

The Combined-Continuum-and-Discrete-Model (CCDM) for simulation of liquid-particle flows

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Abstract

The Combined-Continuum-and-Discrete-Model (CCDM) is a technique that can simulate microscale behaviour of fluid-particle systems. Previous studies have focused on gas-solids flows; however, the technique is equally applicable to liquid-solid systems providing the model is expanded to account for complex fluid-particle interaction forces and changes to interparticle contact behaviour caused by the liquid medium. In this work, liquid-fluidized beds have been simulated using CCDM. Results indicate that modifications to account for the effect of the liquid have little impact on macroscopic system qualities such as minimum fluidization velocity and bed expansion, but a significant improvement in terms of the microscale particle mixing behaviour produced by the model.

Keywords: liquid fluidization; multiphase flow; computer simulation; particle contacts

1. Introduction

Unit operations involving solid particulate materials submersed in liquids are common in industrial processes. Examples include crystallisation, sedimentation, filtration, hydrotransport, and liquid fluidization. Knowledge of the behaviour of liquid-particle systems is clearly of interest to those working in these areas. While some useful information can be obtained from experimental measurements, examination of microscale motion cannot be realised by experimental methods due to the complexity of these systems. Fortunately, computer simulation techniques may be able to provide a solution.

The Combined-Continuum-and-Discrete-Model, or CCDM, is a technique that can simulate microscale behaviour of fluid-particle systems. Previous CCDM-type studies of multiphase systems have focused on gas-solids flows, in particular the behaviour of gas fluidized beds [1, 2]. However, the technique is equally applicable to many industrial liquid-solids flows.

Here we discuss the simulation of liquid-fluidized beds using CCDM. Examination of liquid fluidization allows evaluation of CCDM's usefulness for more general liquid-solids flows. In addition, increases in the number of applications that make use of liquid-fluidized beds in recent years gives an incentive to better understand the behaviour of these systems.

For liquid-particle systems more complex fluid-particle interactions, as well as the effect of the more viscous fluid on particle collisions, must be accounted for in the model formulation. Comparison of results obtained using the original, or 'gas', CCDM, and the modified, or 'liquid', CCDM are presented here.

2. Methodology

CCDM uses a combination of the Discrete Element Method (DEM) for predicting the particle motion, and Computational Fluid Dynamics (CFD) for modelling the behaviour of the continuum fluid.

In DEM [3] simulations, the trajectories and rotations of individual particles are evaluated based on Newton's second law of motion, using a numerical time stepping scheme. Contact forces are calculated at each time step using appropriate contact laws, and resolved into their normal and tangential components. The key assumption in DEM is that disturbances cannot propagate from any particle further than its immediate neighbours, providing a sufficiently small time step is used.

For calculation of the continuum fluid flow, the locally-averaged [4] continuity and Navier-Stokes equations are solved using the SIMPLE method [5] to give the fluid velocity and pressure. This CFD calculation for the fluid is combined with the DEM model of the particles' behaviour by carefully applying Newton's third law of motion to the fluid-particle interaction force. This ensures the two sets of equations, which are solved on different length scales, are correctly coupled.

More details of the CCDM model formulation as applied in gas-solids systems are given in [2]. The modifications to the CCDM which are necessary to correctly simulate liquid-solid systems are described below.

2.1. Fluid-particle interaction forces

In liquid-particle systems, high fluid viscosity and small density difference between the phases means certain fluid-particle interactions that are negligible in gas-particle systems must be considered. In the 'gas' CCDM, only the steady-state drag force is considered. In the 'liquid' CCDM, we consider the added-mass, the Magnus (spin) lift, and the pressure gradient forces, in addition to the steady-state drag force. The overall fluid-particle interaction force is therefore:

$$\mathbf{f}_d = \frac{\pi}{6} \rho_f d_p^3 \left[\frac{3}{4d_p} \left(C_{D0} |\mathbf{u}_f - \mathbf{u}_p| (\mathbf{u}_f - \mathbf{u}_p) \varepsilon^{-\chi+1} + C_m (\mathbf{u}_f - \mathbf{u}_p)^2 \right) + C_a \frac{d}{dt} (\mathbf{u}_f - \mathbf{u}_p) + \left(\frac{d\mathbf{u}_f}{dt} - \mathbf{g} \right) \right] \quad (1.1)$$

