Chemical Engineering Journal 174 (2011) 475–481

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Journal

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

Short communication

Enforcing mass conservation in DPM-CFD models of dense particulate flows

C.L. Wu[a,*], K. Nandakumar[a], A.S. Berrouk[b], H. Kruggel-Emden[c]

[a] Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge 70803, USA
[b] Department of Chemical Engineering, The Petroleum Institute, P.O. Box 2533, Abu Dhabi, United Arab Emirates
[c] Department of Energy Plant Technology, Ruhr-University Bochum, D-44780 Bochum, Germany

ARTICLE INFO

Article history:
Received 22 June 2011
Received in revised form 10 August 2011
Accepted 11 August 2011

Keywords:
Mass conversation
Discrete particle/element modeling
Computational fluid dynamics
Dense particulate flow

ABSTRACT

An improved coupling method is proposed to ensure mass conservation in a previously developed DPM-CFD model (C.L. Wu et al., Three-dimensional discrete particle model for gas–solid fluidized bed on unstructured mesh, Chemical Engineering Journal 152 (2009), 514–529). In enforcing the mass balance for the continuous phase in such algorithms using the single phase flow solvers, any heterogeneity in the particle concentration field (caused by clustering of particles) creates non-zero source terms. It is shown that if this is not handled properly, it can create large numerical errors (of up to 10%) and any oscillation in the flow field manifests itself in a similar error in the mass conservation. By using the conservative form of the equations in integral formulation, the coupling between the DPM and CFD models ensures mass conservation on the global scale in the entire domain, even in the presence of local heterogeneities in the flow field. The method also offers a consistent implementation of mass flow boundaries at the inlet. Numerical results show the superiority of the new coupling method over the previous one in conserving mass and handling transport processes in fluidized beds.

1. Introduction

The discrete particle/element model (DPM or DEM) coupled to computational fluid dynamics (CFD) algorithms has been widely applied to simulate a wide variety of dense fluid-particle flows. The state of the art review of the DPM-CFD modeling technique can be found in the literatures [1,2]. As part of a DPM-CFD algorithm development, both finite difference and finite volume methods have been used to solve the fluid-phase governing equations. Several algorithms have been developed from scratch to simulate dense particulate flows [3–7]. Some of the DPM codes have been designed to work on top of already mature single-phase flow solvers. The merit of such a development lies in taking advantage of the availability, in these mature CFD solvers, of well-established techniques for handling complex geometries and boundary conditions using robust numerical algorithms across several types of physics. Moreover, these mature CFD solvers offer the necessary flexibility for the DPM algorithms to extend to complex transport processes such as those with heat/mass transfer and/or chemical reactions.

In a previous work [8], we proposed a simple, yet efficient, technique to couple the 3D hard-sphere discrete particle model to the commercial CFD solver FLUENT. The continuous phase governing equations are rearranged in a particular way to yield a set of equations similar to those for single phase flow but with specified source terms. Using this rearrangement it has been straightforward to utilize FLUENT single-phase flow solver on arbitrary 3D unstructured mesh. This coupling approach is also applicable for DPM based on soft-sphere particle dynamics.

Several other research groups have been engaged in similar development recently [9–11]. Some researchers have brought to our attention that, contrary to usual expectation, the coupling method in our previous work cannot guarantee the mass conservation of the continuous phase when the finite volume method is applied to discretize such equations. In this short communication, we aim to clarify this issue and present an improved coupling method that can recover the conservation property of the transport equation.

2. DPM-CFD coupling method by Wu et al. (2009)

The governing equations of the continuous phase mainly follow the volume-averaged form of the two-fluid model. The local mass variation rate is balanced by its net convective mass fluxes if there is no inter-phase mass transfer:

$$\frac{\partial}{\partial t}(\varepsilon\rho) + \nabla\cdot(\varepsilon\rho\mathbf{u}) = 0 \tag{1}$$

where p is the density, ε is the void fraction and $\mathbf{u}$ is the velocity of the continuous phase.

* Corresponding author. Tel.: +1 508 869 4193.
E-mail addresses: chunliangwu@gmail.com, chunliangwu@lsu.edu (C.L. Wu).

1385-8947/$ – see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.cej.2011.08.033

The momentum equation reads as:

$$\frac{\partial}{\partial t}(\varepsilon\rho\mathbf{u}) + \nabla\cdot(\varepsilon\rho\mathbf{u}\mathbf{u}) = -\varepsilon\nabla p + \nabla\cdot(\varepsilon\bar{\bar{\boldsymbol{\tau}}}) + \mathbf{S}_p + \varepsilon\rho\mathbf{g} \quad (2)$$

where p is the static pressure and $\bar{\bar{\boldsymbol{\tau}}}$ is the stress tensor. The source term $\mathbf{S}_p$ represents the forces, such as drag, due to particle–fluid interactions.

To utilize directly any single-phase flow solver, the above equations are re-organized into the following form:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = S_c \quad (3)$$

and

$$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\mathbf{u}) = -\nabla p + \nabla\cdot(\bar{\bar{\boldsymbol{\tau}}}) + \rho\mathbf{g} + \mathbf{S}_m \quad (4)$$

where

$$S_c = -\frac{\rho}{\varepsilon}\left(\frac{\partial\varepsilon}{\partial t} + \mathbf{u}\cdot\nabla\varepsilon\right) \quad (5)$$

and

$$\mathbf{S}_m = S_c\mathbf{u} + \frac{1}{\varepsilon}(\mathbf{S}_p + \bar{\bar{\boldsymbol{\tau}}}\cdot\nabla\varepsilon) \quad (6)$$

Eqs. (3) and (4) appear in a form similar to the single-phase governing equations except the additional source terms defined by Eqs. (5) and (6). Thus, their incorporation into a CFD solver is straightforward. All mainstream CFD solvers such as FLUENT, Start-CD, CFX and Open-FOAM have the feature of adding source terms in the transport equations by plugging user-defined functions. When the SIMPLE series algorithm is used to solve the above governing equations (Eqs. (3)–(6)), the source terms are calculated and returned to the solver during iteration. Details of the solution procedure are described in Fig. 1 in Wu et al. [8].

