



The effect of frictional pressure, geometry and wall friction on the modelling of a pseudo-2D bubbling fluidised bed reactor



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ABSTRACT

The two fluid model (TFM) closed by the kinetic theory of granular flows (KTGF) has been developed to a high level of maturity over the past three decades. However, significant uncertainties still remain about the influence of various closure models on the predictions of the hydrodynamics and especially the reactive performance of fluidised bed reactors. The three factors investigated in this study – frictional pressure, geometry (2D/3D) and friction at the walls – all have significant influences on model predictions of the behaviour of a pseudo-2D bubbling fluidised bed reactor. This study aims to quantify the influence of these important factors on simulation output both in terms of hydrodynamics and reactive performance. Simulations designed to evaluate the effects of these factors were carried out over a wide range of fluidisation velocities, bed loadings and particle sizes to reveal significant impacts on the results. Differences in simulation results varied significantly with changes in the three operating variables investigated (fluidisation velocity, bed loading and particle size) and were analysed in detail. Finally, 3D simulations with wall friction and frictional pressure included showed qualitatively very similar hydrodynamic behaviour to that observed in the experiments. Quantitatively, measurements of the bed expansion ratio compared well for different fluidisation velocities and the particle sizes, but some unexplained differences were still observed in response to changes in the bed loading.

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List of symbols

Main symbol definitions

α	volume fraction
ϕ	kinetic energy transfer rate (W/m^3)
φ	angle of internal friction (degrees)
γ	dissipation rate (W/m^3)
λ	bulk viscosity (Pa s)
μ	viscosity (Pa s)
Θ_s	granular temperature (m^2/s^2)
ρ	density (kg/m^3)
ζ	specularity coefficient
τ_s	particle relaxation time (s)
$\bar{\tau}$	stress tensor (Pa)
$\vec{\tau}_s$	particle shear force at the wall (N)

\vec{v}	velocity vector (m/s)
v_r	terminal velocity (m/s)
∇	del operator/gradient (1/m)
C_D	drag coefficient
d	diameter (m)
e_{ss}	particle–particle restitution coefficient
f	drag function
\vec{g}	gravity vector (m/s^2)
$g_{0,ss}$	radial distribution function
H	bed height (m)
\bar{I}	identity tensor
$I_{2D} = \frac{1}{2}S$	S : second invariant of the strain rate tensor (s^{-2})
\vec{J}	diffusive flux ($\text{kg}/(\text{m}^2 \text{ s})$)
K	momentum exchange coefficient ($\text{kg}/\text{m}^3 \text{ s}$)
k	diffusion coefficient ($\text{kg}/\text{m s}$)
p	pressure (Pa)
Re_s	particle slip Reynolds number
S	strain rate tensor (s^{-1})
t	time (s)
$\vec{U}_{s,\parallel}$	particle velocity parallel to wall (m/s)

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Sub- and superscript definitions

0	initial/static
Θ_s	granular temperature
<i>col</i>	collisional
<i>exp</i>	experiment
<i>fric</i>	frictional
<i>g</i>	gas or grain
<i>gs</i>	inter-phase
<i>kin</i>	kinetic
<i>max</i>	maximum packing
<i>s</i>	solids
<i>sim</i>	simulation

Abbreviations

ANOVA	analysis of variance
BER	bed expansion ratio
by	interaction effect
CCD	central composite design
dp	particle diameter
H0	initial static bed height
KTGF	kinetic theory of granular flows
L	linear effect
PS	phase segregation
Q	quadratic effect
SS	sum of squares
TFM	two fluid model
U0	fluidisation velocity
X	reactor performance

1. Introduction

The two fluid model (TFM) closed by the kinetic theory of granular flows (KTGF) [1–3] has been developed to a high level of maturity over the past three decades. For this reason, recent research work involving the TFM for the modelling of fluidised beds has been focusing primarily on specific process applications under the implicit assumption that the underlying models are sufficiently accurate. In terms of model development, the majority of recent research activity has been focused on large scale simulations through a filtered approach (e.g. [4]), but room for improvement still exists in the smaller scale resolved simulations on which these filtered models are based, especially in reactive flows (e.g. [5]).

