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A STRUCTURE-DEPENDENT MULTI-FLUID MODEL FOR GAS-SOLID FLUIDIZATION

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ABSTRACT

In heterogeneous gas-solid flows, meso-scale structures (such as bubbles and clusters) significantly affect the hydrodynamics as well as mass/heat transfer and reaction rate. To be consistent with these structures, we tried to formulate a set of conservation equations with consideration of structures, namely the structure-dependent multi-fluid (SFM) model based on the EMMS (energy-minimization multi-scale) (1) method. It was found that our previous works (2-5) on the coupling of TFM and EMMS drag can be viewed as a simplified solution of SFM with stability condition.

1. INTRODUCTION

Gas-solid fluidization is normally aggregative, featuring dynamic structures over a broad range of spatio-temporal scales. These structures (such as bubbles and clusters) have significant impacts on the flow, mass/heat transfer and reaction rate, and hence have attracted many researchers using computational fluid dynamics (CFD) to investigate those effects. Direct numerical simulation (DNS) as well as various kinds of discrete particle methods may allow detailed analysis of these structures, however, they are normally unaffordable to industrial application due to the limited computing resources. The two-fluid model (TFM) is more suitable for industrial applications, where the flows of the gas and the solids are statistically averaged and assumed as interpenetrating continua (6). The so-called coarse-grained TFM does not reflect the structural effects within each grid and, therefore, is difficult to capture the experimental behavior (7). Here, we try to establish a set of structure-dependent conservation equations, on which the energy-minimization multi-scale (EMMS) drag can be naturally incorporated, as practiced in our previous works (2-5).

2. MODEL FORMULATION

For heterogeneous gas-solid flows from the bubbling to fast fluidization, there exists a bimodal probability distribution over the entire range of solids concentration distribution, one apex corresponding to the particle-rich dense phase and the other to the gas-rich dilute phase (1,8). Thus, it is reasonable to reduce heterogeneous structures into dilute-dense two-phase description. Bearing in mind this two-phase simplification, we may derive a structure-dependent multi-fluid model (SFM) as follows:

2.1 Structure-dependent multi-fluid model

To be consistent with the two-phase structure, the monodisperse gas-solid riser flow is classified into the dense clusters (denoted by subscript c) and the dilute broth (denoted by subscript f) according to the structural characterization in the EMMS model, as shown in Fig. 1. The dense clusters are surrounded and dispersed by the continuous dilute phase. Further we refine such broth-cluster structure by defining four continua of structural sub-elements, namely the dense-phase gas, the dense-phase solid, the dilute-phase gas and the dilute-phase solid (denoted by gc, sc, gf and sf, respectively).

If the dilute and dense phases are homogeneous inside, the gas-solid drag per unit volume of the dilute/dense phase ($\mathbf{F}_{df}$/$\mathbf{F}_{dc}$) can be closed with the classical drag coefficient, such as Wen and Yu correlation (9). Since the dilute-phase gas surrounds the dense-phase particles, there exists an additional drag ($\mathbf{F}_{di}$). The interactions of the gas (solids) between the dilute and dense phases due to transient evolution of clusters are taken into account by the mass exchange terms (Γ_g, Γ_s). For brevity, other interaction forces (such as the lift force, the virtual mass force), and chemical reactions are not included in this work.

