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Evaluation of a filtered model for the simulation of large scale bubbling and turbulent fluidized beds

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ABSTRACT

Full 3D flow simulations of lab and industrial scale dense fluidized beds were carried out using a filtered Eulerian–Eulerian approach. Filtered closures for interphase momentum exchange, solids stresses and additional wall corrections were implemented in the standard equations of motion. These closures had a very large effect on the overall model performance when solved on the large cell sizes required for computationally affordable 3D fluidized bed simulations. Numerical experiments conducted under different fluidization conditions showed that the current model formulation performs well over a wide range of operating conditions. It was found that additional modelling accounting for flow non-uniformity is essential under certain fluidization conditions. The current method for dealing with flow non-uniformity by means of wall corrections yielded good results under vigorous fluidization, but caused a slight inaccuracy at low fluidization velocities. In general, comparisons to a wide range of experimental data showed good quantitative agreement, suggesting that the formulation of the filtered model is highly generic. The filtered approach was also successfully verified in a large scale bubbling fluidized bed reactor by comparisons with a highly computationally expensive, well resolved, non-filtered flow simulation.

1. Introduction

Fluidized bed reactors form an integral part of many process industries in operation today. The intimate inter-phase contact and excellent mixing achieved by these reactors offer a highly favourable environment for any gas–solid or solid catalysed reaction. Fluidized bed reactor performance is very difficult to predict, however, primarily due to the complex and highly interconnected physical phenomena involved. Intricate gas–solid hydrodynamics is tightly coupled to heat transfer and heterogeneous reaction kinetics, presenting a distinctly non-linear modelling problem.

The fundamental flow modelling framework of computational fluid dynamics (CFD) is therefore an ideal candidate for accurately modelling these complex reactors. Simultaneous conservation of mass, momentum, energy and species throughout space and time ensures that the non-linear interactions between all relevant physical phenomena are simulated directly. For this reason, CFD modelling of fluidized beds has enjoyed significant research attention over the past two decades. A Eulerian–Eulerian multiphase flow modelling framework closed by the kinetic theory of granular flows (KTGF) [1–3] is regularly used for this purpose.

Another complicating characteristic of fluidized bed reactors is the formation of mesoscale structures (bubbles in bubbling beds and clusters in risers). The size, shape and nature of these mesoscale structures largely determine the behaviour of a fluidized bed and have to be accounted for in order to correctly predict reactor performance [4]. Generally, however, these controlling structures occur on very small time and length scales, requiring fine grids and small timesteps to resolve accurately. A standard Eulerian–Eulerian KTGF approach can therefore only simulate relatively small-scale 2D fluidized beds and a fully resolved, 3D simulation of an industrial fluidized bed is far beyond the capabilities of today's computational facilities.

In order to attain accurate solutions on computational grids coarse enough to allow for large-scale 3D simulations, a filtered approach may be used where the effects of mesoscale structures, now being smaller than the grid size, are modelled based on averaged values of local flow variables. Such an approach allows for computational speedups of several orders of magnitude, but additional closure relations are required to close the filtered conservation equations.

This work is based on filtered two-fluid models of gas–particle flows as formulated by Sundaresan and co-workers [5,6]. The models were developed in two stages. Firstly, highly resolved simulations of two-fluid models were carried out in periodic domains. The resulting flow-fields were subsequently filtered to obtain filtered constitutive models for fluid–particle drag coefficient, the particle phase pressure and particle phase viscosity. The resulting models depended only on particle and fluid physical properties, particle volume fraction and the

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List of symbols

α	Volume fraction
Δ_f	Filter length (m)
λ	Bulk viscosity (kg/(m·s))
μ	Shear viscosity (kg/(m·s))
ρ	Density (kg/m^3)
$\bar{\bar{\tau}}$	Stress tensor (kg/(m·s^2))
$\vec{v}$	Velocity vector (m/s)
∇	Gradient or del operator (1/m)
C_D	Drag coefficient
c	Drag filter coefficient
d	Diameter (m)
Fr_f	Filter size Froude number
$\vec{g}$	Gravity vector (m/s^2)
$h\ (\alpha_s)$	Scaling function
$\bar{\bar{I}}$	Identity tensor
K	Momentum exchange coefficient (kg/(m^3·s))
p	Pressure (Pa)
Re	Reynolds number
t	Time (s)
V	Volume (m^3)
v_t	Terminal particle velocity (m/s)
x	Distance from the wall (m)

Subscripts

d	Dimensionless
g	Gas
p	Not filtered (i.e. on a particle level, not on a cluster level)
sg	Inter-phase
s	Solid

filter size. Secondly, highly resolved simulations in a wall-bounded domain were carried out in order to derive the required corrections in near-wall regions.

