Powder Technology 228 (2012) 69–83

Contents lists available at SciVerse ScienceDirect

Powder Technology

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

Comparison of phenomenological and fundamental modelling approaches for predicting fluidized bed reactor performance

Schalk Cloete [a], Abdelghafour Zaabout [b], Stein Tore Johansen [b], Shahriar Amini [b,*]

[a] NTNU Department of Energy and Process technology, Trondheim, Norway
[b] SINTEF Materials and Chemistry, Trondheim, Norway

ARTICLE INFO

Article history:
Received 21 December 2011
Received in revised form 26 April 2012
Accepted 28 April 2012
Available online 5 May 2012

Keywords:
Computational fluid dynamics
Phenomenological model
1D model
Fluidized bed reactor
Kinetic theory of granular flows
Central composite design

ABSTRACT

Two approaches to modelling fluidized bed reactors were evaluated and compared in this work: a phenomenological 1D approach based on empirical closures and a more fundamental 2D approach based on computational fluid dynamics (CFD). The fundamental modelling approach should be more accurate and generic, but is several orders of magnitude more computationally expensive than the phenomenological approach. Therefore, the development of accurate, but computationally affordable phenomenological models is a matter of great importance. This work evaluated the behaviour of both modelling approaches over a wide range of operating variables spanning the bubbling fluidization regime. These variables included fluidization velocity, bed height, operating temperature and particle size. Several different closure models were evaluated for the phenomenological approach and it was shown that models for the bubble size, bubble-to-emulsion mass transfer coefficient and solids inside the bubble all have a significant impact on model performance. An optimal combination of closure models used in the phenomenological approach succeeded in providing a good match to data gathered from the more generic fundamental approach. The response of the model to changes in particle size was identified as the area with the greatest potential for further development. More detailed comparisons of axial distributions of important flow variables showed some differences between the predictions of the phenomenological and fundamental modelling approaches. In particular, the hydrodynamic measures of axial void distribution and bubble rise velocity predicted by these two approaches showed some significant differences.

1. Introduction

Modelling of non-linear systems such as fluidized bed reactors is essential for the purposes of optimization, control and scale-up. Various hydrodynamic models have been presented in the literature in order to address this need. Initially, simple contacting models such as plug flow, mixed flow and tanks in series were tested [1]. However, a major advance seen in fluidized bed reactor modelling was the introduction of two-phase theory [2]. According to this theory, the fluidized bed consists of two phases; the emulsion phase where the gas is flowing under minimum fluidization conditions through a dense mass of solids and the bubble phase where no solids are present and the gas can rise at velocities significantly greater than the fluidization velocity. Subsequently, the existence of a third phase in the form of a particle cloud between the bubble and the emulsion phases was also considered [3], especially for beds with fine particles. This cloud phase was neglected for intermediate and coarse particles though. Over the following decades many models were developed for industrial fluidized beds on the basis of this theory [4,5]. Models were developed for gas–solid catalytic cracking [6,7] and for heterogeneous gas–solid reactions [8,9] and were shown to give adequate predictions of process performance.

Despite its success, the simple two phase model (STP) has received criticism for under-predictions of reactor performance because of two inaccurate assumptions: (i) the bubble is free of solids and (ii) the emulsion phase is under minimum fluidization conditions. Alternative approaches were proposed to address these assumptions [10,11]. In addition, the two-phase model was also extended from its basis in bubbling fluidization to the regimes of turbulent [12] and the fast fluidization [13].

Even though such extensions are available, the simple two-phase model (STP) is best applied in the bubbling fluidization regime for which it was originally developed. Even so, the success of the models largely depends on accurate closure laws for the bubble size and the inter-phase mass transfer. Considering the existence of solids inside the bubble may also be necessary to improve model performance.

Several formulations of the bubble size and the mass transfer coefficient are available in the literature, but a clear consensus on the best performing model combination is yet to be reached. Assessment of model performance with respect to different formulations of various constituent models over a wide range of operating conditions covering the bubbling regime is therefore of high importance. For this reason, the response of model performance to changes in four independent

* Corresponding author.
E-mail address: shahriar.amini@sintef.no (S. Amini).

