MESOSCALE MODELING FOR COMPUTATIONAL FLUID DYNAMICS OF CIRCULATING FLUIDIZED BEDS

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Abstract – Gas-solid fluidized bed is a typical dissipative system, featuring meso-scale structures with bimodal distribution of parameters. To account for this characteristic, recent years have witnessed a blossom of meso-scale modeling research from various angles of view. In particular, by integrating the bimodal distribution into the structure-dependent analysis of mass, momentum and energy conservation, we can unify the hydrodynamic equations of the two-fluid model and those of the energy minimization multi-scale (EMMS) model. Further, by extending this structure-dependent analysis to the extremum behavior of energy dissipation, we find that the minimum energy dissipation rate applies only to the uniform flow in gas-dominated regime, but fails in the particle-fluid compromising fluidization regime. In contrast, the EMMS principle of compromise in competition can well describe the variational behavior of meso-scale structures, and hence the EMMS-based multi-scale computational fluid dynamics has been successfully applied in predicting fluidization behavior in both academy and industry. The concept of EMMS meso-scale modeling has been recently extended to the realm of hybrid computing, enabling us a quasi-real-time computation. Such a big jump of capability will radically modify our research mode, bringing us to the new paradigm of virtual process engineering.

MESO-SCALE STRUCTURE: THE KEY TO FLUIDIZATION

Gas-solid fluidization is a typical dissipative system with multiscale structure. When reviewing the history of fluidization, one can readily find the flow structure has always been treated as the key factor, which can be evidenced by numerous researches following the pioneering work on, to mention but a few, the motion of bubbles (Davidson, 1961; Jackson, 1963; Kunii and Levenspiel, 1991), clusters (Yerushalmi et al., 1976; Li and Kwauk, 1980; Li et al., 1991; Grace et al., 1997) and aggregates (Agbim et al., 1971; Chaouki et al., 1985) and so on. However, the multiscale feature of flow structure, in particular, its meso-scale characteristics, was not widely recognized as the key to understand fluidization until in recent 30 years (Li, 1987; Li et al., 1988; Matsen, 1988; Li et al., 1993; Li and Kwauk, 1994; Ge et al., 2008; Li et al., 2009; Li et al., 2013; Sundaresan, 2000; Sundaresan, 2011; van der Hoef et al., 2008), reflecting a shift of angle of view over the research of fluidization.

In a fluidized bed, particles are agitated by a fluid or external force field to manifest a fluid-like behavior. With variation of operating conditions and material properties, the fluid and particles in a fluidized bed can be homogeneously or heterogeneously dispersed, as distinguished by Wilhelm and Kwauk (1948) in terms of “particulate” and “aggregative” fluidization. The heterogeneous flow structure covers a broad range of scales with respect to time and space (Li and Kwauk, 1994; Li and Kwauk, 2003). And these scales can be defined in a relative manner: the scale with respect to the smallest space being observed, say, a single particle in the discrete element method (DEM) (Tsuji et al., 1993) or a local cell in continuum-based computational fluid dynamics (CFD), can be termed the micro-scale; the scale with respect to the whole vessel or reactor can be termed the macro-scale; then, the wide span of scales between the micro- and macro- scales can be termed the meso-scale (Li, 1987; Li et al., 1990; Li et al., 1993; Li et al., 2009; Wang et al., 2010). In other words, the micro-scale normally refers to the scale of the element investigated, on which the knowledge is comparatively well understood and can be treated as the input or the basis; the macro-scale refers to the scale of the system consisting of elements, on which the operation/ design is to be optimized. The meso-scale, bridging between the micro-scale elements and macro-scale system, bears the dynamic and nonequilibrium information of flow structures that greatly affects the performance of flow, heat/mass transfer and reactions (Li et al., 1988; Li et al., 1993; Li, 1998; Wang et al., 2005; Ge et al., 2007; Ge et al., 2008; Dong et al., 2008a; Wang et al., 2011). As a result, the meso-scale structure is the key to understand the complex behavior of fluidization.

CHARACTERIZATION OF MESO-SCALE STRUCTURE: DISSIPATIVE WITH BIMODAL DISTRIBUTIONS

In a gas flow, the gas density, hydrodynamic velocity and temperature vary throughout the gas but the inhomogeneity tends to be smoothed within the mean free path via intermolecular collisions and related transport of mass, momentum and energy. For a typical molecular gas, the mean free path is much smaller than the scale of Kolmogorov eddies (Gidaspow, 1994). Such a clear separation between the micro-scale (mean free path) and the meso-scale (Kolmogorov eddies) allows defining a series of "scale independent" parameters such as flux or mass density for the gas. And a homogeneous, local equilibrium state can be achieved in a macroscopically nonequilibrium gas flow.

In contrast to a molecular gas flow, fluidization and rapid granular flow are dissipative, lacking scale separation with respect to both space and time (Campbell, 1990). In particular, the stronger the inelasticity is, the harder it is to separate the micro- and meso- scales (Wang and Chen, 2015). Owing to this lack of scale separation, the inherent meso-scale structure is also termed microstructure in rapid granular flows (Goldhirsch, 2003), and the parameters for a fluidized bed become "scale dependent". Such scale dependency does not vanish with the dwindling of the computational cell in CFD simulation (Hong et al., 2016). Indeed hydrodynamic description based on local equilibrium assumption cannot be satisfied for granular materials, as indicated in Du et al. (1995) by means of a one-dimensional system of inelastic particles.