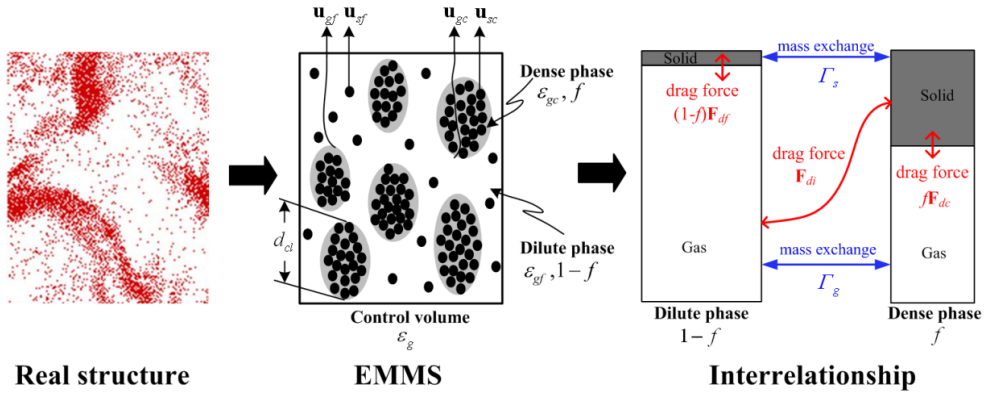

Fig. 1 The schematic diagram of modeling for heterogeneous gas-solid flows (10)

Following the Eulerian spatial averaging method, we can derive the conservation equations for four continua as follows:

Continuity equation for the dense-phase gas:

$$\frac{\partial}{\partial t}(f\varepsilon_{gc}\rho_g)+\nabla\cdot(f\varepsilon_{gc}\rho_g\mathbf{u}_{gc})=\Gamma_g \quad (1)$$

Continuity equation for the dense-phase solid:

$$\frac{\partial}{\partial t}(f\varepsilon_{sc}\rho_s)+\nabla\cdot(f\varepsilon_{sc}\rho_s\mathbf{u}_{sc})=\Gamma_s \quad (2)$$

Continuity equation for the dilute-phase gas:

$$\frac{\partial}{\partial t}[(1-f)\varepsilon_{gf}\rho_g] + \nabla\cdot[(1-f)\varepsilon_{gf}\rho_g\mathbf{u}_{gf})] = -\Gamma_g \quad (3)$$

Continuity equation for the dilute-phase solid:

$$\frac{\partial}{\partial t}[(1-f)\varepsilon_{sf}\rho_s] + \nabla\cdot[(1-f)\varepsilon_{sf}\rho_s\mathbf{u}_{sf})] = -\Gamma_s \quad (4)$$

Momentum conservation equation for the dense-phase gas:

$$\frac{\partial}{\partial t}(f\varepsilon_{gc}\rho_g\mathbf{u}_{gc}) + \nabla\cdot(f\varepsilon_{gc}\rho_g\mathbf{u}_{gc}\mathbf{u}_{gc}) = -f\nabla p + \nabla\cdot(f\boldsymbol{\tau}_{gc}) + f\rho_g\mathbf{g} - f\mathbf{F}_{dc} + \Gamma_g\mathbf{u}_g^i \quad (5)$$

Momentum conservation equation for the dense-phase solid:

$$\frac{\partial}{\partial t}(f\varepsilon_{sc}\rho_s\mathbf{u}_{sc}) + \nabla\cdot(f\varepsilon_{sc}\rho_s\mathbf{u}_{sc}\mathbf{u}_{sc}) = -\nabla p_{sc} + \nabla\cdot(f\boldsymbol{\tau}_{sc}) + f\varepsilon_{sc}(\rho_s-\rho_g)\mathbf{g} + f\mathbf{F}_{dc} + \mathbf{F}_{di} + \Gamma_s\mathbf{u}_s^i \quad (6)$$

Momentum conservation equation for the dilute-phase gas:

$$\frac{\partial}{\partial t}[(1-f)\varepsilon_{gf}\rho_g\mathbf{u}_{gf}] + \nabla\cdot[(1-f)\varepsilon_{gf}\rho_g\mathbf{u}_{gf}\mathbf{u}_{gf}] = -(1-f)\nabla p + \nabla\cdot[(1-f)\boldsymbol{\tau}_{gf}] + (1-f)\rho_g\mathbf{g} - (1-f)\mathbf{F}_{df} - \mathbf{F}_{di} - \Gamma_g\mathbf{u}_g^i \quad (7)$$

