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Grid independence behaviour of fluidized bed reactor simulations using the Two Fluid Model: Effect of particle size

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

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

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ABSTRACT

It is well known that particle size has a significant influence on the grid independence behaviour of fluidized bed reactor simulations carried out using the Two Fluid Model (TFM) approach. The general rule of thumb states that the cell size should scale linearly with the particle size so that the cell size is always at most a factor of 10 larger than the particle size. In this study, however, the effect of particle size on grid independence behaviour was shown to be unexpectedly large. In particular, a five-fold increase in particle size permitted the use of a 63 times larger cell size, implying a $63^3 \approx 250{,}000$ times speedup for resolved simulations in the planar 2D domain considered in this study. Thus, the general rule of thumb was found to be overly cautious, especially for larger particles. Closer investigation revealed the particle relaxation time to be a very good predictor of the grid independent cell size. Although this finding needs to be confirmed for parameters other than only the particle size, this relation can theoretically be used to greatly shorten the time-consuming grid independence studies that are required before any fluidized bed simulation campaign. In general, the rapid increase in cell size allowed by larger particle sizes showed that reasonably accurate industrial scale simulations (5 m inner diameter reactor) are already possible in 2D for large particles (~600 μm). If the 2D grid independence behaviour assessed in this study is extendible to 3D, larger particle sizes in the range of 500–1000 μm can already be simulated in full 3D for reactor sizes ranging from 1–4 m. Simulation of smaller particle sizes (<200 μm) will remain out of reach for many decades to come, however, and a filtered coarse grid approach will definitely be required to make such simulations possible.

1. Introduction

Fluidized bed reactors are widely used in the process industry for applications involving gas–solid reactions or solid catalysed reactions. The excellent heat and mass transfer characteristics of these reactors are highly advantageous from a process engineering point of view and it can therefore be assumed that the number of process applications utilizing this technology will only increase in the future.

Fluidized bed reactors are challenging to design and scale up, however, primarily due to the complex transient process nature created by the formation of mesoscale particle structures inside the bed. These particle structures are observed as clusters in risers and bubbles in bubbling fluidized beds and result from the non-linear drag interaction between the gas and the solids. When designing a fluidized bed reactor, these structures cannot be ignored because they have a profound influence on all transport phenomena inside the reactor.

This complex hydrodynamic behaviour of fluidized bed reactors is closely coupled to reaction kinetics and heat transfer considerations. For example, the formation of the structures has a negative influence on the overall reaction rate by concentrating particles (and therefore surface area for reaction) in dense clusters that have a low gas permeability [1]. The result is a severe mass transfer limitation because reacting gases cannot penetrate fast enough into the cluster. Thus, if this cluster effect is not accurately accounted for in the reactor design and scale up considerations, reactor performance will be greatly over-predicted, leading to misleading design guidelines.

In this work, the fundamental modelling framework of computational fluid dynamics (CFD) is proposed as a suitable modelling tool. Because of its fundamental basis in the conservation of mass, momentum, species and energy, CFD is capable of inherently capturing the complex mesoscale structure formation and the resulting non-linear interactions that make fluidized bed reactors a difficult modelling challenge.

CFD approaches for modelling fluidized bed reactors have been developed to a good level of maturity over the past three decades, primarily based on the kinetic theory of granular flows (KTGF) [2–4] where the random uncorrelated motions of particles are likened to the motions of molecules in a gas. This approach has been used extensively in the literature and some favourable hydrodynamic validation studies have also been performed [5–7]. However, the primary limitation of these methods is the fine spatial and temporal resolution required to

* Corresponding author at: Department of Process Technology, SINTEF Materials and Chemistry, Richard Birkelands Vei 3, 7034 Trondheim, Norway. Tel.: +47 46639721.
E-mail address: shahriar.amini@sintef.no (S. Amini).

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Nomenclature

Main symbol definitions

α	volume fraction
Δ_{lin}	linearized grid size
ϕ	kinetic energy transfer rate (W/m^3)
γ	dissipation rate (W/m^3)
Θ_s	granular temperature (m^2/s^2)
μ	viscosity (Pa·s)
ρ	density (kg/m^3)
ς	specularity coefficient
$\overline{\overline{\tau}}$	stress tensor (Pa)
$\vec{\tau}_s$	particle shear force at the wall (N)
τ_s	particle relaxation time (s)
τ_{Ss}	Stokes relaxation time (s)
$\vec{v}$	velocity vector (m/s)
∇	del operator/gradient (1/m)
Ar	Archimedes number
C	molar concentration (mol/m^3)
C_D	drag coefficient
d	diameter (m)
$\vec{g}$	gravity vector (m/s^2)
$g_{0,ss}$	radial distribution function
$\bar{I}$	identity tensor
$\vec{J}$	diffusive flux (kg/(m^2·s))
K	momentum exchange coefficient (kg/(m^3·s))
k	reaction rate constant (m/s)
k_{Θ_s}	granular temperature diffusion coefficient (kg/(m·s))
M	molar mass (kg/mol)
N	moles (mol)
p	pressure (Pa)
R	gas constant (8.314 J/(K·mol))
Re	Reynolds number
R_H	heterogeneous reaction rate (mol/(m^3·s))
S	source term (kg/m^3·s)
T	temperature (K)
t	time (s)
U	fluidization velocity (m/s)
$\vec{U}_{s,\|\|}$	particle velocity parallel to wall (m/s)
V	volume (m^3)
X	reactor performance parameter
Y	mass fraction