Wang and Chen (2015) summarized three dissipative features that need to be considered for granular flow and fluidization. Firstly, the granular temperature could be anisotropic (Breault et al., 2005; Jung et al., 2005) or even a tensor (Goldhirsch, 1999); energy equipartition is violated for binary granular materials (Meer and Reimann, 2006; Wang and Menon, 2008) and the so-called turbulent granular temperature can be separated on the scale of clusters from the fluctuation of single particles (Jung et al., 2005). All these facts challenge the role of granular temperature in characterizing the granular behavior in fluidization.

Secondly, different from the Maxwellian distribution for molecular gases, non-Maxwellian distribution has been found as a key feature of fluidized particles except for extremely dilute condition (Kudrolli and Henry, 2000; Losert et al., 1999; Olafsen and Urbach, 1999; Rouyer and Menon, 2000). In a vibro-fluidized bed, it was found that the local velocity distribution of the velocity component in the vibration direction is asymmetric and, in particular, appears to be a bimodal distribution which comprises two peaks in the zones near the boundary, where the energy is supplied, and decays into nearly Maxwellian distribution via inelastic collisions away from the boundary (Chen et al., 2012; Chen et al., 2013). The means of energy input and dissipation directly dominate the shape of the velocity distribution (van Zon and MacKintosh, 2004). In an air-fluidized bed, the energy input comprises drag-induced agitation from both over the boundary and inside the bed. Gaussian and non-Gaussian and even bimodal distributions can be found as expected to exist locally and alternately in such cases (Wang et al., 2017).

Thirdly, bimodal distribution is also dominant with respect to the solid concentration in fluidized beds. For a circulating fluidized bed, e.g., one peak of the bimodal distribution corresponds to the dense "cluster" phase and the other to the dilute "broth" phase (Li and Kwauk 1994; Lin et al., 2001). For a bubbling fluidized bed, this bimodal structure can be characterized by "emulsion" and "bubble" phases (Davidson et al., 1977).

In all, how to account for the meso-scale features of fluidization, which are dissipative and can be characterized by bimodal distribution of parameters, constitutes a major challenge to our understanding of fluidization.

MESOSCALE STRUCTURE: CHALLENGE TO COMPUTATIONAL FLUID DYNAMICS

Multiphase flow and relevant computational fluid dynamics (CFD) have received rapidly growing interest in chemical engineering community in recent decades. As expected the prediction of flow structure in fluidized beds has been the focus of pioneering researches (Gidaspow, 1994). Ding and Gidaspow (1990) captured the bubbling phenomena inside a fluidized bed by integrating the kinetic theory of granular flow (KTGF) with the two-fluid model (TFM). Tsuo and Gidaspow (1990) captured the clustering phenomena of coarse particles inside a high-velocity fluidized bed. In the era of early development, TFM was widely utilized, in which the particles were assumed uniformly distributed at local equilibrium and thus their collective behavior can be treated as one homogeneous continuum. Experimental correlations obtained under the condition of homogeneous fluidization or fixed bed were used to close the drag force (say, Wen and Yu, 1966; Richardson and Zaki, 1954). And the kinetic theory for molecular gas was extended to for granular

flow by introducing inelastic collisions to account for the momentum transfer between particles (Gidaspow, 1994).

When a dense circulating fluidized bed (CFB) riser with fine particles was simulated, as encountered in fluid catalytic cracking (FCC) processes, the situation is quite different. Uniform distribution was predicted which deviates much from realistic clustering phenomenon on the meso-scale (Agrawal, 2001; Xiao et al., 2003; Yang et al., 2003). These meso-scale structures could be finer than the grid size used in computational fluid dynamics (CFD) simulations (Wang and Li, 2007; Hong et al., 2016).Some argued if the grid is fine enough to the size of 10 times the particle diameter (or even smaller), then the conventional TFM with closures derived from homogeneous systems may well predict the flow behavior (Agrawal et al., 2001; Wang et al., 2009; Parmentier et al., 2012; Fullmer and Hrenya, 2016). Lu et al. (2009) simulated a CFB riser with FCC particles and pointed out that the fine-grid TFM simulation may improve the results but it is not sufficient to predict correctly the solids flux whereas the solids flux is an important factor to characterize the flow state of a circulating fluidized bed. Benyahia (2012b) refined the grid size of the case in Lu et al. (2009) to 1mm and found that the refinement of grid helps to predict the S-shaped axial profile, but the predicted solids flux is still much higher than experimental data. Hong et al. (2016) performed a series of fine-grid TFM simulation of fluidized beds that cover the regimes from bubbling, turbulent to circulating fluidization. They found bubbling fluidization can be well predicted and the discrepancy increases when simulating turbulent fluidization and confirmed that fine-grid TFM simulation with homogeneous drag fails to predict reasonable solids flux in CFB. Discrete description of the solid phase, as in CFD-DEM (Xu et al., 2007; Benyahia and Sundaresan, 2011) and multi-phase particle-in-cell (MPPIC) (Li et al., 2012), does not help improve the solids flux prediction. Wang and Chen (2015) attributed this discrepancy to the local equilibrium assumption used in these approaches. Wang et al. (2017) found through high-speed camera measurement that the particle velocity largely follows Maxwellian distribution in the emulsion and bubble phases but manifests bi-modal distribution over their interface, and such bimodal distribution becomes more dominant with increase of gas velocity. In addition, Lu et al. (2011) indicated that the effect of meso-scale structure varies with material properties and operating conditions, in particular, it decays with the increase of particle diameter or Archimedes number, so, it is easier to reach grid-independent solution for low-velocity, coarse particle fluidization.