Momentum conservation equation for the dilute-phase solid:

$$\frac{\partial}{\partial t}[(1-f)\varepsilon_{sf}\rho_s\mathbf{u}_{sf}] + \nabla\cdot[(1-f)\varepsilon_{sf}\rho_s\mathbf{u}_{sf}\mathbf{u}_{sf}] = -\nabla p_{sf} + \nabla\cdot[(1-f)\boldsymbol{\tau}_{sf}] + (1-f)\varepsilon_{sf}(\rho_s-\rho_g)\mathbf{g} + (1-f)\mathbf{F}_{df} - \Gamma_s\mathbf{u}_s^i \quad (8)$$

It should be noted that the above momentum equations are written in forms of the hydrodynamic model B (6) where the gas pressure gradient only acts on the gas phase. The stress tensor ($\boldsymbol{\tau}_k$) takes the Newtonian form as

$$\boldsymbol{\tau}_k = \varepsilon_k\mu_k\left[\nabla\mathbf{u}_k + (\nabla\mathbf{u}_k)^T\right] + \varepsilon_k(\lambda_k - \frac{2}{3}\mu_k)(\nabla\cdot\mathbf{u}_k)\mathbf{I} \quad (9)$$

$\mathbf{u}^i$ is the interface gas/solid velocity between the dilute and dense phases. In principle, this set of governing equations (Eqs. 1-8) could be solved to obtain the independent variables (i.e., p, f, $\boldsymbol{\varepsilon}_{gf}$, $\boldsymbol{\varepsilon}_{gc}$, $\mathbf{u}_{gf}$, $\mathbf{u}_{gc}$, $\mathbf{u}_{sf}$, $\mathbf{u}_{sc}$), provided that the parameters (i.e., $\boldsymbol{\tau}_{sf}$, $\boldsymbol{\tau}_{sc}$, p_{sf}, p_{sc}, Γ_g, Γ_s, $\mathbf{F}_{df}$, $\mathbf{F}_{dc}$, $\mathbf{F}_{di}$) be closed elaborately. Direct solution of such set of SFM equations is harder than TFM. Thus, we tried to reduce the current SFM into available TFM with structure-dependent closures.

2.2 Restoration to the EMMS model

2.2.1 Mass balance

Combining the mass balance equations for the gas and the solids, we can derive the mass balance for the gas:

$$\mathbf{U}_g = f\mathbf{U}_{gc} + (1-f)\mathbf{U}_{gf}, \tag{10}$$

and for the solids:

$$\mathbf{U}_s = f\mathbf{U}_{sc} + (1-f)\mathbf{U}_{sf}. \tag{11}$$

2.2.2 Force balance

For a lumped description of a steady-state reactor, the dominant factors of the force balance are the drag force, gravity and the buoyancy due to the pressure drop, while other terms such as the accelerations, stresses and the inter-phase mass exchange can be ignored. Thus, the force balance equations in SFM can be simplified into the following forms.

Force balance for the dense-phase solid:

$$f\mathbf{F}_{dc} + \mathbf{F}_{di} = -f\varepsilon_{sc}(\rho_s - \rho_g)\mathbf{g}. \tag{12}$$

Force balance for the dilute-phase solid:

$$\mathbf{F}_{df} = -\varepsilon_{sf}(\rho_s - \rho_g)\mathbf{g}. \tag{13}$$

Force balance for the dense-phase gas:

$$f\mathbf{F}_{dc} = -f\nabla p + f\rho_g\mathbf{g}. \tag{14}$$

Force balance for the dilute-phase gas:

$$(1-f)\mathbf{F}_{df} + \mathbf{F}_{di} = -(1-f)\nabla p + (1-f)\rho_g\mathbf{g}. \tag{15}$$

Eliminating the gas pressure gradient from Eqs. (14) and (15) yields the pressure drop balance between the dilute and dense phases:

$$\mathbf{F}_{df} + \frac{\mathbf{F}_{di}}{1-f} = \mathbf{F}_{dc}. \tag{16}$$

Eqs. (10-13) and (16) exactly revert to the EMMS model. If we include the inertial terms to account for the dynamic change within each grid, we can derive the set

of equations of the unsteady state EMMS model. Recent exploration on the meso-scale structure reveals that, both bubble and cluster based EMMS models (2,5) can be unified under the umbrella of a generalized SFM, which can be used for simulating both bubbling and circulating fluidized beds with fair agreement with experimental data (11).

