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Short communication

Grid independence behaviour of fluidized bed reactor simulations using the Two Fluid Model: Detailed parametric study

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ABSTRACT

This short communication builds on previous work on the grid independence behaviour of the Two Fluid Model in reactive bubbling fluidized bed simulations. Regarding hydrodynamic grid independence behaviour (the numerical accuracy with which phase segregation was resolved), the particle relaxation time was confirmed as being directly proportional to the cell size achieving sufficiently grid independent behaviour. This relationship held over different particle sizes, particle densities, gas densities, gas viscosities and drag laws, but the slope of the proportionality changed for particle relaxation times above 0.4. For reactive grid independence behaviour (the numerical accuracy with which reactor performance was resolved), the relationship between the particle relaxation time and the sufficiently grid independent cell size was more complex, depending not only on the resolution of phase segregation, but also on the kinetic rate implemented and on the permeability of the emulsion phase. Simple and practical rules of thumb were proposed for estimating the sufficiently grid independent cell size for hydrodynamic and reactive simulations. For most practical purposes, the simpler and more accurate hydrodynamic grid independent cell size correlation can safely be used to run sufficiently accurate bubbling fluidized bed reactor simulations.

1. Introduction

Grid independence behaviour of fluidized bed simulations carried out using the Two Fluid Model (TFM) closed by the Kinetic Theory of Granular Flows (KTGF) remains a very important research topic even today, three decades after this approach was first proposed [1–3]. Firstly, TFM-KTGF simulations are used to derive industrial scale filtered models (e.g. [4–6]) which are enjoying significant research attention at present. Secondly, as shown in the first part of this work [7], larger particle sizes have much less stringent grid size requirements than smaller particle sizes and industrial sized beds using large particles (~500 μm) can already be simulated with current computational capacities.

These important applications of resolved TFM simulations require tedious and time-consuming grid independence studies to be completed for every set of operating conditions simulated. Often, when a parametric CFD study is carried out, only one grid independence study is completed on the assumption that these guidelines can be used over the entire parameter space. This assumption is often invalid, however, implying that varying degrees of numerical error could be confounding the results obtained over the parameter space.

The first part of this work showed that grid independence behaviour scaled very well with the particle relaxation time. This correlation could be used to significantly shorten the grid independence work that must be done before each resolved TFM simulation campaign, but was only evaluated for simulations carried out with different particle sizes. This second part of the work is therefore completed to assess this correlation by varying a broader range of simulation parameters that have a direct influence on the particle relaxation time.

2. Simulations

The simulation setup and data processing strategy followed in this short communication is identical to that reported in the first part of this work [7] except for the reaction kinetic description outlined in Section 2.1 below.

2.1. Reaction kinetics

A simple, catalytic conversion of five different gas species A, B, C, D and E to gas species A^*, B^*, C^*, D^* and E^* respectively was simulated to

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Nomenclature

Main symbol definitions

α	volume fraction
Δ	sufficiently grid independent cell size (m)
ε	void fraction
ρ	density (kg/m^3)
a	acceleration (m/s^2)
Ar	Archimedes number ($\frac{gd_s^3\rho_g(\rho_s-\rho_g)}{\mu_g^2}$)
c_3	proportionality constant (s)
c_4	proportionality constant (m)
d	particle diameter (m)
g	gravitational acceleration (m/s^2)
k	reaction rate constant (s^{-1})
m	mass (kg)
R^H	heterogeneous reaction rate (mol/(m^3 s))
Y	mass fraction

Sub- and superscript definitions

emul	emulsion
g	gas
hydro	hydrodynamic
react	reactive
s	solids

occur on the surface of microscopic solid grains (S) within the particles used in the fluidized bed:

$$A + S \rightarrow A* + S$$
$$B + S \rightarrow B* + S$$
$$C + S \rightarrow C* + S$$
$$D + S \rightarrow D* + S$$
$$E + S \rightarrow E* + S.$$

Mass transfer limitations were neglected on the assumption that mass transfer is much faster than the reaction rate on the surface of the grains. The validity of this assumption was confirmed in a previous publication by the authors [8].

The physical and chemical properties of all species were specified to be identical so that the reactions would not influence the hydrodynamics resulting in a non-linear interaction. This will significantly simplify the interpretation of results, enabling clearly decoupled conclusions regarding hydrodynamic and reaction kinetic grid independence to be drawn from each simulation.

