Chemical Engineering Journal 171 (2011) 301–313

Contents lists available at ScienceDirect

Chemical Engineering Journal

journal homepage: www.elsevier.com/locate/cej

Two- and three-dimensional CFD modeling of Geldart A particles in a thin bubbling fluidized bed: Comparison of turbulence and dispersion coefficients

Benjapon Chalermsinsuwan [a,b,*], Dimitri Gidaspow [c], Pornpote Piumsomboon [a,b]

[a] Fuels Research Center, Department of Chemical Technology, Faculty of Science, Chulalongkorn University, 254 Phayathai Road, Patumwan, Bangkok 10330, Thailand
[b] Center for Petroleum, Petrochemicals, and Advanced Materials, Chulalongkorn University, 254 Phayathai Road, Patumwan, Bangkok 10330, Thailand
[c] Department of Chemical and Biological Engineering, Illinois Institute of Technology, 10 West 33rd Street, Chicago, IL 60616, USA

ARTICLE INFO

Article history:
Received 15 October 2010
Received in revised form 30 March 2011
Accepted 3 April 2011

Keywords:
Bubbling fluidized bed
Computational fluid dynamics (CFD)
Dispersion coefficient
Hydrodynamics
Multiphase flow
Turbulence

ABSTRACT

A comprehensive understanding of turbulence and dispersion is essential for the efficient design of a conventional fluidized bed reactor. However, the available information is restricted to that in a two-dimensional (2-D) plane, because of the experimental and simulation limitations. It is, therefore, of importance to evaluate the remaining third dimension of the system and compare these results with the corresponding data obtained from the 2-D analysis for validation. In this study, computational fluid dynamics (CFD) based upon the kinetic theory of granular flow with a modified interphase exchange coefficient was successfully used to compute the system hydrodynamics of fluid catalytic cracking (FCC) particles in a thin bubbling fluidized bed with 2-D and three-dimensional (3-D) computational domains. In addition, the shortcoming of the current CFD model was evaluated. With respect to the bed height, the bed expansion ratio and solid volume fraction revealed similar results from both 2-D and 3-D computational domains. The turbulent granular temperature was higher than that of the laminar ones in the lower section of the bed while the laminar granular temperature dominates the system in the upper section. However, the granular temperatures obtained from the 3-D computational domain were slightly lower than that from the 2-D computational domain. The computation also showed that the dispersion coefficients are in good agreement with the literature measurements and so the 2-D computational domain can be used to simulate the bubbling fluidized bed system. Finally, all the evaluated system hydrodynamic values in the thin radial system direction were lower in the 3-D computational domain than in the thick radial system direction.

1. Introduction

Fluidized beds are types of reactor that can be used to perform a variety of gas–solid multiphase reacting flows, such as fluid catalytic cracking (FCC) and coal combustion units [1,2]. In these types of reactor, a gas is passed through solid particles at high enough velocities to suspend the solids and cause them to behave as a fluid. As the gas velocity passing through the solid particles increases, a series of changes in the motion of the solids is formulated as flow regimes. These regimes, arranged in order of increasing velocities are; bubbling, turbulent, fast fluidization and pneumatic transport [3].

At present, the bubbling regime has received more attention than the other three regimes because of its unique characteristics. The occurrence of bubbles is the major characteristic of this regime which then exerts an influence on the gas–solid mixing and reaction conversion. For Geldart B and D particles, the gas velocity, when in excess of the required velocity to maintain the dense phase of the minimum fluidization condition, flows through the solids in the form of a bubble [4]. For Geldart A particles, the solid does not start bubbling as the gas velocity reaches the minimum fluidization condition, but the bed starts expanding [5] due to the role of the interparticle forces. The solid starts to bubble when the gas velocity exceeds the minimum bubbling condition. For Geldart C particles, the solids are very fine and very difficult to fluidize and so there is no bubbling regime [6]. Although there have been a number of published studies on the bubbling regime, most of them have been focused on the macroscopic viewpoint, such as the alteration of the flow pattern with operating conditions [7–9]. Studies from a microscopic viewpoint are still lacking in the literature, despite the fact that this will allow a better understanding of the fundamental parameters describing the system

* Corresponding author at: Department of Chemical Technology, Faculty of Science, Chulalongkorn University, 254 Phayathai Road, Patumwan, Bangkok 10330, Thailand. Tel.: +66 2218 7682; fax: +66 2255 5831.
E-mail address: benjapon.c@chula.ac.th (B. Chalermsinsuwan).