The above difficulties encountered in simulation of meso-scale structures reflect a challenge to the development of CFD. To meet this challenge, recent years have witnessed a blossom of meso-scale modeling for CFD simulation (Li et al., 1993; Li and Kwauk, 1994; Agrawal et al., 2001; Yang et al., 2003; Wang et al., 2010; van der Hoef et al., 2008; Sundaresan, 2011; Schneiderbauer and Pirker, 2014; Wang et al., 2015; Fullmer and Hrenya, 2017). Indeed, though disputes over the applicability of TFM, or rather, the assumption of local equilibrium, may last for a longer period of time for multiphase flow modeling, meso-scale modeling is always desired to establish structure-dependent closures, as fine-grid resolution of a fluidized bed reactor is hardly affordable to current computing resources. In particular, the effect of meso-scale structure on the effective drag force, which is the dominant factor for fluidization, has become a hot topic in recent years.

MESO-SCALE MODELING: BEYOND LOCAL EQUILIBRIUM ASSUMPTION

The efforts on meso-scale modeling can be generally classified into two approaches: the correlative and the variational (Li et al., 2003). The correlative normally refers to a bottom-up methodology, where one may start from certain basic model at lower level and perform highly resolved simulations to resolve flow structures and obtain constitutive closures for a higher level model. For example, some obtain the effective drag coefficients for coarse-grid simulation from direct numerical simulations (van der Hoef et al., 2008; Zhou et al., 2014) or fine-grid TFM simulations over periodic domains or realistic fluidized beds (Agrawal et al., 2001; Igci et al., 2008; Parmentier et al. 2012; Schneiderhauer and Pirker, 2014).

The correlative approach is normally conducted over a domain with size comparable to the element of higher level simulation, then, it resolves the flow structures at scales larger than the element, but not those occurring at a sub-element scale (Ge et al., 2008). Thus, the accuracy of drag closures obtained from the correlative approach depends on two issues: first, whether the local equilibrium is assumed for the element and, if yes, whether this assumption is sufficient to reveal all the meso-scale structures; second, whether the domain is characteristic of the flow field in a realistic fluidized bed. Aside from the disputes over the local equilibrium assumption as discussed above, the second issue also deserves more attention. In particular, if the lower-level simulation is performed over a periodic domain where the drag force balances the gravity, the flow structure is expected to be different from the realistic one, as for a fluidized bed, particles (or a computational cell) are always subject to local force imbalance and acceleration (Wang et al., 2010).

Recent progress in high performance computing allows fully resolved direct numerical simulations (DNS) of gas-solid two-phase flow (Ma et al., 2006; van der Hoef et al., 2008; Zhou et al., 2014; Liu et al., 2017; Tenneti and Subramaniam, 2014), from which one may obtain the effective drag closure by integrating the interfacial forces over particles tracked. Integration of the stress over the surface of a particle gives its interphase forces, in which the drag represents the time-independent component of the longitudinal force (along direction of relative velocity), besides the time-dependent longitudinal forces (e.g., added mass force, Basset force), transversal or lift forces perpendicular to relative velocity and the buoyancy irrelevant to slip (Crowe and Michaelides, 2006). For a many-particle system, the effective drag force is actually an averaged term defined on the macroscopically steady state, referring to the total interphase force divided by the volume of gas-particle mixture that may include other non-local contributions owing to interstitial flow field. So it is not surprising that fully resolved DNS results revealed that the drag correction may depend, besides void fraction and slip velocity (Wang et al., 2010; Igci and Sundaresan, 2011; Igci et al., 2012), further on the sub-grid gradient of void fraction (Li et al., 2017; Fullmer and Hrenya, 2016; Zhou et al., 2014) and even more.

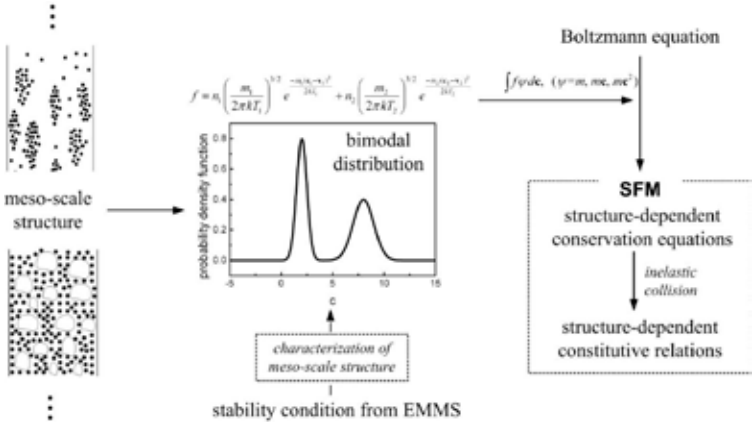

Fig. 1. General framework of EMMS-based meso-scale modeling based on bimodal distribution (Wang and Chen, 2015)

The variational approach embraces structure parameters in its conservation equations and resorts to certain regime-specific, variational stability conditions to determine the structures and relevant constitutive relations. The typical example is the energy-minimization multi-scale (EMMS) model proposed by Li and Kwauk (1994), which will be presented in section 5.

