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Numerical prediction of flow hydrodynamics of wet molecular sieve particles in a liquid-fluidized bed

Guodong Liu[a,b,*], Peng Wang[a], Huilin Lu[b], Fan Yu[b], Yanan Zhang[b], Shuai Wang[b], Liyan Sun[b]

[a] *School of Municipal and Environmental Engineering, Harbin Institute of Technology, Harbin, China*
[b] *School of Energy Science and Engineering, Harbin Institute of Technology, Harbin, China*

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ABSTRACT

The Eulerian–Eulerian framework was used in the numerical simulation of liquid hydrodynamics and particle motion in liquid-fluidized beds. The kinetic theory of granular flow, which accounts for the viscous drag influence on the interstitial liquid phase, was used in combination with two-fluid models to simulate unsteady liquid–solid two-phase flows. We focus on local unsteady features predicted by the numerical models. The solid fraction power spectrum was analyzed. A typical flow pattern, such as core annular flow and particle back-mixing near the wall region of liquid–solid fluidized beds is obtained from this calculation. Effects of the restitution coefficient of particle–particle collisions on the distribution of granular pressure and temperature are discussed. Good agreement was achieved between the simulated results and experimental findings.

Introduction

Liquid–solid fluidized beds are applied extensively in the chemistry, biotechnology, food science, environment, and other industries, because of their favorable mass and heat transfer ability, high operational flexibility, and reduced back-mixing of phases. They have therefore become the focus of much research work.

Molecular sieve particles are used extensively in wastewater treatment because of their porous structure. The porous structure has a large surface area per unit mass, which results in a strong affinity for organic compounds in the wastewater and therefore makes molecular sieve particles ideal sorbents or filter media for their removal. Molecular sieve particles are robust and easy to fluidize and are therefore used extensively as fluidization materials in the wastewater treatment industry.

The modeling of liquid–solid fluidized bed reactors is challenging because of their complex flow behavior and the amount of interaction between liquid and solid phases. Computational fluid dynamics (CFD) is one of the most promising tools for modeling flow behavior. CFD aims to include key mechanisms to predict accurate flow fields and other characteristics of fluidized beds for design, scale-up, and optimization. In the literature, two different CFD models are usually used to simulate fluidized bed flow characteristics. One is the Eulerian–Lagrangian model and the other is the Eulerian–Eulerian two-fluid model. The Lagrangian model solves equations of motion for each particle by taking particle–particle collisions and forces acting on the particle into account, whereas the Eulerian–Eulerian two-fluid model assumes that the liquid and particle phases are continuous, and considers full interpenetration of the two phases in the continuum and momentum equations. To achieve closure, the kinetic theory of granular flow is used with a granular temperature to consider the conservation of fluctuating solids energy. Conservation equations of mass and momentum of both phases result from the statistical average of instantaneous local transport equations (Gidaspow, 1994). The Eulerian–Eulerian two-fluid model is often preferred over others because it is less computationally resource demanding. Recently, considerable attention has been given to the application of CFD to liquid–solid fluidized beds by the Eulerian–Eulerian two-fluid model.

From a traditional point of view, liquid–solid fluidized beds should be comparatively simpler to model than gas–solid fluidized beds because of the homogeneity of hydrodynamics. However, since inter-particle collisions and particle–wall collisions are taken

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* Corresponding author at: Harbin Institute of Technology, School of Energy Science and Engineering, No. 92 West Dazhi Street, Harbin 150001, China. Tel.: +86 045186412258.
E-mail address: gdliu@hit.edu.cn (G. Liu).

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into account (Gidaspow & Lu, 1998), and because of the existence of a liquid film that separates particles as they approach each other, liquid–solid hydrodynamic behavior will become more complex. In literature, CFD has been applied explicitly to liquid–solid fluidized beds (Cheng & Zhu, 2008; Cornelissen, Taghipour, Escudié, Ellis, & Grace, 2007; Lettieri, Di Felice, Pacciani, & Owoyemi, 2006). Researchers have used Eulerian–Eulerian approaches, simplified the fluidized bed as two-dimensional and assumed all particles to be spherical and of uniform size. In all cases, the liquid was tap water; however, particles differed in diameter and density. As mentioned previously, particle collisions may not occur among approaching adjacent particles because of the liquid film between collision particles. To consider this effect, Gidaspow and Lu (1998) suggested an effective restitution coefficient of close to one, whereas for other cases, the coefficients of restitution were less than one, which implied inelastic collisions among particles. Recently, Yang and Hunt (2006) took the effective coefficient of restitution as a function of binary Stokes number, and found that the restitution coefficient of particle–particle collisions was less than one but increased with increasing binary Stokes numbers. In the liquid–solid flow system, because of the acceleration and rotation of particles, the surrounding fluid would apply additional forces to the particles. The virtual mass and lift forces could represent such fluid effects. A number of researchers neglected the virtual mass force and lift force effects when simulating liquid–solid flows (Lettieri et al., 2006; Cornelissen et al., 2007; Panneerselvam, Savithri, & Surender, 2007; Cheng & Zhu, 2008; Gevrin, Masbernat, & Simonin, 2008; Reddy & Joshi, 2009; Hadinoto & Chew, 2010). However, compared with gas–solid two-phase flow, liquid–solid two-phase flow is more dependent on virtual mass force and lift force because of the liquid flow medium, which has a higher density and viscosity. Razzak, Agarwal, Zhu, and Zhang (2008) considered the effect of lift force because of velocity gradients in the liquid-phase flow field but neglected the virtual mass force. Huang (2011) simulated the effect of virtual mass force of liquid–solid flow. It was demonstrated that the virtual mass force played an important role in the CFD simulation of liquid–solid fluidization, and should be considered in CFD simulations. For the effect of different drag laws on liquid–solid two-phase flow, Reddy and Joshi (2009) used the drag coefficient model proposed by Joshi (1983) and Pandit and Joshi (1998) with an energy balance approach where few assumptions were made. Others (Limtrakul, Chen, Ramachandran, & Dudukovic, 2005; Cornelissen et al., 2007; Panneerselvam et al., 2007; Cheng & Zhu, 2008; Mazzei & Lettieri, 2008; Gevrin et al., 2008) used equations based on empirical correlations. Cornelissen et al. (2007) compared empirical drag laws and discovered that the Gidaspow (1994) drag model agreed better with experimental values, but this approach was neglected because of its abrupt change in drag at a bed voidage of 0.8, which could cause numerical instabilities (van Wachem & Almstedt, 2003). However, in this simulation, the Lu and Gidaspow (2003) drag model was used because of its perfect modification of the Gidaspow (1994) drag model, which avoided abrupt changes in drag force at a bed voidage of 0.8.