0032-5910/$ – see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.powtec.2012.04.063

Nomenclature

α	Volume fraction
δ	Bubble fraction
ε	Void fraction
ϕ	Kinetic energy transfer rate (kg/m.s^3)
γ	Dissipation rate (kg/m.s^3)
μ	Viscosity (kg/m.s)
Θ_s	Granular temperature (m^2/s^2)
ρ	Density (kg/m^2)
ς	Specularity coefficient
$\bar{\bar{\tau}}$	Stress tensor (kg/m.s^2)
$\vec{\tau}_s$	Particle shear force at the wall (N)
$\vec{v}$	Velocity vector (m/s)
∇	Del operator/Gradient (1/m)
Ar	Archimedes number
C	Molar concentration (mol/m^3)
D	Diffusivity (m^2/s)
d	Diameter (m)
g	Gravitational constant (9.81 m/s)
$\vec{g}$	Gravity vector (m/s^2)
$g_{0,ss}$	Radial distribution function
H	Bed height (m)
h	Height within the reactor (m)
$\bar{\bar{I}}$	Identity tensor
$\vec{J}$	Diffusive flux (kg/(m^2.s))
K	Momentum exchange coefficient (kg/(m^3.s))
K	Mass transfer coefficient (1/s)
k	Diffusion coefficient (kg/m.s)
k	Reaction rate constant (m/s)
M	Molar mass (kg/mol)
N	Moles (mol)
p	Pressure (Pa)
R	Gas constant (8.314 J/K.mol)
R^H	Heterogeneous reaction rate (mol/m^3 s)
S	Source term (kg/m^3 s)
T	Temperature (K)
t	Time (s)
U	Velocity (m/s)
$\vec{U}_{s,\|\|}$	Particle velocity parallel to wall (m/s)
V	Volume (m^3)
x	Mass fraction
Y	Species mass fraction
z	Axial distance (m)

Sub- and superscript definitions

0	Inlet
Θ_s	Granular temperature
A	Species A
b	Bubble
br	Bubble rise
c	Cloud or core
e	Emulsion
ex	Expanded bed
g	Gas or grain
gs	Inter-phase
i	Species index
max	Maximum packing
mf	Minimum fluidization
n	Reaction order
p	Particle
s	Solids
st	Static

Abbreviations

by	Interaction effect
d	Particle diameter
H	Initial static bed height
L	Linear effect
Q	Quadratic effect
SS	Sum of squares
T	Temperature
U	Fluidization velocity

variables (fluidization velocity, static bed height, particle size, and temperature) is studied in this work.

Computational fluid dynamic (CFD) modelling based on the standard two fluid model closed by the kinetic theory of granular flows (KTGF) [14–16] was chosen to assess 1D model performance. This methodology has been used extensively in the published literature over the past three decades and has been hydrodynamically validated (e.g. [17]). CFD also offers great flexibility to investigate the effects of changes in any conceivable independent variable and is therefore an ideal tool to use in the present study where a wide range of independent variables will be investigated. Physical experimentation over such a wide range of variables would be prohibitively complex and expensive.

2. Simulations

Both phenomenological 1D and fundamental 2D simulations were performed and compared in this work. The theoretical bases behind these approaches will be presented separately below.

2.1. 1D model theory

The simple two phase model (STP) was used as a basis for the 1D modelling conducted in this study. Several additions were made to the STP in its standard form.

2.1.1. Standard STP model equations

The fluidized bed is assumed to consist of two phases; the particle-rich emulsion phase and the particle-lean bubble phase. The STP model assumes that the bubbles are solid-free and reactions occur only in the emulsion phase where the gas flows upwards at minimum fluidization velocity. The equation system (Eqs. (1)–(15)) solved in this modelling approach is given in Table 1. This combination of closure relations were chosen based on their popularity in the open literature and successful comparisons to experimental data [9,11].

2.1.2. Model enhancements and alternative formulations

Eq. (7) and Eq. (11) were used for the bubble size and mass transfer in initial 1D simulations. Alternative model formulations were subsequently evaluated in the form of Eq. (6) for the bubble size as well as variations on Eq. (10) and its constituents and Eq. (13) for the mass transfer. The best performing model combinations were retained for any subsequent simulations.

The STP formulation was also improved by considering the existence of solid particles inside the bubble. A simple initial model was derived from CFD for this purpose.

2.1.3. Solution strategy

The system of equations given in Table 1 was solved using an algorithm implemented in MATLAB. The entire reactor was divided into constant sections with a height of Δz. Hydrodynamic parameters (bubble size and velocity, the mass transfer coefficient, etc.) were determined in each section, after which the mole balance equations were solved to get the axial species concentration. A Runge–Kutta method