As the bubbles are spherical, the detected chord-length of this pierced bubble is represented as a dotted line between two triangles in Fig. 1(b).

Results and discussion

Comparison of local and global bubble rise velocity

In Fig. 2, all locally detected bubble rise velocities are plotted over the detected chord-length (open blue[1] circles). Most of the blue circles are broadly scattered above the full line representing the Davidson and Harrison correlation (Eq. (3)), which was used for the simulation the global BRV.

All blue circles in Fig. 2 lie on the left side of the Davison and Harrison correlation, because the chord-length is usually smaller than the bubble diameter. Fig. 2 shows that more than a constant factor is needed to shift the detected mean BRV to the right that it matches the Davidson and Harrison correlation Eq. (3). The dashed line, which illustrates the detected local mean BRV, largely overestimates the simulated mean BRV for a given bubble diameter, especially for smaller bubbles. With increased bubble size the difference between both is approaching zero, because the possible pierce positions are shifted toward the centerline of the bubbles. If a correlation would have been developed based on the locally detected BRV data, the global BRV would be considerably overestimated, because the BRV would be connected to the measured chord-length which is usually smaller.

To overcome the problem of correlating the BRV to the detected chord-length more sophisticated four-point probes were developed, which are able to correlate the measured 3-dimensional BRV to the corresponding bubble size (Guet et al., 2003; Luther et al., 2004). However, applying such a four point probe, the locally measured number weighted mean BRV would still be larger than the simulated number weighted mean BRV present in the bed, which is described in the next section in more details.

In Fig. 2, additionally different mean BRVs are depicted: the locally detected mean BRV based on all detected bubbles shown as blue circles (diamond, number averaged), the global mean BRV of all simulated bubbles (green circle, number averaged) and the corrected (see next section) mean BRV (black cross) are depicted.

When the number weighted mean BRV of all locally detected bubbles is compared to the global simulated BRV, the local measurement largely overestimates the simulated bubble rise velocity for the underlying Gamma distribution. In addition, the detected mean chord-length is a little bit smaller than the mean bubble size simulated. The change in mean chord-length is discussed in all details by (Rüdisüli et al., 2012a), whereas the changes in the mean BRV are discussed and corrected in the following.

In Fig. 3(a), the relative differences between the detected local and simulated global mean BRV are plotted as a function of the simulated global mean bubble diameter. The simulated global mean bubble diameter is changed by using different shape and scale factors for the underlying Gamma distribution in the Monte Carlo model. For visualization, several Gamma distributions for different shape factors are plotted in Fig. 3(b) and distributions for different scale factors in Fig. 3(c).

The set of curves in Fig. 3(a) depicts that the local detected mean overestimates the simulated global mean BRV between 5 and 40%, depending on the chosen bubble size distribution. For systems of large bubbles, where the mean bubble size is exceeding the half of the reactor diameter (145 mm), the difference is approaching zero, which is e.g. the case for slugging. Large bubbles however are normally avoided in fluidized bed reactors, because usually the available exchange surface between bubble and dense phase shall be maximized to increase mass transfer and chemical conversion (Fan, 1989; Safoniuk et al., 2002). For small bubble sizes the relative differences are as high as 40% as can be seen in Fig. 3(a).

To explain why the locally detected mean BRV is larger than the mean BRV of the bed, one has to look at the pierce probability of a bubble with known size (Fig. 4). The pierce probability is increased to unity with increased bubble size, which means larger bubbles are more probably pierced than small ones. Hence, in the analyzed system, where the BRV is assumed to be proportional to the square root of the bubble size, the mean bubble rise velocity is overestimated. A similar result would be obtained, if e.g. the correlation

[1] For interpretation of color in Fig. 2, the reader is referred to the web version of this article.