In the above coupling approach, the mass source term Eq. (5) is highly dependent of the void fraction and its gradient. The void fraction is calculated by an analytical method that accounts for the fractional volume of a particle shared by several finite volume cells [12]. Several methods can be employed to evaluate the scalar gradient under unstructured mesh, among which the Green–Gauss method was used in Wu et al. [8]. It reads as:

$$\nabla\varepsilon = \frac{1}{\Delta V}\sum_f \bar{\varepsilon}_f\mathbf{A}_f \quad (7)$$

$\mathbf{A}_f$ is the face normal vector pointing out of the cell and ΔV is the cell volume. The summation is taken over all the cell faces. We will discuss later the calculation procedure for the void fraction at the cell face $\bar{\varepsilon}_f$.

For continuity or mass conservation, it is expected that the mass inflow is balanced by the mass outflow in simulations such as fluidization where no particle moves in or out of the domain. However, it has been found that the mass conservation was not guaranteed in typical simulations based on the above-described coupling method. Fig. 1 shows the net gas mass flow (normalized by the inflow rate) monitored in a fluidized bed simulation. In this simulation, a jet at the bed bottom center is introduced to quickly generate heterogeneous flow structure. The Gidaspow's drag formula is used in all the simulation of the present work. This drag formula is a combination of the Ergun equation developed for dense regimes and Wen & Yu's correlation used for dilute regimes [13]. The parameters used in the simulation are listed in Table 1. It can be seen that there is always 6–14% net mass inflow in a periodic variation, which suggests that the mass imbalance might be correlated to any periodicity in the flow field.

One may first think that this is the result of an insufficient precision of the equation (Eq. (7)) used to compute the void fraction gradient. In fact, the problem originates from the rearrangement of Eq. (1) into Eq. (3) in order to facilitate its implementation in a single-phase solver. Indeed, Eq. (3) is not in a conservative form as it is the case of Eq. (1). They are mathematically equivalent and both can achieve same precision of discretization, but the integral of Eq. (3) in space cannot ensure mass conservation as we shall explain below.

Table 1
Bed configuration and parameters used in simulations for both coupling methods.

Bed dimension	0.25 m × 0.02 m × 0.6 m
CFD mesh dimension	50 × 2 × 80
Stagnant bed height	0.28 m
Central jet width	0.01 m
Gas density	1.225 kg/m^3
Gas viscosity	1.8×10^{-5} kg/m s
Minimum fluidization velocity u_{mf}	1.04 m/s
Background gas velocity	1.0 m/s
Gas jet velocity	20 m/s
Collision dynamics	Soft sphere model
Particle number	186,805
Particle density	2250 kg/m^3
Particle diameter	0.002 m
DPM time step	5×10^{-6} s
CFD time step	0.0001 s
Convergence criteria	0.0001

We denote the whole solution domain by Ω, which is meshed into fine cells. For a general FVM solver and given a constant density of the continuous phase, the re-arranged continuity equation (Eq. (3)) integrated over a cell P with volume ΔV reads as:

$$b \equiv \sum_f \Lambda_f + \frac{\rho}{\varepsilon_P^{n+1}}\left(\frac{\varepsilon_P^{n+1}-\varepsilon_P^n}{\Delta t} + \mathbf{u}_P^{n+1}\cdot\nabla\varepsilon_P^{n+1}\right)\Delta V = 0 \quad (8)$$

Under the same conditions, integrating Eq. (1) over a cell P yields:

$$\rho\frac{\varepsilon_P^{n+1}-\varepsilon_P^n}{\Delta t}\Delta V + \sum_f \varepsilon_f^{n+1}\Lambda_f = 0 \quad (9)$$

where $\Lambda_f = \rho\mathbf{u}_f\cdot\mathbf{A}_f$ is the interstitial mass flux of the continuous phase through the cell face f. Eq. (9) can ensure mass conservation since the mass flux at the cell faces is shared by its neighboring cells.

One can easily prove, by considering the 1D steady flow case, that Eqs. (8) and (9) cannot be retrieved from each other regardless of the method used to calculate the void fraction gradient. This is simply because of the non-uniformity of the void fraction field. This is a common feature of all differential equations written in a non-conservative form. If we sum Eq. (8) over all the cells and given that, for fluidization, there is no net particle flow, we obtain:

$$b_\Omega = \sum_{bf}\Lambda_{bf} + \sum_P \frac{\rho}{\varepsilon_P^{n+1}}(\mathbf{u}_P^{n+1}\cdot\nabla\varepsilon_P^{n+1})\Delta V = 0 \quad (10)$$

The first summation is taken over all the boundary faces while the second one is over all the cells. The first summation should be equal to zero according to the mass conservation of the continuous phase:

$$\sum_{bf}\Lambda_{bf} = 0 \quad (11)$$

Or equivalently the integral of the mass source term over the whole domain is zero:

$$\sum_P \frac{\rho}{\varepsilon_P^{n+1}}(\mathbf{u}_P^{n+1}\cdot\nabla\varepsilon_P^{n+1})\Delta V = 0 \quad (12)$$

Since the continuous phase is often considered as incompressible, the pressure-based algorithm such as SIMPLE is most favorable to