ARTICLE IN PRESS
PTEC-11854; No of Pages 9
Powder Technology xxx (2016) xxx–xxx
Contents lists available at ScienceDirect
Powder Technology
journal homepage: www.elsevier.com/locate/powtec

Multiscale modeling of rapid granular flow with a hybrid discrete-continuum method

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ARTICLE INFO

Article history:
Received 22 October 2015
Received in revised form 12 April 2016
Accepted 10 August 2016
Available online xxxx

Keywords:
Hybrid discrete-continuum method
Multiscale simulation
Discrete element model
Continuum model
Granular flow

ABSTRACT

Both discrete and continuum models have been widely used to study rapid granular flow, discrete model is accurate but computationally expensive, whereas continuum model is computationally efficient but its accuracy is doubtful in many situations. Here we propose a hybrid discrete-continuum method to profit from the merits but discard the drawbacks of both discrete and continuum models. Continuum model is used in the regions where it is valid and discrete model is used in the regions where continuum description fails, they are coupled via dynamical exchange of parameters in the overlap regions. Simulation of granular channel flow demonstrates that the proposed hybrid discrete-continuum method is nearly as accurate as discrete model, with much less computational cost.

1. Introduction

Granular matter which consists of macroscopic particles can widely be found in nature and in industry [1,2]. A better understanding of granular matter is not only desirable for physicists, but also for engineers from various sectors, such as mining, pharmaceutical and chemical industries [3]. Extensive theoretical, numerical and experimental studies have been devoted to this fascinating area [4–6], however, our understanding is still far from satisfactory after several decades' efforts due to its dissipative, non-linear and non-equilibrium characteristics, reflected by the lack of a general theory for describing its hydrodynamics [4,7].

To simulate granular flow, both macroscopic continuum model and microscopic discrete model have been extensively used [8,9]. Continuum model, solving the conservation equations of mass, momentum and energy, is very useful for analyzing and designing industrial processes involving a large number of discrete particles. However, it is much less mature compared with the classical fluid mechanics theory for molecular gas or liquid fluid, mainly due to the dissipative nature of particle-particle interactions and the resultant lack of scale separation [10,4], and the formation of heterogeneous structures, such as particle clustering structure [11]. Continuum method may also be inadequate in situations when no accurate boundary condition can be formulated or due to the existence of Knudsen layer [12,13]. On the other hand, discrete model [14] tracks the motion of each particle according to Newton's law, and accordingly, provides detailed information about the dynamics of granular flow. Unfortunately, discrete model is computationally extremely demanding for engineering applications.

In this study, a hybrid discrete-continuum method is developed for modeling granular flow, taking the merits of both continuum and discrete methods but discarding their drawbacks. The idea is to concurrently couple physical descriptions at different scales to solve the dilemma that has been described, as in the hybrid atomistic-continuum methods for rarefied gas flows [15], dense fluids [16,17] and solid mechanics [18]. Continuum model is used to model the majority of simulation domain while discrete method is used within the domains where continuum description is inadequate.

2. Method

2.1. Continuum method

The hybrid discrete-continuum method is based on domain decomposition as illustrated in Fig. 1. The method has been used in the study of micro- and nano-fluid flow [17,16,19]. The simulation domain is divided into a continuum region located at the center of the channel and two discrete regions near the two side walls. Two overlap regions are constructed to ensure the continuity of mass and momentum in the entire simulation domain. In the continuum region, Navier-Stokes equation combined with kinetic theory of granular flow is applied [20]. The governing equations are numerically solved with finite difference method on a staggered grid [21,22]. The mass and momentum conservation equations are given as follows,

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http://dx.doi.org/10.1016/j.powtec.2016.08.017