Sub- and superscript definitions

A	species A
g	gas
gs	interphase
i	species index
n	reaction order
s	solids

accurately resolve the mesoscale structures. Thus, simulations of industrial scale fluidized bed reactors are not computationally affordable for the majority of cases.

The most promising approach for meeting this challenge is to model the effects of these mesoscale structures on grid sizes that can be larger than the structure itself. An increasing body of literature focusing on the subject is already available (e.g. [8–11]). However, the additional modelling included in this filtered approach introduces a substantial degree of uncertainty simply due to the complex nature of the subgrid clustering phenomena. After more than a decade of development, current closures for the drag and solids stresses appear to function reasonably well with uncertainties still present in areas with large flow gradients such as near-wall regions [12]. A first closure for first order heterogeneous reactions has recently been proposed [13] and heat transfer correlations are yet to be developed.

Therefore, this work strives to find the real limits of an approach which is mature already today: the TFM/KTGF approach. It is well known that the grid independence behaviour of TFM simulations is strongly correlated with the particle size simulated. In general, fluidized beds using larger particle sizes can be simulated on coarser grids with cell sizes often specified at 10 times the particle size as a general rule of thumb. With the consistent exponential increase in computational capacity and availability, it can therefore be reasoned that the particle size that can be directly simulated in an industrial scale fluidized bed will gradually decrease with time. Some guidelines can be found in this work regarding the size of fluidized bed that can be directly simulated with existing models and a specified particle size using computational capacities available today.

2. Simulations

2.1. Model equations

The equation system for the well-known TFM KTGF approach will be briefly outlined below. This approach has been confirmed to give adequate representations of the hydrodynamics of fluidized bed units [6,14,15], although it should be stated that the 2D approximations of 3D cylindrical beds will lead to systematic deviations within the parameter space of interest [16] and that the simulation becomes very sensitive to exact cluster resolution when fast reactions are simulated [17]. The complete equation system can be viewed in [1].

2.1.1. Conservation equations

The continuity and momentum equations for the gas and solids phases are given below:

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

$$\frac{\partial}{\partial t}\left(\alpha_g\rho_g\vec{v}_g\right)+\nabla\cdot\left(\alpha_g\rho_g\vec{v}_g\vec{v}_g\right)=-\alpha_g\nabla p+\nabla\cdot\overline{\overline{\tau}}_g+\alpha_g\rho_g\vec{g}+K_{sg}\left(\vec{v}_s-\vec{v}_g\right) \tag{2}$$

$$\frac{\partial}{\partial t}\left(\alpha_s\rho_s\right)+\nabla\cdot\left(\alpha_s\rho_s\vec{v}_s\right)=0 \tag{3}$$

$$\frac{\partial}{\partial t}\left(\alpha_s\rho_s\vec{v}_s\right)+\nabla\cdot\left(\alpha_s\rho_s\vec{v}_s\vec{v}_s\right)=-\alpha_s\nabla p-\nabla p_s+\nabla\cdot\overline{\overline{\tau}}_s+\alpha_s\rho_s\vec{g}+K_{gs}\left(\vec{v}_g-\vec{v}_s\right) \tag{4}$$

The solids stresses $\left(p_s \text{ and } \overline{\overline{\tau}}_s\right)$ are modelled according to the KTGF. Interphase momentum exchange ($K_{gs}=K_{sg}$) was modelled according to the formulation of Syamlal and O'Brien [4]. The drag law is the most important factor which influences the particle size-related grid independence behaviour of the TFM and the full formulation is presented in Section 3.2.

Species are conserved only for the gas phase.

$$\frac{\partial}{\partial t}\left(\alpha_g\rho_gY_{gi}\right)+\nabla\cdot\left(\alpha_g\rho_g\vec{v}_gY_{gi}\right)=\nabla\cdot\alpha_g\vec{J}_{gi}+\alpha_gS_{gi} \tag{5}$$

No energy conservation was included under the assumption of isothermal flow. This is usually a good assumption due to the excellent mixing achieved in fluidized bed reactors.