Chemical Engineering Science 102 (2013) 76–86

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

An analytical model to describe the motion of a low concentration of spherical particles within a Newtonian fluid

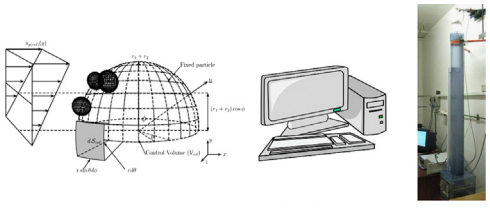
J.M. Wilms [a,*], G.J.F. Smit [b], G.P.J. Diedericks [b]

[a] Mechanical and Mechatronic Engineering, University of Stellenbosch, Private Bag X1, 7602 Matieland, South Africa
[b] Division of Applied Mathematics, University of Stellenbosch, Private Bag X1, 7602 Matieland, South Africa

HIGHLIGHTS

- Closure of the fluid–solid drag with a Representative Unit Cell model (RUC).
- Derivation of a particle viscosity term for modelling of particle–particle interaction.
- Numerical and physical settling tube experiments for validation of the model.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 13 May 2013
Received in revised form
23 July 2013
Accepted 27 July 2013
Available online 2 August 2013

Keywords:
Particle interaction
Two-phase flow
Fluid–solid drag
Closure modelling
Settling-tube

ABSTRACT

In this paper a particle–particle interaction term is derived and incorporated into the two-fluid analytical model of Smit et al. (2011). This model was developed for low concentration spherical particle motion in a Newtonian fluid and the inclusion of particle interactions is required for instances where particles collide. Moreover, such a modification serves as a first step towards the modelling of higher particle concentrations. A brief overview of the analytical derivation of the model by Smit et al. (2011) is included for clarity and a detailed derivation of the newly developed particle–particle interaction term is given. In this derivation, particle interaction is described using impulse mechanics with a collision sphere model in a centre of mass reference frame for collision detection. The updated model is included into an existing Fortran 95 program and validated with experimental data obtained by the authors from camera- and settling tube procedures.

1. Introduction

The motion of discrete particles within a Newtonian fluid is frequently modelled by treating the combination of phases as a single fluid phase or by evaluating the constituent phases as individual fluids. Alternatively, two-phase motion is described by modelling each of the discrete particles with Newton's second law and then tracking their individual motions. The first two methods constitute the classical Euler approach and require the specification of an empirical particle viscosity which places a limitation on the physical analysis of the particle motion. The latter, Discrete Element Method (DEM), has become more popular with the increase in computational resources but is, however, expensive in this regard and often dependent on parallel computing over multiple processors.

The empirical nature of the mixture- or the two-fluid approach and the computational cost of tracking schemes are avoided in the method described here. The model derived by Smit et al. (2011) uses the Navier–Stokes mass- and momentum conservation equations to impart the motion of the fluid but attempts to preserve the discrete nature of the particles by constructing their mass- and momentum conservation equations on the basis of Newton's second law. Instead of tracking the particles, the equations derived for a single particle are averaged over a Representative Elementary

* Corresponding author. Tel.: +27 763034492.
E-mail addresses: fine.wilms@gmail.com, fine@sun.ac.za (J.M. Wilms).

0009-2509/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ces.2013.07.043

Volume (REV). The REV is a volume which should contain both continuum and particle phases, and should be representative of the entire domain. More information on the criteria to which an REV should adhere may be found in the work of Whitaker (1967) and Bachmat and Bear (1986). The original REV integration procedure, applied in the averaging of the fluid phase, is, however, substituted with summation in this work to account for the particles' disjoint nature.

Averaging of the momentum conservation equations yields surface integral terms. The integral terms over the phase-separating face embody momentum transfer between the phases. They emerge in each of the phases' momentum conservation equations identically but with opposite sign, thus ensuring that momentum is conserved over the entire domain. These terms are closed with a Representative Unit Cell (RUC) model, which is a rectangular volume of minimum dimensions into which the geometric properties of the REV may be embedded. The RUC was first developed by Du Plessis and Masliyah (1988) and has been modified here to incorporate the relative slip velocity.

Momentum transfer may, however, also occur between the particles themselves, due to particle–particle collisions. Interaction of this type resides in the integral term over interfaces which are established when particles come into close proximity of each other. It is consequently isolated to the particle phase momentum conservation equation. The aforementioned interaction was not included by Smit et al. (2011) and is described here using impulse mechanics with a collision sphere model in a centre of mass reference frame for collision detection.

The model is coded in Fortran 95 and the numerical velocity data, yielded, is validated with empirical data from settling-tube experiments.

2. Two-phase flow model

The two-phase flow model for low concentration spherical particle motion through a Newtonian fluid excluding particle interaction was discussed in Smit et al. (2011). A brief overview is given here of the averaging procedures used and a detailed discussion is presented for the derivation of a particle–particle interaction term.