In a bubbling fluidized bed, the bimodal distribution corresponds to the coexistence of emulsion and bubbles, and in a circulating fluidized bed, it corresponds to the coexistence of clusters and broth. In the intermediate region, turbulent fluidization features rapid and alternate dominance between voids and clusters. As shown in Fig. 1 (Wang and Chen, 2015), by incorporating a combination of two Maxwellian distribution with respect to the dense and dilute phases into the Boltzmann equation, in principle, we can obtain the structure-dependent conservation equations for the mass, momentum, energy and granular temperature (Chen et al., 2017; Wang et al., 2016). The structure parameters in these conservation equations can be determined empirically from with experimental correlations, or by satisfying certain regime-specific EMMS stability condition, as presented in the following sections.

a) Structure-dependent analysis of mass, momentum and energy

By defining structure-based sub-elements to account for the bimodal distribution of parameters, we can derive a set of structure-dependent multi-fluid model (SFM) equations for the mass and momentum of the gas/solid in the dense and dilute phases, respectively (Hong et al., 2012). In line with the observed velocity distribution (Wang et al., 2017), both the dense and dilute phases can be assumed to be homogeneous and at local equilibrium state. The gas in the dilute broth surrounds the clusters in a CFB (Hong et al., 2012), or, the dense emulsion surrounds the gas bubbles in a bubbling fluidized bed (Hong et al., 2013; Luo et al., 2017; Shi et al., 2011), thus, there are additionally a meso-scale drag over the interface together with dynamic mass exchange of gas and particles between the dilute and dense phases. Direct solution of SFM equations is rather difficult, if not impossible, as its number of variables and conservation equations, apart from the mass exchange terms that need to be closed, are twice that of TFM. A simple way out is to sum the SFM equations

for the dilute and dense phases, thus yield a set of TFM-like equations, where the continuity equations are the same as TFM but the momentum equations differ in structure-dependent drag force and solid stress to be closed, as follows:

$$\frac{\partial}{\partial t}(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\mathbf{v}_{\mathrm{g}})+\nabla\cdot(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\mathbf{v}_{\mathrm{g}}\mathbf{v}_{\mathrm{g}})=-\varepsilon_{\mathrm{g}}\nabla p_{\mathrm{g}}+\nabla\cdot\boldsymbol{\tau}_{\mathrm{ge}}+\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\mathbf{g}-\mathbf{F}_{\mathrm{de}}+\nabla\cdot\boldsymbol{\tau}_{\mathrm{Dg}}, \tag{1}$$

$$\frac{\partial}{\partial t}(\varepsilon_{\mathrm{s}}\rho_{\mathrm{s}}\mathbf{v}_{\mathrm{s}})+\nabla\cdot(\varepsilon_{\mathrm{s}}\rho_{\mathrm{s}}\mathbf{v}_{\mathrm{s}}\mathbf{v}_{\mathrm{s}})=-\varepsilon_{\mathrm{s}}\nabla p_{\mathrm{g}}-\nabla p_{\mathrm{sc}}+\nabla\cdot\boldsymbol{\tau}_{\mathrm{sc}}+\varepsilon_{\mathrm{s}}\rho_{\mathrm{s}}\mathbf{g}+\mathbf{F}_{\mathrm{de}}+\nabla\cdot\boldsymbol{\tau}_{\mathrm{Ds}}, \tag{2}$$

where ε denotes volume fraction, ρ density, $\boldsymbol{\tau}$ shear stress tensor, $\mathbf{F}_{\mathrm{de}}$ effective drag force vector, $\mathbf{v}$ velocity vector, p pressure, subscripts g and s denote gas and solid phase, and subscripts e denote effective term and D diffusive term, respectively. The effective drag force includes the contributions from the drag forces in the dense phase $\mathbf{F}_{\mathrm{dc}}$, dilute phase $\mathbf{F}_{\mathrm{df}}$ and interphase $\mathbf{F}_{\mathrm{di}}$, as follows:

$$\mathbf{F}_{\mathrm{de}}=f\mathbf{F}_{\mathrm{dc}}+\mathbf{F}_{\mathrm{di}}+(1-f)\mathbf{F}_{\mathrm{df}}, \tag{3}$$

where f denotes the volume fraction of dense phase, subscripts c, f, i denote the dense phase, dilute phase and interphase, respectively. And the effective solid stress $\boldsymbol{\tau}_{\mathrm{sc}}$ is given by

$$\boldsymbol{\tau}_{\mathrm{sc}}=f\boldsymbol{\tau}_{\mathrm{sc}}+(1-f)\boldsymbol{\tau}_{\mathrm{sf}}\ . \tag{4}$$

Further, the SFM energy conservation for the gas phase can be derived by summing the dot products of the momentum equation and gas velocity in both the dilute and the dense phases, as follows (Song et al., 2014):

$$W_{\mathrm{T,g}}+W_{\tau\mathrm{,g}}=W_{\mathrm{k,g}}-\rho_{\mathrm{g}}\mathbf{U}_{\mathrm{g}}\cdot\mathbf{g}+W_{\mathrm{st}}+W_{\mathrm{d,g}}, \tag{5}$$

where $W_{\mathrm{T,g}}$ and $W_{\tau\mathrm{,g}}$ denote the net power of the gas pressure and shear stress exerted per unit volume, respectively, $W_{\mathrm{k,g}}$ the variation rate of the kinetic energy of gas per unit volume; the second term on the RHS denotes the variation rate of gas gravity potential per unit volume, W_{st} the power consumed for suspending and transporting particles per unit volume, and $W_{\mathrm{d,g}}$ the energy dissipation rate of gas per unit volume.