1385-8947/$ – see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.cej.2011.04.007

Nomenclature

C	Scale factor (–)
C_{D0}	Drag coefficient (–)
d_p	Particle diameter (m)
D	Dispersion coefficient (m^2/s)
e	Restitution coefficient between solids or particles (–)
e_W	Restitution coefficient between particle and wall (–)
g	Gravity force (m/s^2)
g_0	Radial distribution function (–)
h	Height of system outlet (m)
H	Height of system (m)
H_i	Height of quasi-steady state solid bed (m)
H_0	Height of initial solid bed (m)
I	Unit tensor (–)
I_{2D}	Second invariant of the deviator of the rate of strain tensor (Pa)
l	Thickness of system (m)
n	Unit vector (–)
P	Pressure (kPa)
Re	Reynolds number (–)
t	Time (s)
T_L	Lagrangian integral time scale (s)
u	Superficial velocity (m/s)
v	Velocity (m/s)
$v_{s,\text{slip}}$	Slip velocity of solid phase at the wall (m/s)
$v_{s,W}$	Velocity of solid phase at the wall (m/s)
$v_{t,W}$	Tangential velocity of solid phase at the wall (m/s)
v'	Velocity fluctuation (m/s)
W	Width of system (m)
x	Radial x-direction (–)
y	Axial y-direction (–)
z	Radial z-direction (–)

Greek letters

β_{gs}	Interphase exchange coefficient (kg/m^3 s)
$\beta_{gs,\text{new}}$	Modified interphase exchange coefficient (kg/m^3 s)
ε	Volume fraction (–)
$\varepsilon_{s,\max}$	Volume fraction of solid phase at maximum packing (–)
ϕ	Specularity coefficient (–)
φ	Angle of internal friction (°)
γ_s	Collisional dissipation of solid fluctuating energy (kg/m s^3)
γ_W	Collisional dissipation of solid phase fluctuating energy at the wall (kg/m s^3)
κ_s	Conductivity of solid fluctuating energy (kg/m s)
μ	Viscosity (kg/m s)
θ	Granular temperature (m^2/s^2)
θ_t	Turbulent granular temperature (m^2/s^2)
θ_W	Granular temperature at the wall (m^2/s^2)
ρ	Density (kg/m^3)
τ	Stress tensor (Pa)
ω	Correction factor correlation (–)
ξ	Bulk viscosity (kg/m s)

Subscripts

g	Gas phase
s	Solid phase
x	Radial x-direction
y	Axial y-direction
z	Radial z-direction

hydrodynamics, and so enable scientists and engineers to design better and more efficient reactors [10].

The hydrodynamics of bubbling fluidized bed reactors deals with the dynamic phenomena of the gas–solid suspension inside the reactor. The parameters describing these hydrodynamics include the turbulence and dispersion coefficients. Tartan and Gidaspow [11] stated that using a kinetic theory based particle image velocimetry apparatus, there are two kinds of turbulence in the fluidization, as measured by granular temperature. A "laminar" granular temperature, which represents random oscillations of individual solids and measures the solid's fluctuating kinetic energy, and a "turbulent" granular temperature, which represents the motion of the bubble or cluster of solids and measures the normal Reynolds stress. These terminologies are named after the method to compute the oscillations or movements. The laminar oscillation is obtained by computing the instantaneous velocity while the turbulent oscillation is obtained by the hydrodynamics or averaged instantaneous velocity, which is typically used as the turbulent velocity in turbulence theory. This methodology has then been applied to characterize the information in many fluidization systems in both experimental and simulation conditions [12–16]. Dispersion coefficients are a parameter for measuring the quality of mixing and their definition is based on the kinetic theory of granular flow [17]. As such it is a measure of the spread of solids with reference to the spatial location. Similar to turbulence, there are two kinds of mixing; a "laminar" type due to individual particle oscillations and a "turbulent" type due to bubble or cluster of solid oscillations [15,18]. In addition, many researchers have tried to compute these parameters using other methodologies, such as tracer injection [19–22] and thermal inspection [23]. However, these methodologies were mainly restricted to considering the dispersion coefficient only in the axial direction, ignoring all other directions. Recently, Breault [24] summarized that the reported dispersion coefficients (from the available literature) can vary up to five orders of magnitude. Given that our current understanding of both turbulence and dispersion coefficients is somewhat restricted to a two-dimensional (2-D) plane, albeit due to the experimental and simulation limitations, the values in the other system dimensions are interesting to discover and compare with the data obtained from 2-D studies.

Computational fluid dynamics (CFD) is a branch of fluid mechanics that uses numerical methods and algorithms to solve problems and analyze phenomena that involve fluid and chemically reacting flows [25]. For gas–solid systems, two different approaches might be used for the calculation, namely the Lagrangian and the Eulerian approaches. The Lagrangian approach should be used when the solids in the system occupy a low volume fraction while the Eulerian approach should be used when the solid volume fraction in the system is high. For the bubbling fluidized bed, the Eulerian approach is thus more suitable for the calculation. This approach separately solves the conservation equations for each phase. Among the various attempts to close the gas–solids flow, the kinetic theory of granular flow is the most widely applied theory as a constitutive equation [26–30]. This theory is basically an extension of the classical kinetic theory of gases with the addition of the solid fluctuating kinetic energy and the solids collision descriptions. Although CFD is anticipated to make valuable contributions in predicting the performance of a bubbling fluidized bed, there are currently no universal CFD models that can be applied to all systems [31–34], as will be discussed in the following sections. Therefore, more attention should be focused in this area.

This study aims to determine the turbulence or granular temperature and the axial and radial dispersion coefficients for gas and solids in a thin bubbling fluidized bed using CFD simulation with 2-D and three-dimensional (3-D) computational domains. As stated above, it was the first literature that studies and compares these