2.1. The fluid phase

The REV averaging procedure for fluid quantities, ψ, which are assumed to be finite, continuous and differentiable is given by

$$\psi_f = \frac{1}{U_f}\iiint_{U_f} \psi \, dU_f, \tag{1}$$

where U_f is the volume of the fluid phase within the REV. The application of the averaging procedure, given by Eq. (1), yields the following averaged momentum conservation equation for the fluid phase:

$$\rho_f \frac{\partial \epsilon_f \underline{v}_f}{\partial t} + \rho_f \nabla \cdot \left(\epsilon_f \underline{v}_f \underline{v}_f\right) = \rho_f \underline{g} \epsilon_f - \epsilon_f \nabla p_f + \mu_f \nabla \cdot \left(\epsilon_f \nabla \underline{v}_f\right) + \underline{I}_{fs}, \tag{2}$$

where the drag force between fluids and solids is summarised in, $\underline{I}_{fs}$, as

$$\underline{I}_{fs} = \frac{1}{U_o}\int_{S_{fs}} \left(-\tilde{p}_f \underline{\underline{1}} + \underline{\underline{\tau}}_f\right) \cdot \underline{n}_f \, dS. \tag{3}$$

In Eqs. (2) and (3), ρ_f is the density of the fluid phase; $\underline{v}_f$ and $\underline{v}_s$ are the average velocities of the fluid- and solid phases, respectively; $\underline{g}$ is the gravitational acceleration; and μ_f is the dynamic viscosity of the fluid. The average fluid pressure is denoted by p_f and the fluid volume fraction is the ratio of fluid-to-total volume, given by, $\epsilon_f = U_f/U_o$. The shear stress between the fluid and the solid is denoted by $\underline{\underline{\tau}}_f$ and the integral is taken over the fluid–solid interface, S_{fs}.

The averaged mass conservation equation for the fluid phase is given by

$$\frac{\partial \epsilon_f}{\partial t} + \nabla \cdot \epsilon_f \underline{v}_f = 0. \tag{4}$$

2.2. The solid phase

The solid phase is composed of discrete, solid, rigid particles which are, apart from when they collide, completely surrounded by the fluid phase. In consideration of the solid phase's disjoint nature, the averaging procedure of Eq. (1) is adapted to

$$\gamma_s = \frac{1}{U_s}\sum_{i=1}^{n} \gamma_i \nu_i, \tag{5}$$

where U_s denotes the combined solid volume which consists of all solid particle volumes, ν_i, within the REV whereas γ_i is a property associated with particle i and is defined at its centroid. The averaged mass conservation for the solid phase is given by

$$\frac{\partial \epsilon_s \rho_s}{\partial t} + \nabla \cdot \left(\epsilon_s \underline{v}_s\right) = 0, \tag{6}$$

where ρ_s is the density of the solid phase, the solid volume fraction is given by $\epsilon_s = U_s/U_o$, and the average solid velocity is denoted by $\underline{v}_s$.

The momentum conservation of a single particle is given by

$$m_i \frac{d\underline{v}_i}{dt} = m_i \underline{g} + \sum \underline{F}, \tag{7}$$

where m_i is the mass of particle i; $\underline{v}_i$ denotes its velocity and the last term in Eq. (7) represents all external forces apart from gravity, $\underline{g}$. Summation of Eq. (7) over all particles in an REV and subsequent application of Eq. (5) yields the following for the averaged solid phase momentum equation

$$\rho_s \frac{\partial}{\partial t}\epsilon_s \underline{v}_s + \rho_s \nabla \cdot \epsilon_s \underline{v}_s \underline{v}_s = \epsilon_s \rho_s \underline{g} - \underline{I}_{fs} + \frac{1}{U_o}\int_{S_{ss}} \underline{\underline{\sigma}}_i \cdot \underline{n}_i \, dS, \tag{8}$$

The particle stress is denoted by σ_i. Following Enwald et al. (1997), Crowe et al. (1998), Soo (1990), and Kleinstreuer (2003) the particle stress is assumed to be a linear combination of stress induced by the surrounding continuum, σ_f, and stress instigated by neighbouring particles, σ_{ss}

$$\underline{\underline{\sigma}}_i = \underline{\underline{\sigma}}_f + \underline{\underline{\sigma}}_{ss}. \tag{9}$$

The particle induced stress may in itself be decomposed in a frictional and a kinetic-collisional component (Enwald et al., 1997; Dartevelle, 2003). For dilute flows it is assumed that the frictional component may be dropped and it follows that the particle stress may be written as

$$\underline{\underline{\sigma}}_i = \underline{\underline{\sigma}}_f + \underline{\underline{\sigma}}_{kc}, \tag{10}$$

where σ_{kc} denotes the kinetic-collisional shear stress. Following Enwald et al. (1997) and Dartevelle (2003) this is composed of a pressure and a shearing component. For the purpose of the current work it is assumed that the small grain size and dilute concentrations yield a particle pressure which, when compared to the shear, may be considered negligible. It follows that the particle shear stress is given by

$$\underline{\underline{\sigma}}_i = -p_f \underline{\underline{1}} + \underline{\underline{\tau}}_f + \underline{\underline{\tau}}_{kc}. \tag{11}$$

In Eq. (11) the fluid stress has been decomposed into a pressure, p_f, and a shearing component, $\underline{\underline{\tau}}_f$, whilst $\underline{\underline{\tau}}_{kc}$ denotes the kinetic-collisional particle shear stress. The latter stress can physically