It is obvious that the SFM reduces to the TFM if there is no difference between the dilute and dense phases. On the other hand, if one models a fluidized bed at steady state, then the drag force, gravity and gas pressure dominate the flow behavior of the system, whereas the other factors, such as acceleration, stress and mass exchanges can be neglected. Then the mass and momentum equations of the SFM reduce to the hydrodynamic part of the EMMS model, as detailed in Hong et al. (2012) and Chapter 6 of Li et al. (2013). Similarly, the SFM energy conservation equation can also reduce to the same form as the EMMS energy decomposition for a steady state description of a fluidized bed, i.e., $W_{\mathrm{T,g}}=W_{\mathrm{st}}+W_{\mathrm{d,g}}$. Thus the SFM, which stems from the meso-scale nature with bimodal distribution of gas-solid flow, can be viewed as a more general model that covers the realms of both TFM and EMMS. And it paves the fundamental base of why one can integrate the EMMS drag in CFD simulation. It is worth noting that the structure parameters in Eqs. (1)-(4) still need closure relations to solve the reduced SFM equations, which will be detailed in the following sections.

b) Structure-dependent analysis of energy dissipation

Bearing in mind the dissipative features of gas-fluidized bed, in particular, the bimodal velocity and density distributions, we can further extend the SFM analysis to the energy dissipation. As detailed in Tian et al. (2017), by deriving the structure-dependent internal energy equation and incorporating it into the thermodynamic relation between internal energy and entropy, we can finally obtain the structure-dependent energy dissipation relation. For an isothermal fluidized bed under steady state, the energy dissipation due to heat transfer and viscous stress can be neglected, and then the total energy dissipation rate per unit volume, E_{d}, can be written as follows:

$$E_{\mathrm{d}}=f\mathbf{F}_{\mathrm{dc}}\cdot\left(\mathbf{v}_{\mathrm{gc}}-\mathbf{v}_{\mathrm{sc}}\right)+\mathbf{F}_{\mathrm{di}}\cdot\left(\mathbf{v}_{\mathrm{gf}}-\mathbf{v}_{\mathrm{sc}}\right)+\left(1-f\right)\mathbf{F}_{\mathrm{df}}\cdot\left(\mathbf{v}_{\mathrm{gf}}-\mathbf{v}_{\mathrm{sf}}\right), \tag{6}$$

where $\mathbf{v}_{\mathrm{gc}}$, $\mathbf{v}_{\mathrm{sc}}$, $\mathbf{v}_{\mathrm{gf}}$ and $\mathbf{v}_{\mathrm{sf}}$ denote the velocities of dense-phase gas, dense-phase particle, dilute-phase gas and dilute-phase particle, respectively. By accounting for the force balance between drag and gravity in the dilute and dense phases, it reads

$$E_{\mathrm{d}} = \varepsilon_{\mathrm{g}}\varepsilon_{\mathrm{s}}\left(\mathbf{v}_{\mathrm{s}} - \mathbf{v}_{\mathrm{g}}\right)\left(\rho_{\mathrm{s}} - \rho_{\mathrm{g}}\right)\cdot\mathbf{g}. \tag{7}$$

According to the method of Lagrange multipliers, the extremum point of the energy dissipation rate is located over the bounds of the domain, and the energy dissipation rate decreases monotonically with mean void fraction ε_g. Indeed by sweeping the structure parameters, one can readily find that at a given superficial gas velocity, a homogeneous state is predicted with $E_d \rightarrow \min$ such that void fraction approaches to $\varepsilon_{\mathrm{uni}}$, where $\varepsilon_{\mathrm{uni}}$ denotes the maximum value of void fraction in homogeneous fluidized system.

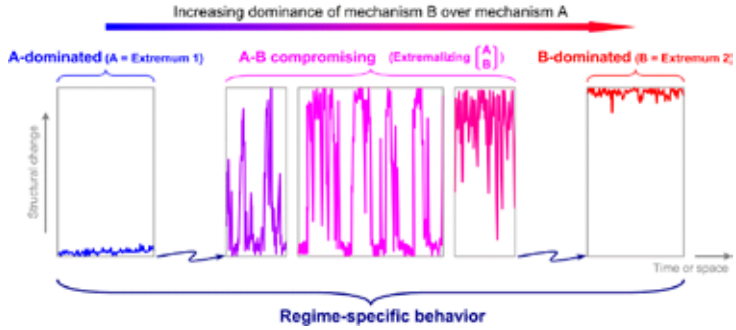

Fig. 2. According to the principle of compromise in competition, three regimes occur successively with changing the relative dominance of Mechanism B over Mechanism A (Li, 2016).

To account for the meso-scale, inhomogeneous flow structures prevalent in CFB, Li and his colleagues proposed the meso-science based on the EMMS principle of compromise in competition (Li et al., 2013; Li and Huang, 2014; Li, 2016; Li et al., 2016), unfolding a new viewpoint in searching for the generality of the extremum behavior of multiphase complex systems. According to this principle, in a fluidized bed, two dominant mechanisms corresponding to different regimes should be first distinguished, alternately, with respect to time and space, and their compromise gives rise to the stability condition of the EMMS model, $N_{\mathrm{st}} \rightarrow \min$. In a broader sense, Li (2016) indicated that, as depicted in Fig. 2, two variational criteria, governing separate dominant mechanisms, are both involved in shaping the structures of complex systems. Either of the two alone may be only designated as either an A-dominated or B-dominated regime governed exclusively by a single mechanism. That is right the case of the above energy dissipation analysis, which only corresponds to the B-dominated regime in Fig. 2. However, in the A-B compromising regime to which the gas-solid flow in a fluidized bed belongs, as emphasized in Li et al. (2016), eventually, two extrema have to compromise in their competition to reach their respective relative extremal values with a mutual constraint, although these values are different from those without compromise, and further, searching a single variational criterion in terms of dissipation rate is right for either A- or B-dominated regime, as practiced in thermodynamics, but not likely in the A-B compromising regime due to multiple dissipative mechanisms with different extremum behaviors. Even if a single extremal function does exist, it should not be in terms of total dissipation. Such a mechanism of the dissipation and variational behavior of fluidization paves a solid base for the EMMS model proposed decades ago, as will be revisited in the following section.