2.3 Reduction to TFM+EMMS

Combining the corresponding mass/momentum equations in SFM for gas and solids, we get the following mass/momentum equations similar to TFM.

Mass conservation for the gas:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g) = 0 \quad . \tag{17}$$

Mass conservation for the solids:

$$\frac{\partial}{\partial t}(\varepsilon_s \rho_s) + \nabla \cdot (\varepsilon_s \rho_s \mathbf{u}_s) = 0 \quad . \tag{18}$$

Momentum conservation for the gas:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g \mathbf{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g) = -\nabla p + \nabla \cdot \boldsymbol{\tau}_{ge} + \rho_g \mathbf{g} - \beta_{Be}(\mathbf{u}_g - \mathbf{u}_s) + \nabla \cdot \boldsymbol{\tau}_{Dg} \quad . \tag{19}$$

Momentum conservation for the solids:

$$\begin{aligned} \frac{\partial}{\partial t}(\varepsilon_s \rho_s \mathbf{u}_s) + \nabla \cdot (\varepsilon_s \rho_s \mathbf{u}_s \mathbf{u}_s) = & -\nabla p_{se} + \nabla \cdot \boldsymbol{\tau}_{se} + \varepsilon_s (\rho_s - \rho_g)\mathbf{g} \\ & + \beta_{Be}(\mathbf{u}_g - \mathbf{u}_s) + \nabla \cdot \boldsymbol{\tau}_{Ds} \end{aligned} \quad . \tag{20}$$

where

$$\varepsilon_k = f \varepsilon_{kc} + (1 - f)\varepsilon_{kf} \quad , \tag{21}$$

and

$$\mathbf{u}_k = \frac{f \varepsilon_{kc} \mathbf{u}_{kc} + (1 - f)\varepsilon_{kf} \mathbf{u}_{kf}}{\varepsilon_k} \quad . \tag{22}$$

The effective drag coefficient (β_{Be}) can be written as follows:

$$\beta_{Be} = \frac{f\mathbf{F}_{dc} + \mathbf{F}_{di} + (1-f)\mathbf{F}_{df}}{\mathbf{u}_g - \mathbf{u}_s}. \quad (23)$$

which exactly reverts to our definition in previous multiscale CFD approaches, which feature a combination of TFM equations and EMMS drag. The structural stress (τ_e), the diffusion stress (τ_D) and the structural pressure (p_{se}) are the same as in Hong *et al*. (10). In particular, the closure of F_{di} is the most critical part, which may differ with the characterization of meso-scale structures in terms of e.g. bubble or cluster. More details should be referred to Hong *et al*. (11).

Compared with the type-B model of TFM, the reduced SFM differs in its formulation of the stress, drag force and diffusion stress by including the structural effects. If the flow is homogeneous within each grid, the traditional TFM can be viewed as a specific case of SFM.

3. SIMPLIFIED SOLUTION OF SFM: MULTI-SCALE CFD

As mentioned above, the TFM and EMMS model can be unified under the umbrella of a more generalized, stability-constrained SFM. And our previous works (2-5) on Multi-scale CFD can be viewed as a simplified solution of SFM.