C_{D0} , the steady state drag coefficient, and the exponent χ are functions of the particle Reynolds number, Re , as given in [6]. C_m , the Magnus lift force coefficient, is also a function of Re , and is calculated as described in [7]. C_a is the added-mass coefficient, taken to be 0.5. The final term on the right-hand side is the pressure gradient force [8].

2.2. Particle-particle and particle-wall contacts

In liquid-particle systems, interparticle collisions differ significantly from those in gas-particle systems due to the effect of hydrodynamic lubrication forces between the

particle surfaces which depend on the fluid density and viscosity. To account for this in the ‘liquid’ CCDM, each particle’s coefficient of restitution was taken to be a function of the particle Stokes number, based on the relation given in [9]:

$$e_{liquid} = e_{gas} \left(1 - \frac{St_c}{St} \right) \quad (1.2)$$

where e_{gas} is the particle coefficient of restitution in air, and St_c is the critical impact Stokes number, below which rebound does not occur. In this work, St_c was set equal to 10 [9]. St , the particle Stokes number, is given by:

$$St = \frac{mv}{6\pi\mu r^2} = \frac{Re}{9} \frac{\rho_p}{\rho_f} \quad (1.3)$$

3. Simulation conditions

Solid phase		Fluid phase	
Particle shape	Spherical	Fluid	water
Number of particles	1600	Viscosity, μ	$1.00 \times 10^{-3} \text{ kgm}^{-1}\text{s}^{-1}$
Particle diameter, d	$5.00 \times 10^{-3} \text{ m}$	Density, ρ_f	$1.00 \times 10^3 \text{ kgm}^{-3}$
Particle density, ρ_p	$2,750 \text{ kgm}^{-3}$	Bed width	$2.00 \times 10^{-1} \text{ m}$
Spring constant, k_n	$1.50 \times 10^6 \text{ Nm}^{-1}$	Bed height	1.00 m
Sliding friction, γ	0.3	Bed thickness	$5.00 \times 10^{-3} \text{ m}$
Dry damping coefficient, η	1.10 kgs^{-1}	Cell width	$1.00 \times 10^{-2} \text{ m}$
Time step, Δt	$5.00 \times 10^{-7} \text{ s}$	Cell height	$1.00 \times 10^{-2} \text{ m}$

Table 1. Parameters used in the simulations.

An initial packing was generated by allowing randomly distributed particles to fall under the influence of gravity, without fluid effects. This packing was used in the fluidized bed simulations with both the original and modified CCDM models. A uniform fluid inlet velocity across the base of the bed was used in all cases.

4. Results and discussion

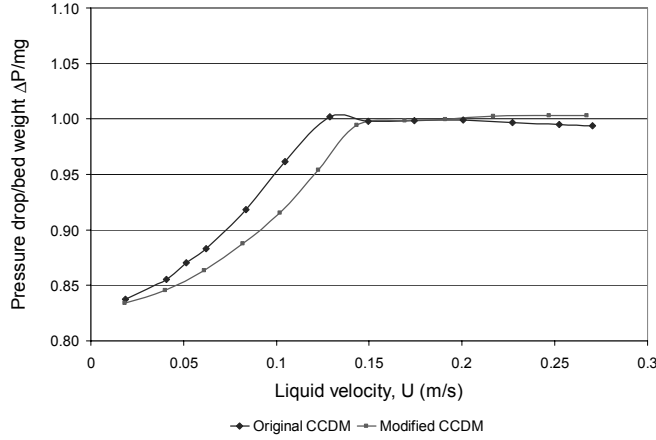


Figure 1: Relationship between liquid velocity and pressure drop for both CCDM models

Figure 1 shows the evolution of the bed pressure drop as the liquid velocity is increased. The curve reaches a plateau at the minimum fluidization velocity, U_{mf} . In the cases shown $U_{mf} = 0.13 \text{ ms}^{-1}$ for the original CCDM and 0.15 ms^{-1} for the modified CCDM. These values are higher than predicted from the Richardson-Zaki equation, which gives U_{mf} as 0.08 ms^{-1} .