EMMS MODEL AND APPLICATION: DRAG, HEAT/MASS TRANSFER AND REACTIONS

a) EMMS model

In the EMMS model (Li et al., 1988; Li and Kwauk, 1994), the meso-scale structure was characterized with a dense phase consisting of spherical clusters and a dilute phase with homogeneously dispersed particles. The cluster diameter was assumed inversely proportional to N_{st}, which tends to minimum according to the principle of compromise in competition (Li et al., 2013; Li and Huang, 2014). As presented above, the EMMS model features a set of structure-dependent mass and momentum conservation equations plus a stability condition of N_{st} tending to minimum, with which all the structure parameters can be resolved by following a nonlinear programming scheme, the detail of which is referred to Ge and Li (2002).

Besides predicting flow states of fluidized beds, the EMMS model is highlighted with its unique ability to predict the choking, an instability phenomenon first identified by Zenz (1949). In a pneumatic transport riser, by decreasing gradually the gas flow rate under a fixed solids flux, the choking is defined to describe an

abrupt rise of pressure drop per unit length of pipe and an apparent collapse into a condition of slug flow (if the pipe diameter is small and comparable to the scale of meso-scale structure). The solid flux at the choking point represents the saturation carrying capacity of the gas at the corresponding superficial velocity. Apart from the factors of geometrical design and blower insufficiency (Bi et al., 1993; Yang et al., 2004), the choking-induced operation instability was found closely related to the bi-stable state predicted by using the EMMS model (Ge and Li, 2002). When that occurs, two flow states with different solid concentrations satisfy simultaneously the minimum of N_{st} and hence both flow states coexist physically at specific set of operating conditions with the same saturation carrying capacity. When applying the EMMS model to predict the flow regime transitions over a wide range of operating conditions, we can define the intrinsic flow regime map that is free from the limitation of any geometric factors, over which one can readily distinguish the gas-dominated dilute-phase transport, the particle-fluid compromised dense-phase transport and in between the choking or continuous transition area that are separated by the critical point (Wang et al., 2007; Wang et al., 2008b; Wang et al., 2010). On the other hand, the flow state of a fluidized bed is determined by not only the hydrodynamics but also the geometric factors such as the size of reactors and the coupling between interconnected sections in the whole loop of the system. Indeed the scale up effects of fluidized bed reactors heavily relies on such factors. And that requires CFD modeling with detailed spatial resolution. The EMMS model is a structure-based option to provide closure relations for CFD, in particular, the drag.

b) EMMS drag

The EMMS model was originally proposed for predicting time-averaged behavior of fluidized beds on the reactor scale. To integrate with CFD, the EMMS drag was proposed (Li et al., 1993) and Yang et al. (2003) introduced acceleration into the EMMS model to account for the force imbalance between the effective gravity of particles and the drag force. In this way, a simplified EMMS drag coefficient can be determined based on information of cross-sectionally averaged gas velocity and solid flux. Use of this EMMS drag was found to enable correct prediction of solid flux and axially S-shaped profiles of voidage, whereas the use of homogeneous drag was found to overpredict the solids flux by a factor of nearly ten.

Later study revealed that the EMMS stability condition should be satisfied only at large enough scales, e.g., the reactor scale, which mismatches the scale at which a CFD grid applies (Li et al., 2004). Based on this understanding, the EMMS model was extended to describe the meso-scale structures at the sub-grid level (Wang and Li, 2007). To coordinate the hydrodynamics and the stability condition at different scales, the extended EMMS drag model (EMMS/matrix) adopts a two-step scheme. Namely, the first step is to determine the meso-scale parameters in terms of the diameter and void fraction of clusters (d_c and ε_{gc}) under the constraint of the global stability condition $N_{st}\rightarrow$min. In the second step, with known relation of d_c and ε_{gc}, the sub-grid version of EMMS model with accelerations for the dilute and dense phases is coupled with CFD in each cell, determining the drag coefficient. In literature, some may misinterpret the EMMS drag is coupled with the TFM. However, as the EMMS drag is consistent with SFM conservation equations, so that once the EMMS drag is used, the governing equations should be the SFM (Hong et al., 2012; 2013; Song et al., 2014).

Use of EMMS drag enables reliable CFD prediction of apparent flow regime map for CFB, which is associated with not only hydrodynamics but also geometric factors (Wang et al., 2008b; Wang et al., 2010). The apparent flow regime changes gradually with riser height. A short riser whose whole range of pipe is affected by the inlet/outlet effect may skip the choking transition. This dependency of the flow regime on the riser height is at least one of the major reasons that cause disputes in literature about understanding of the choking phenomena. By comparison, Ullah et al. (2013) pointed out that the use of homogeneous drag fails to predict the bi-stable state and choking through drift flux analysis.