This approach was demonstrated to achieve good results in riser flows of Geldart A particles [7], but has not been thoroughly evaluated for application in dense bubbling and turbulent fluidized beds. These flow regimes will be the focus of the current study and will present a thorough test for the generality of the current modelling approach. If good results can be attained for a wide range of bubbling and turbulent fluidization cases in addition to the aforementioned favourable riser flow results, it can be interpreted as a very positive result for the filtered modelling approach as it stands now and serve to encourage both academia and industry to further develop this approach. A good generic agreement should encourage academia to extend this approach to also include species, energy and reaction kinetic filtering and encourage industry to start employing and testing this approach in real-world problems involving reactor hydrodynamics. Such an increased focus would significantly accelerate the development of a model capable of making real contributions to industrial fluidized bed reactor design and operation.

Two bed configurations will be considered in the present work: a lab-scale fluidized bed filled with Geldart A particles and operated in the bubbling and turbulent regimes as well as an industrial scale bubbling fluidized bed filled with large Geldart D particles. 3D simulation of the hydrodynamics in these beds lies beyond the capacities of present computational resources, implying that a filtered approach is mandatory for achieving sufficiently accurate numerical solutions.

2. Simulations

Numerical simulations will be based on a multiscale modelling approach proposed by Igci et al. [5]. In this approach, filtered closures are derived from small scale, well resolved simulations.

2.1. Model equations

The equation system is based on the Eulerian–Eulerian multiphase flow modelling approach, where the two participating phases (gas and solid) are treated as inter-penetrating continua or fluids. This approach is often referred to as the two fluid model (TFM).

2.1.1. Conservation equations

Mass and momentum are conserved for each phase individually.

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

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

$$\frac{\partial}{\partial t}\left(\alpha_g\rho_g\vec{v}_s\right) + \nabla\cdot\left(\alpha_g\rho_g\vec{v}_g\vec{v}_g\right) = -\alpha_g\nabla p + \nabla\cdot\bar{\bar{\tau}}_g + \alpha_g\rho_g\,\vec{g} + K_{sg}\left(\vec{v}_s\vec{v}_g\right) \tag{3}$$

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

In the above equations, all variables represent filtered values.

Since this is only a hydrodynamic study, no conservation of energy or species are included.

2.1.2. Closures

Standard hydrodynamic simulations of fluidized beds are generally closed by the KTGF, modelling subgrid motions of particles on grids much larger than the particle size. In addition to modelling particle scale phenomena, the filtered approach also models mesoscale phenomena by accounting for the presence of subgrid particle structures. Simulations can therefore be carried out on grid sizes larger than the subgrid structures. Filtered closures are added on top of the KTGF closures so that, when no filtering is required, the KTGF closure is used. The KTGF will not be presented in detail here, however, since it is not the primary focus of the study and is well documented in numerous other works (e.g. [4,8]).

The equation setup used in this paper was received through a personal communication directly from Sundaresan and co-workers and represents the latest and most accurate formulations according to the filtering methodology outlined in two recent publications [5,6]. While a previous study [7] validated these formulations in riser flows, this study aims to carry out validation studies in the bubbling and turbulent fluidization regimes, thereby fully assessing the generality of the modelling approach.

The first filtered closure is that of interphase momentum transfer ($K_{sg} = K_{gs}$) in Eqs. (3) and (4). This is done by modifying the subgrid drag law for the particle [9] by a factor between zero and one. The momentum interaction coefficient is therefore reduced to account for the larger amount of slip experienced by a conglomerate of particles.

$$K_{sg} = K_{sg,p}(1 + c) \tag{5}$$

$$K_{sg,p} = \frac{3}{4}C_D\frac{\alpha_s\alpha_g\rho_g\left|\vec{v}_s - \vec{v}_g\right|}{d_s}\alpha_g^{-2.65} \tag{6}$$

$$C_D = \frac{24}{\alpha_g \mathrm{Re}_s}\left[1 + 0.15\left(\alpha_g\mathrm{Re}_s\right)^{0.687}\right] \tag{7}$$