Since the flow hydrodynamics of wet molecular sieve particles is important in the operation of a liquid fluidized bed to remove organic contaminants in wastewater treatment, it is essential that experimental and numerical simulations be used to study detailed fluidization behavior of wet molecular sieves. Limited research exists in this area. We conducted a detailed investigation into the hydrodynamics of wet molecular sieves at a series of fluidization velocities by numerical simulation based on our experimental device. Local unsteady features of particle flows were predicted by numerical models. The solid fraction power spectrum was analyzed to study the corresponding flow patterns. We also considered the effect of restitution coefficient of wet molecular sieves, and discuss their influence on granular pressure and temperature distributions.

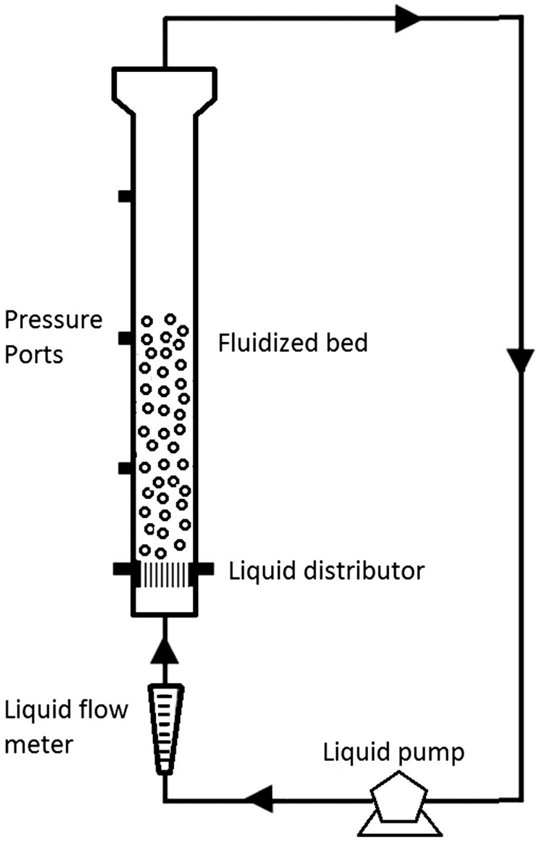

Fig. 1. Schematic of experimental liquid–solid fluidized bed.

Experimental

To test the capability of the CFD model in simulating liquid–solid fluidized bed flow behavior, simulation results from the proposed CFD model and experimental results from the bed voidage of liquid–solid fluidized beds were compared. Liquid–solid fluidization experiments must be conducted at laboratory scale, where all inputs are characterized as well as possible. Liquid–solid fluidization provides a comparatively simpler behavior and facilitates better characterization of fluid and particle properties.

The liquid–solid experimental fluidized bed is shown schematically in Fig. 1. The Plexiglas column has an inner diameter of 0.10 m and a height of 1.037 m. Molecular sieves ($3/4CaO{\cdot}1/4Na_2O{\cdot}Al_2O_3{\cdot}2SiO_2{\cdot}9/2H_2O$) are used extensively in wastewater treatment because of their powerful absorption ability. Solids used were spherical molecular sieve particles of 2.4 mm mean diameter with a solid particle diameter distribution as shown in Fig. 2. Tap water was used.

Liquid flow velocity measurements were performed using the ultrasonic technique (Fluxus F601, Flexim, Germany). Bed expansion height was measured using graph paper marked along the column length.

Liquid–solid two-fluid model

In this work, an Eulerian–Eulerian two-fluid model was used (see Appendix A). This model assumes that the liquid–solid phases are continuous and fully interpenetrating within each control volume, and conservation of mass and momentum is maintained for the liquid and solid phases. Among the various attempts to formulate particulate flow, the kinetic theory of granular flow, which considers the conservation of solid fluctuation energy by introducing the concept of granular temperature $\theta = 1/3\langle c\rangle^2$, was used