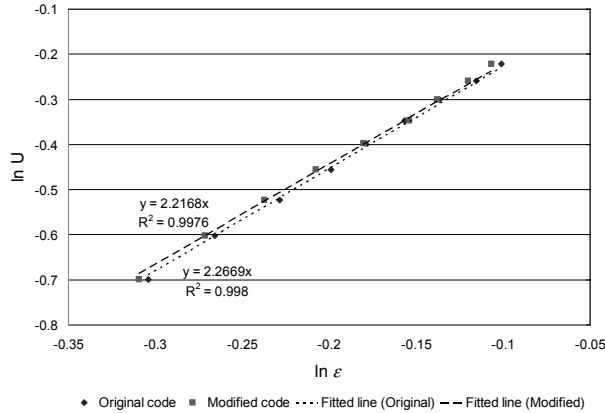


Figure 2: Richardson-Zaki bed expansion, both models – gradients give the value of exponent n

Figure 2 shows the relationship between voidage and liquid velocity, U . Both fitted lines have similar gradients: 2.27 for the original CCDM; 2.22 for the modified CCDM. These values are close to the theoretical value of $n = 2.4$ for systems with a terminal $Re > 500$ (in this system terminal $Re = 2800$).

While Figures 1 and 2 suggest that the modifications have not had a great impact on the macroscopic system behaviour, since the differences in U_{mf} and bed expansion between the two versions of CCDM are small, results from the modified CCDM exhibit quite significant differences in terms of particle-scale mixing and flow behaviour. Figures 3

and 4 show snapshot images of fluidized beds simulated with the original (Fig. 3) and modified CCDM (Fig. 4).

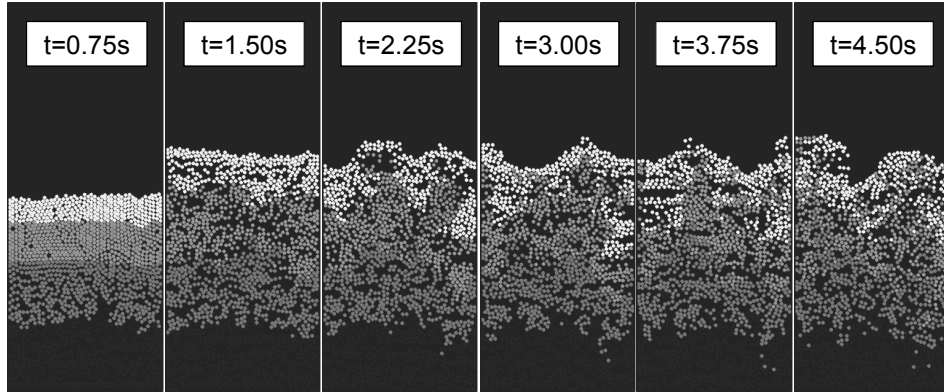


Figure 3: Snapshot images of bed fluidized at 0.4 ms^{-1} , as simulated with original CCDM model. (Particles coloured according to initial position to allow visual observation of mixing).

