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Comparison of heat transfer models in DEM-CFD simulations of fluidized beds with an immersed probe

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ABSTRACT

The basic mechanisms governing the process of surface-to-bed heat transfer in fluidized beds and their relative importance have not been fully characterized yet, mainly owing to the lack of reliable data at the particle scale. Numerical simulations based on the discrete element method may prove successful in predicting the evolution of the fluid and particles' temperature fields. In the present work, microscopic models of the fluid–particle, particle–particle, fluid–surface and particle–surface heat transfer have been implemented in a DEM–CFD hydrodynamic code. Details are discussed on the methodology adopted to include immersed objects in the computational domain. Thus, three approaches to represent particle-particle heat transfer are analysed and compared against experimental values, taken from the literature, of the heat transfer coefficient between a hot fluidized bed and a spherical probe. Unfortunately, some parameters appearing in the formulations are difficult to determine, so reasonable estimates are calculated and used in the simulations. Under conditions similar to the experiments, simulation predictions of the heat transfer coefficient range from 43 to 340 W/(m^2 K) depending on the model used, while the experimental values are located around 160 W/(m^2 K). The variability of these numerical results confirms their sensitivity to the particle–particle mechanism considered. Finally, it is shown that using the model that produces results in agreement with experiments the heat flows due to the particle convective and the fluid convective transfer are of comparable importance.

1. Introduction

Fluidized bed reactors operating at high temperatures are often encountered in industry, where tube bundles or surfaces are immersed to provide or remove the heat necessary to the process. However, research studies on hot bubbling beds are much more limited in numbers, often due to the increased complexity of the system and difficult accurate measurements. Therefore, a successful design of industrial units very often relies upon empirical correlations and expensive scale-up of real plants. To render predictions on the behaviour of the system so problematic is the combination of complex two-phase hydrodynamics and the intimately related heat and/or mass transfer and chemical reactions. Models and correlations available in the literature generally offer limited validity [1]. Even the most widely used theories, such as those based on the packet renewal model [2], appear based on assumptions not easily verifiable.

Progresses in understanding the mechanisms governing the process are being made thank to new experimental techniques (see e.g. Refs. [3,4]) and detailed computational models (see e.g. Ref. [5]). Among the most promising approaches belonging to the latter category is a combination of the DEM (Discrete Element Method, [6]) and CFD (see e.g. [7,8]). In the recent years, these are being expanded to incorporate effects due to fluid–solid and solid–solid thermal energy exchange in fluidized beds [9]. One of the earliest computational works based on a combined DEM–CFD approach including thermal effects was devoted to the characterization of the heat transfer in pneumatic transport lines [10]. More recently, Zhou et al. [11] used a DEM–LES approach with thermal exchange and chemical reaction for fluidized bed coal combustion and Malone and Xu [12] simulated the flow and heat transfer in large-particle liquid-fluidized beds with heated walls.

The aim of this paper is to present the results of an extension of a computer code previously developed for DEM–CFD simulations of gas- and liquid-fluidized bed hydrodynamics [13] and mixing of fluidized binary beds [14] to include the energy balance and the effects of particle-scale heat transfer. Microscopic models describing transfer of thermal energy between two particles, between a particle and the fluid and between the two phases and immersed objects exist in the literature (see e.g. Refs [15–18]). Some of them have been obtained from theoretical considerations, while others are attempts to find possible explanations for the disagreement between oversimplified models and experimental data. Integrated with DEM–CFD simulations, these models are expected to allow important progresses in characterizing heat transfer at the macroscopic scale (e.g. [10]). To explore this possibility in fluidized bed applications, various heat transfer approaches have been incorporated into the model with the aim to carry out simulations of a fluidized bed with an immersed

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spherical probe and compare them with experimental data available in the literature [19]. A brief discussion of the equations utilized is presented in Section 2, along with the extensions required to include surfaces internal to the computational domain for both solid and fluid phases. In Section 3 the microscopic models utilized to represent the various heat transfer mechanisms and their implementation are discussed. The simulations of the fluidized bed behaviour and the comparison of the predictions with experimental data are illustrated in Section 4.

2. Extension of the DEM–CFD model with immersed boundaries

As in the conventional Discrete Element Method [6], the particles' trajectories are obtained by integration of the Newton–Euler equations governing the translational and rotational motion, respectively. For each particle considered the following equations are integrated:

$$m\mathbf{a} = m\mathbf{g} + \sum_{j=1}^{Nc} \mathbf{f}_{c,j} + V_p \nabla p + \mathbf{f}_d \tag{1}$$

$$I\boldsymbol{\alpha} = \sum_{j=1}^{Nc} \mathbf{f}_{c,j} \times \mathbf{R} \tag{2}$$

where m and I are particle mass and moment of inertia. In Eq. (1) the force contributions considered are gravitation, the sum of the contact forces $\mathbf{f}_c$ and the fluid–particle hydrodynamic interaction, subdivided into a pressure gradient term and the drag. In Eq. (2) the only force contributions causing a torque on the particle are assumed to be the contact forces applied at the contact point, i.e. hydrodynamic actions promoting rotation are neglected. Thus, the torque arises from the cross product of the cumulative contact force by the vector $\mathbf{R}$ pointing from the particle centre to the contact point. The contact forces are conveniently decomposed into normal and tangential contributions and a non-linear model [20] is adopted to relate the contact forces to the macroscopic particle–particle and particle–wall displacement and relative velocity.