Pseudo-2D domains are especially useful when it comes to assessing resolved TFM simulations. These domains allow for easy access to local experimental data which can be used to thoroughly evaluate the accuracy of small scale simulations. For example, it has recently been found that the friction on the large front and back walls of a pseudo-2D fluidised bed has a very large influence on the solids velocity observed in the unit. When simulating a pseudo-2D unit on a 2D plane using the standard TFM, it was found that the mean solids velocities occurring inside the reactor can be over-predicted by a factor of four [6]. This very large discrepancy was attributed to the neglected friction between the particles and the large front and back walls in the 2D simulation and this will be further studied in this work over a range of fluidisation velocities, particle sizes and bed loadings.

Although the aforementioned study found that the transition from a 2D to a 3D simulation domain had no influence on the solids velocity profiles in itself, this conclusion might not be generally valid. In order to facilitate measurements of the particle velocity using particle image velocimetry combined with digital image analysis (PIV/DIA), relatively large particles (500 μm) have been used. These large particles formed large flow structures which maintained distinctly 2D behaviour in the thin bed. Smaller particle sizes, on the other hand, will form smaller particle structures which could be smaller than the thickness of the bed, thereby possibly creating an influence related to the choice between a

2D and 3D simulation geometry. This effect will also be further studied in this work.

In addition, another potential source of error, the influence of the frictional pressure, will be investigated in this work. The majority of published literature on the subject simply uses granular pressure models derived for the kinetic and collisional regimes also in the frictional regime. This is not technically correct because the normal stresses resulting from prolonged contact at very high solids packing are very different in nature compared to the short lived collisions and the sub-scale translations in the collisional and kinetic regimes. A limited number of papers [7–9] have looked at this effect and found a moderate impact of the frictional pressure on the bubble dynamics and bed expansion. This paper will therefore further evaluate this factor over a wider range of flow conditions.

2D planar simulations without the inclusion of frictional pressure have been compared to pseudo-2D experiments before. One of the most cited studies about the validation of the 2D TFM approach in a bubbling fluidised bed [10] used a pseudo-2D experimental setup and found good comparisons with regard to bed expansion ratio and local solids volume fraction profiles measured with an optical probe. In our previous study [6], bed expansion ratios over a range of fluidisation velocities were evaluated and it was confirmed that the simulated bed expansion ratios mirrored experimental observations almost exactly.

Simulation predictions of the bed expansion under different bed loadings and particle sizes were less accurate, but despite the very large discrepancy in the particle velocity, the predictions of the bed expansion ratio were still acceptable. It therefore appears that the macroscopic hydrodynamic behaviour is not very sensitive to the correct prediction of the solids velocity.

The ultimate aim of such models, however, is to accurately simulate a fluidised bed reactor. Therefore, this study will also include reaction kinetics to investigate the effect of the inclusion of wall friction and frictional pressure not only on the bed hydrodynamics, but also on reactor performance (the degree of conversion achieved). The results will serve as a guideline for subsequent simulation comparisons to reactive experiments performed in a pseudo-2D bubbling fluidised bed reactor.

The decision to limit the scope of this work to the detailed investigation of only three factors (frictional pressure, geometry (2D/3D) and friction at the walls) was based on extensive efforts to improve the match with quantitative and qualitative experimental results reported in Sections 4.1.5 and 4.2 of this work. All three selected factors influence the frictional momentum transfer in the pseudo-2D domain which, due to the large wall/volume ratio, is particularly sensitive to frictional forces exerted by the walls. Other closure models also have an influence on the solution, but the most important of these, the drag law and the particle–particle restitution coefficient in particular, have been explored in quite some detail in the literature to date (e.g. [10–14]). This work will therefore include only a brief assessment of these and other potentially important factors.

2. Simulations*2.1. Model equations*

Conservation equations are solved for each of the two phases present. The continuity equations for the gas and solids phases are given below:

$$\frac{\partial}{\partial t} (\alpha_g \rho_g) + \nabla \cdot (\alpha_g \rho_g \vec{v}_g) = 0 \quad 1$$

$$\frac{\partial}{\partial t} (\alpha_s \rho_s) + \nabla \cdot (\alpha_s \rho_s \vec{v}_s) = 0. \quad 2$$

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