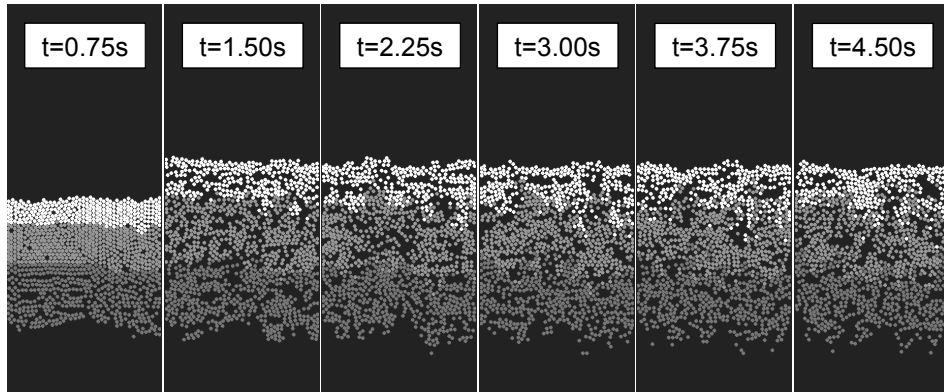


Figure 4: Snapshot images of bed fluidized at 0.4 ms^{-1} , as simulated with modified CCDM model. (Particles coloured according to initial position to allow visual observation of mixing).

In Figure 3, the uneven and unsteady nature of the bed surface is apparent, and a certain degree of mixing is exhibited, whereas in Figure 4 the bed has a smooth surface and is not as well-mixed. The animations from which these snapshots are taken show distinct differences in the flow behaviour of the two beds: the simulation with the original CCDM exhibits bubbling behaviour akin to that observed in a gas-fluidized bed; while the modified CCDM produces a smoother fluidization with less bubbling, as is commonly observed in liquid fluidized beds.

Figure 5, which shows distributions of particles' axial (a) and radial (b) component velocities, supports this finding. There is a noticeable difference in both plots. Results from the original CCDM exhibit greater deviation from the mean value (close to zero in all cases), indicative of greater mixing; while distributions from the modified CCDM are more tightly grouped around the mean, as expected from the lesser degree of mixing observed in Figure 4.

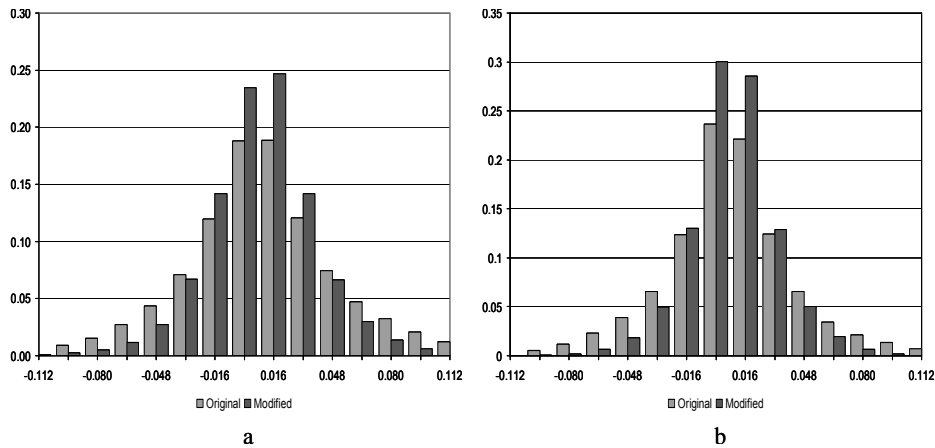


Figure 5: Individual particle component velocity distributions for fluidized beds, velocity 0.4 ms^{-1}
 (a) Axial velocity distribution; (b) Radial velocity distribution.

5. Conclusions

The Combined-Continuum-and-Discrete-Model (CCDM) has been applied to simulate liquid-fluidized beds. Inclusion of additional fluid-particle interaction forces and revision of the way interparticle contacts are treated resulted in similar values to the original CCDM in terms of macroscopic bed properties, but better results in terms of the particle-scale mixing behaviour. Further studies are being performed in order to determine the relative sensitivity of the model to each of the individual fluid-particle interaction forces, and of the revised contact mechanics.

Acknowledgments

The authors would like to thank Nexia Solutions Ltd. and the Engineering and Physical Sciences Research Council for financial support to Mr. Malone in the form of CASE studentship award number GR/P03711/01.

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