From the point of view of DEM, the presence of immersed surfaces requires a slight modification of the standard algorithm to include also contact detection and evaluation of the displacements and corresponding contact forces between each particle and the surfaces. This does not cause heavy complications as approaches similar to the particle–particle case can be easily applied. Special care must be paid to edges and vertices, especially in the contact detection step. Also, the collision with the surface edge shall be modelled through special force–displacement laws, eventually including orientation-dependent stiffness. However, this specific aspect is neglected in the present work, due to the lack of mathematical expressions with the required simplicity.

By setting up the computational model, the code is able to simulate the effect of elementary linear or circular (arcs) walls in 2D or planes and spherical surfaces in 3D (both solid or shallow) inserted into a bed of particles, allowing to create objects of complex shape through any combination of these elements (Fig. 1).

From the point of view of the fluid phase, the inclusion of internal surfaces sets a number of complications. Prior to describing the special treatment of immersed objects let us briefly recall the equations governing the continuous phase hydrodynamics. Considering a compressible fluid, the continuity and momentum balance equations in their locally-averaged form [21] are:

$$\frac{\partial \rho_f \varepsilon}{\partial t} + \nabla \cdot \rho_f \varepsilon \mathbf{u} = 0 \tag{3}$$

$$\frac{\partial \rho_f \varepsilon \mathbf{u}}{\partial t} + \nabla \cdot \rho_f \varepsilon \mathbf{u}\mathbf{u} = -\varepsilon \nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{F}_{FP} + \rho_f \varepsilon \mathbf{g} \tag{4}$$

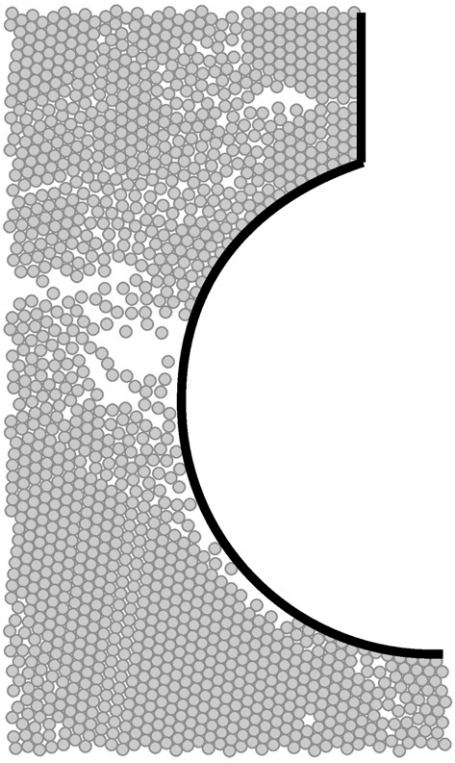

Fig. 1. An enlarged view on particles moving around a circular probe.

where the fluid density ρ_f, velocity $\mathbf{u}$, pressure p, deviatoric stress tensor $\boldsymbol{\tau}$ and voidage ε appear and the fluid–particle interaction force is lumped into the term $\mathbf{F}_{FP}$, in turn determined as

$$\mathbf{F}_{FP} = \frac{-\sum_i \mathbf{f}_{di} \cdot w(x_i - \bar{x})}{\boldsymbol{\Omega}} \tag{5}$$

In Eq. (5) the fluid–particle interaction term has been expressed with reference to the computational cell volume $\boldsymbol{\Omega}$ and explicitly related to the drag force on each particle in the cell, weighted by a bilinear function w of the distance between the particle centre and the four nearest cells' centres (see e.g. [7]). Assigned velocity is used as boundary condition at the inlet boundary, no-slip on the walls and assigned pressure at the outlet boundary. These equations are numerically solved using the *finite volume method* on a staggered grid, through the SIMPLE algorithm.

In the presence of immersed objects the fluid flow can become very complicated. One way to tackle the problem would be to use discretization schemes on body-fitted unstructured grids like those used in finite element simulations of mechanical elements. However, this would require sacrificing the advantages of the finite volume scheme on conventional structured grids. Another simpler but more grossly approximated way is to keep the rectangular grid spacing and set special cells as occluded by the immersed body. In other words, the smooth object surface is approximated by a number of coarse rectangular cells where the fluid velocity components are set to zero, as required by the no-slip conditions, and the pressure gradient is assumed to be zero in the direction normal to the surface. Fig. 2 shows schematically the cells involved in the description of the curvilinear surface and what kind of conditions are imposed on the velocity and pressure in those cells. Arrows shown on the cell faces (typical of staggered grid arrangements) denotes those velocity components that in calculations are set to zero. Analogously, straight lines connecting circles (that denote positions where the pressure is calculated) indicate cell couples where the pressure differences between the two cell centres are set to zero. This approach was implemented in the