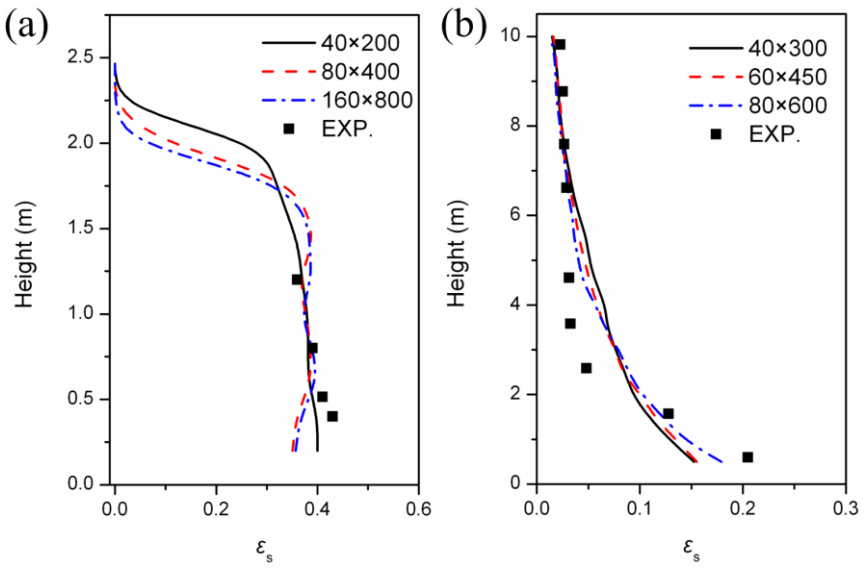

Fig. 2 Comparison of axial solids concentration for (a): bubbling (ID 0.267 m, 2.464 m high; ρ_p = 1780 kg/m^3, d_p =65 μm, ε_{mf} = 0.4) and (b): circulating fluidized beds (ID 0.09m, 10.5 m high; ρ_p = 930 kg/m^3, d_p =54 μm, ε_{mf} = 0.4). Both cases are fluidized with ambient air.

For example, to verify the bubble-based EMMS model recently developed by Hong *et al*. (11), we present the comparison of axial profiles of solids concentration with experimental data for two simulation cases. Simulations were first performed for 20 seconds of physical time, and then the time-averaged analysis was carried out over the remaining 10 seconds. Fig. 2(a) and 2(b) are based on bubbling fluidized bed with U_g=0.2 m/s (12) and fast fluidized bed with

U_g=1.52 m/s and G_s=14.3 kg/(m^2s) (1), respectively. The simulation results of bubbling bed are in reasonable agreement with experimental data. For the case of circulating fluidized bed, deviation exists at the bottom part of the riser, which may be caused by 2D simplification of the inlet region or improper estimation of the initial solids inventory. Further analysis is still needed with regard to this issue. The solids mass flow rate of CFB is monitored at the outlet of riser and the entrained particles are recirculated into the solid inlet. The predicted value of solids flux is about 15.31~16.77 kg/(m^2s) which agrees with experimental value (14.3 kg/(m^2s)), with standard deviation of about 5.30~5.74 kg/(m^2s). In general, we found that the SFM with bubble-based EMMS closure is suitable for flow regimes from bubbling to fast fluidization.

4. CONCLUSION

To be consistent with the dilute-dense two-phase structure, a structure-dependent multi-fluid model was proposed, and then simplified and compared with the traditional TFM and the EMMS models. It was found that the SFM may reduce to the TFM with structure-dependent closures and the hydrodynamics equations of the EMMS model. In other words, the SFM unifies the TFM and the hydrodynamics equations of the EMMS model with different structural characterization. Simulations of a bubbling- and a circulating- fluidized beds are compared with experimental data, showing applicable to wide flow regimes.

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NOTATION

f volume fraction of dense phase
$\mathbf{F}$ drag force, N/m^3
$\mathbf{g}$ gravitational acceleration, m/s^2
G_s solids flux, kg/(m^2s)
p pressure, Pa
$\mathbf{u}$ velocity, m/s
$\mathbf{U}$ superficial velocity, m/s

Greek letters

β drag coefficient, kg/(m^3s)
Γ mass exchange, kg/(m^3s)
ε volume fraction
$\mathbf{I}$ unit tensor
λ bulk viscosity, Pa·s
μ viscosity, Pa·s
ρ density, kg/m^3
τ stress tensor, Pa

Subscripts

c	dense phase
f	dilute phase
g	gas phase
i	meso-scale interphase
mf	minimum fluidization
p	particles
s	solid phase

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