Such geometric factor related disputes may be resolved by resorting to the so-called “virtual experiment” through 3D, full-geometry simulations of CFB (Zhang et al., 2008). Recent simulation even included dynamic adjustment of mechanical valve in simulation and investigated its effects on the choking transition (Liu et al., 2015b). With rapid development of parallel computing technology and new numerical schemes, we can expect such approach will enable us in near future a more vivid and even real-time tool to probe the complex behavior in CFB reactors. The experiment and computation are more integrated than ever before, making the so-called “virtual process engineering” come true (Ge et al., 2011).

c) EMMS mass transfer & reactions

Although the effects of meso-scale structure on the flow have been extensively investigated in recent years, the mass transfer study receives much less attention. There are three possible reasons for this situation (Wang and Chen, 2015, Liu et al., 2015). Firstly, mass transfer interacts with multiphase reactions and flow,

complicating its dependency on structure. Due to the unclear understanding of meso-scale structure, Breault (2006) reported that the mass transfer coefficient for CFBs may differ by up to 5 orders of magnitude. Secondly, the importance of mass transfer on the overall reaction rate is often underestimated. For fine particles reacting with surrounding gas under high slip velocity, as is the case in FCC, it is normally assumed that the fluid-particle mass transfer rate is so high that the overall reaction rate is controlled by the slower step, the surface reaction. However, the meso-scale structure may reduce the mass transfer rate in the same way as it affects the drag coefficient, making realistic behavior being dominated by both surface reaction and mass transfer. The last and the most easily overlooked reason lies in the oversimplified concept of intrinsic kinetic rate (Levenspiel, 1999), which is based on the assumption that the reaction and transport phenomena are separable. However, the observed catalytic reaction mechanism may be affected by the cavity size of molecular sieves (Tian et al., 2015) and elementary reactions may be inseparable from particle concentration (Turns, 2000). Indeed, how to bridge the gap between the elementary kinetics on the scale of molecules and the so-called intrinsic kinetic rate on the scale over a single particle or within a CFD grid is actually ambiguous. The CFD based reaction modeling is hence hard to be theoretical.

In spite of the above difficulties, Wang et al. (2005) proposed an EMMS mass transfer model and Dong et al. (2008a; 2008b) extended it to the sub-grid level by adopting the two-phase structure information determined with the EMMS/Matrix model. Besides the mass transfer in homogeneous mixture of the dilute or dense phase, the meso-scale mass exchange between the dilute and dense phases was also taken into account. Such an approach has been unified under the umbrella of the SFM framework recently (Liu et al., 2015). The meso-scale structure parameter was found necessary to be included as an independent variable to account for the mass transfer besides the normally used Reynolds number. Indeed the scattered data of mass transfer coefficient reported by Breault (2006) can be well explained by the difference in newly added structure parameter. Similar trend has also been predicted by using the filtered approach (Holloway et al., 2012).

INDUSTRIAL APPLICATION

a) Two modes of CFB application

CFBs have been widely applied in industrial processes such as alumina calcination, combustion and gasification, FCC, chemical looping processes and so on (Werther & Hartge, 2014). Besides material properties and operating conditions that are normally viewed as key parameters, the modes of operation and geometric factors are also important factors. Generally, two modes of operation can be distinguished in CFBs (Reh, 1996; Squires et al., 1985): one has been developed from refinery technology where catalyst particles are fluidized and circulated with a “controlled recycle”, as in FCC and methanol to olefins (MTO) reactors (Ye et al. 2015); the other has been developed from processes involving internal combustion where solid particles are circulated with an “undelayed recycle”, such as in a CFB combustor (CFBC) or alumina calciner (Reh, 1996). In CFD simulations, we may distinguish these two modes of operation by fixing solids flux G_s and mean solids volume fraction ε_s, respectively (Mei et al., 2017). When fixing mean solids volume fraction or solid inventory, the solids flux is self-adjusted by circulating all the solids through the loop seal back to the side inlet, as shown in Fig. 3. It is found that the FCC and CFBC modes generally have the same dependence of solids flux on the mean solids volume fraction or solids inventory. However, during the choking transition, the FCC mode of operation needs longer transitional time between different flow states; thus the FCC system may have insufficient time to respond to valve adjustments or flow state change, easily leading to the operating instability.

b) Catalytic processes: FCC and MTO

Indeed the choking-related operating instability was a big problem encountered by SINOPEC when trying to revamp the widely used FCC units in petroleum refineries. The products from the FCC process normally contain large amount of olefins. To reduce the olefin content in gasoline, the Research Institute of Petroleum Processing (RIPP) of SINOPEC developed a novel multiple-section reactor, called the maximizing iso-paraffins (MIP), which was distinguished from conventional FCC reactors by an enlarged section in the middle of the riser tube, where the olefins are transformed into iso-paraffins and aromatics through alkene-isomerization and hydrogen-transfer reactions. Due to this enlarged section design, the superficial gas velocity in the reaction zone is decreased and falls into the choking regime, which is seldom encountered in previous design of FCC units with higher gas velocity. CFD simulation with EMMS drag helped to nail down this problem for the MIP units and thereby provided solution to avoid it (Lu et al., 2007).

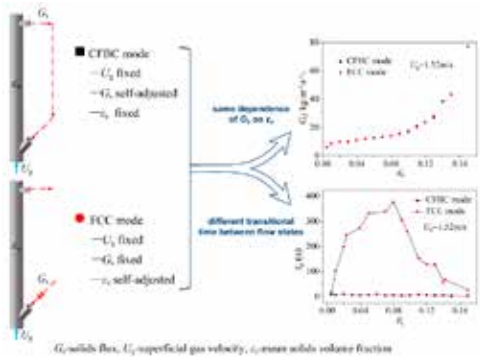

Fig. 3. Comparison between two modes of CFB operation: FCC vs CFBC (Mei et al., 2017).