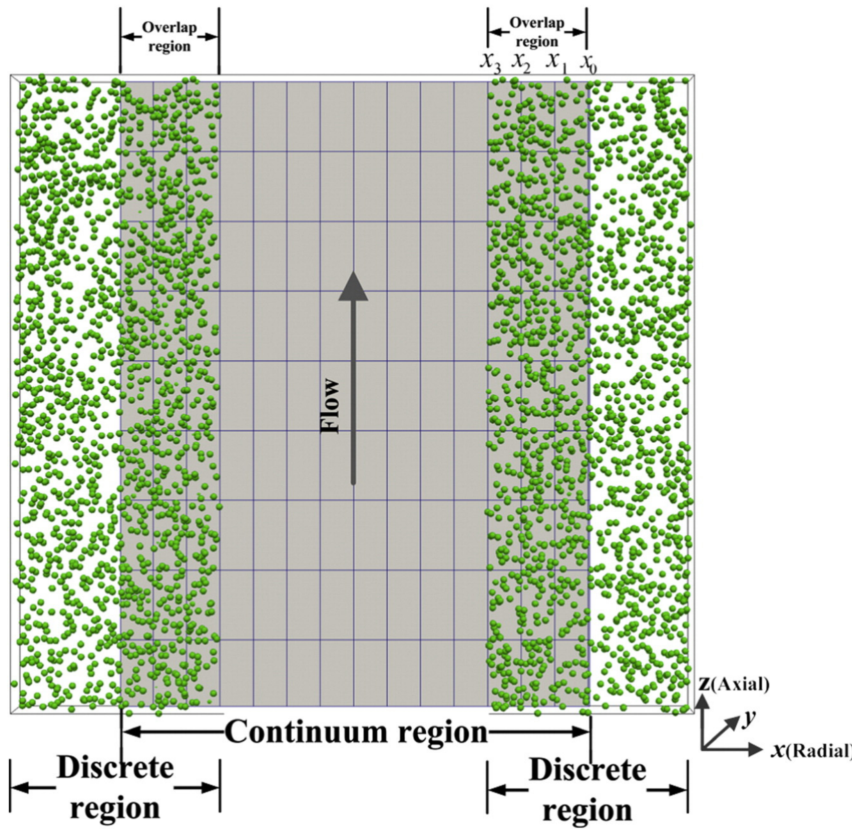

Fig. 1. Schematic of the granular channel flow simulated by the hybrid discrete-continuum method. The simulation domain is divided into a continuum region located at the center of the channel and two discrete regions near the two side walls. They coincidentally have two overlap regions and each overlap region is further divided into three parts: a discrete boundary layer (x_2-x_3), a buffer layer (x_1-x_2) and a continuum boundary layer (x_0-x_1).

$$\frac{\partial}{\partial t}(\phi_s\rho_s) + \nabla\cdot(\phi_s\rho_s\mathbf{U}_c) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\phi_s\rho_s\boldsymbol{U}_c) + \nabla\cdot(\phi_s\rho_s\boldsymbol{U}_c\boldsymbol{U}_c) = -\nabla p_s + \nabla\cdot\tau_s \tag{2}$$

where p_s and τ_s are the granular pressure and solid stress tensor, respectively. The stress tensor is linearly related to the rate-of-strain tensor,

$$\tau_s = \mu_s\left(\nabla\boldsymbol{U}_c + \nabla\boldsymbol{U}_c^T\right) + \left(\lambda_s - \frac{2}{3}\mu_s\right)(\nabla\cdot\boldsymbol{U}_c)\boldsymbol{I} \tag{3}$$

where μ_s is shear viscosity and λ_s is bulk viscosity. The particulate phase stresses are closed using kinetic theory of granular flow which solves a separate conservation equation for granular temperature.

$$\frac{3}{2}\left[\frac{\partial(\phi_s\rho_s\Theta_s)}{\partial t} + \nabla\cdot(\phi_s\rho_s\boldsymbol{U}_c\Theta_s)\right] = (-p_s\boldsymbol{I} + \tau_s):\nabla\boldsymbol{U}_c + \nabla\cdot(k_s\nabla\Theta_s) - \gamma \tag{4}$$

where k_s is heat conductivity of granular phase given by:

$$k_s = \frac{150\rho_s d_p\sqrt{\Theta_s\pi}}{384(1+e)g_0}\left[1 + \frac{6}{5}\phi_s g_0(1+e)\right]^2 + 2\rho_s\phi_s^2 d_p(1+e)g_0\sqrt{\frac{\Theta_s}{\pi}} \tag{5}$$

The solids pressure, shear and bulk viscosity are expressed as:

$$p_s = \phi_s\rho_s\Theta_s + 2\rho_s(1+e)\phi_s^2 g_0\Theta_s \tag{6}$$

$$\mu_s = \frac{4}{5}\rho_s d_p\phi_s^2 g_0(1+e)\sqrt{\frac{\Theta_s}{\pi}} + \frac{\phi_s\rho_s d_p\sqrt{\pi\Theta_s}}{6(3-e)}\left(1 + \frac{2}{5}(1+e)(3e-1)\phi_s g_0\right) \tag{7}$$

$$\lambda_s = \frac{4}{3}\phi_s\rho_s d_p g_0(1+e)\sqrt{\frac{\Theta_s}{\pi}} \tag{8}$$

The energy dissipation due to inelastic collision is expressed as:

$$\gamma = \frac{12(1-e^2)g_0}{d_p\sqrt{\pi}}\rho_s\phi_s^2\Theta_s^{3/2} \tag{9}$$

Within these formulations, g_0 is the radial distribution function that is given as follows:

$$g_0 = \left[1 - \left(\frac{\phi_s}{\phi_{s,\max}}\right)^{1/3}\right]^{-1} \tag{10}$$

The tangential velocity and granular temperature at the wall are calculated using Johnson and Jackson model [23] in the pure continuum simulations:

$$u_{s,w} = -\frac{6\mu_s\phi_{s,\max}}{\sqrt{3}\pi\varphi\rho_s\phi_s g_0\sqrt{\Theta_s}}\frac{\partial u_{s,w}}{\partial n} \tag{11}$$

$$\Theta_{s,w} = -\frac{k_s\Theta_s}{\gamma_{s,w}}\frac{\partial\Theta_{s,w}}{\partial n} + \frac{\sqrt{3}\pi\varphi\rho_s\phi_s u_{s,slip}^2 g_0\Theta_s^{3/2}}{6\phi_{s,\max}\gamma_{s,w}} \tag{12}$$