The five reactions included in the system were set to run at different rates so that the influence of reaction rate on grid independence behaviour could be determined.

$$\begin{aligned} R_A^H &= 20\alpha_s\rho_g\frac{Y_A}{Y_A+Y_{A*}} \\ R_B^H &= 40\alpha_s\rho_g\frac{Y_B}{Y_B+Y_{B*}} \\ R_C^H &= 80\alpha_s\rho_g\frac{Y_C}{Y_C+Y_{C*}} \\ R_D^H &= 160\alpha_s\rho_g\frac{Y_D}{Y_D+Y_{D*}} \\ R_E^H &= 320\alpha_s\rho_g\frac{Y_E}{Y_E+Y_{E*}} \end{aligned} \quad (1)$$

The reaction rates in each cell (molar rate of change from species A to A^*, B to B^* etc. per unit volume) were then implemented as a source term into the species conservation equation. Since the species had identical properties and the reaction occurred in a 1:1 stoichiometric ratio, no mass or momentum source terms were required.

3. Results and discussion

Results will be presented in two main sections: an analysis of the hydrodynamic grid independence behaviour of the model and a similar analysis of the reactive grid independence. Nine new cases were simulated (Table 1), each over at least 5 different cell sizes.

3.1. Hydrodynamic grid independence

The hydrodynamic grid independence was quantified according to the phase segregation performance measure (the volume average of the RMS of the solids volume fraction over the bed region as described in [7]). Since the formation of structures (clusters and bubbles) is the primary factor influencing all transport phenomena occurring inside fluidized bed reactors, it is very important that the grid is sufficiently fine to capture these structures with at least reasonable accuracy. The phase segregation performance measure is a good indicator of the degree of structure resolution.

Following the same methodology as that outlined in the first part of this work [7], the particle relaxation time for each of the cases in Table 1 was calculated at different solids volume fractions. In this case, the particle relaxation time at a solids volume fraction of 0.02 produced a good fit as illustrated in Fig. 1, although it should be stated that the fit remains good in the volume fraction range of 0–0.05 ($R^2 > 0.98$). As discussed in [7], the solids volume fraction at which the particle relaxation time is calculated has a significant influence on the quality of the fit achieved and, in this case, the quality of the fit increasingly deteriorated above a solids volume fraction of 0.05. In this case, the solids volume fraction range of 0–0.05 makes physical sense because it is the typical volume fraction experienced by freely moving particles inside the bubble. These particles will join into the surrounding solids structure if sufficient streamline curvature is resolved so that the particles' inertia cause deviations from the carrier phase streamlines [7].

It is clear that the correlation holds very well for all cases except for case 3 (the largest particle size) where the grid independent cell size is predicted to be smaller than that shown by the actual simulation. When also adding the five cases completed in the first part of this work [7], it is shown that case 3 is not an anomaly, but rather an indicator of a changing trend. The previous study investigated five particle sizes (200, 400, 600, 800 and 1000 μm) with a particle density of 2500 kg/m^3, a gas density of 0.3 kg/m^3 and a gas viscosity of 4.5E − 5 kg/(m·s). The larger particle sizes in this previous study resulted in higher particle relaxation times than those shown in Fig. 1.

The clear shift in the proportionality between the sufficiently grid independent cell size and the particle relaxation time around a relaxation time of 0.4 s is evident from Fig. 2. In the first part of this work [7], this step change was not observed because of an insufficient number of data points (5 cases) and a single proportionality using the particle relaxation time at a solids volume fraction of 0.3 was established. The larger dataset available in this study (14 cases) clearly shows that this was not the complete picture and that the particle relaxation time at a

Table 1
Fluidization velocity and material properties for the different cases considered in this study.

Case	Particle size (μm)	Particle density (kg/m^3)	Gas density (kg/m^3)	Gas viscosity (10^{-5} kg/(m·s))	Fluidization velocity (m/s)
1	200	2500	1.2	2.50	0.273
2	400	2500	1.2	2.50	0.523
3	800	2500	1.2	2.50	1.080
4	400	1250	1.2	2.50	0.322
5	400	5000	1.2	2.50	0.844
6	400	2500	0.3	2.50	0.777
7	400	2500	4.8	2.50	0.340
8	400	2500	1.2	1.25	0.687
9	400	2500	1.2	5.00	0.389