Scale up of fluidized bed reactors is regarded as a major challenge to chemical reaction engineering. CFD-aided approach allows detailed investigation of the coupling between hydrodynamics and reactions within different sized reactors, and hence can be expected to boost the traditionally experiment-based approach with probably lower cost. Recent collaboration between the Institute of Process Engineering (IPE) and Dalian Institute of Chemical Physics (DICP) reexamine the scale-up effect of the MTO reactors as a starting point for further development of more catalytic processes. MTO process developed by DICP differs from FCC in following aspects (Tian et al., 2015; Ye et al., 2015): different catalysts for highest selectivity to ethylene provided with certain amount of coke deposition (MTO: SAPO-34 zeolite catalyst; FCC: zeolite Y catalyst with larger pores); different reactors for longer residence time of particles (MTO: densely bubbling or turbulent fluidization bed; FCC: circulating fluidized bed riser or pneumatic transport) and different thermal conditions (MTO: exothermic; FCC: endothermic).

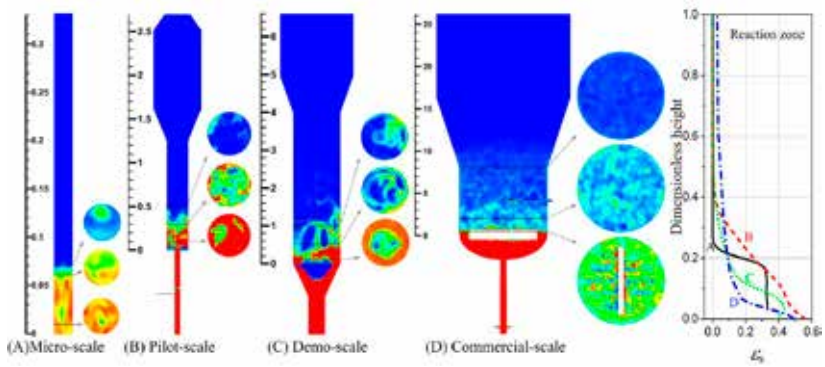

Fig. 4. Instantaneous distribution of solid concentration of different scaled MTO reactors (Lu et al., 2017).

To take into account these difference, we conducted the following studies: 1) A CSTR (continuous stirred tank reactor) model was established to predict the steady-state coke content, and then incorporated it into CFD by initializing the coke concentration to speed up reactive simulations (Lu et al., 2016); 2) A two-step EMMS/bubbling drag model was developed such that coarse-grid simulation of densely bubbling or turbulent fluidize beds can be realized with weak dependence on grid size (Luo et al., 2017). Lumped reaction kinetics was used in simulation to reduce the complexity of catalytic kinetics. Fig. 4 shows snapshots of transient distribution of solid concentration in different sized reactors during the process of scale up. For the reaction behaviors, the predictions of both micro-scale and pilot-scale reactors are in good agreement with the experimental data. However, the predictions of both demo-scale and commercial reactors show deviation from the experimental (Lu et al., 2017). The lumped reaction kinetics was as normal obtained through fitting experimental data over a micro-scale fluidized bed. As discussed above, it cannot be counted on as intrinsic kinetics and depends on the specific conditions of multiphase flow and mass transfer in the fluidized bed. So it can be expected that there will be discrepancy when applying such kinetics in larger-

scale reactors, even the flow behavior can be well predicted. That definitely requires more efforts in future in exploring the mechanism of the coupling between reaction and meso-scale structures.

c) CFB Combustor

Owing to its advantage in low emission and fuel flexibility, CFB boiler for utility power generation has been widely applied in the past decades. To achieve an efficient design and scale-up of CFB boilers, one needs to grasp the complex multiphase flow and reaction behavior, which is greatly affected by air distribution, staged air injection and penetration, separation performance of parallel cyclones and interactions between different compartments and so on. That urgently requires systematic understanding of the whole system. Such ability was highlighted in recent years with the development of 3D, full-loop coarse-grid simulation with meso-scale modeling (Zhang et al., 2008; Zhang et al., 2010; Lu et al., 2013).

To mention but one outcome obtained through 3D, full loop simulation that is hard to investigate with simplified 2D simulation. The performance of parallel cyclones is important to achieve steady circulation of solid materials in large CFB boilers. In practice, lower efficiency was found when a CFB has more than one cyclone. Grace et al. (2007) stated "when two-phase suspensions are conveyed through identical parallel flow paths, the flow distribution can be significantly non-uniform in practice". This phenomenon has been verified experimentally (Kim et al. 2006; Masnadi et al. 2010; Yue et al. 2008), and is a good example of compromise between two dominant mechanisms. Experimental measurement of solid flux is difficult, especially in a commercial CFBB. Previous CFD simulations of cyclone mainly focused on the cyclone itself without consideration of the non-uniform gas inflow from the furnace. Through 3D full-loop simulation, Zhang et al. (2010) pointed out that the averaged solid fluxes for two cyclones of a 150MWe boiler could be quite different. From one instant to another, the fluxes exhibit a seesaw phenomenon, that is, the peak flux alternates in these two cyclones: when one cyclone reaches a maximum flux, the other is near a minimum, and vice versa. This phenomenon was also validated by snapshots showing alternate accumulation of solids near the cyclone inlets at the top of the furnace (Fig. 5). Such ability facilitates in-depth understanding of non-uniform flow in commercial CFBB and enables optimal design and scale-up (Jiang et al., 2014).

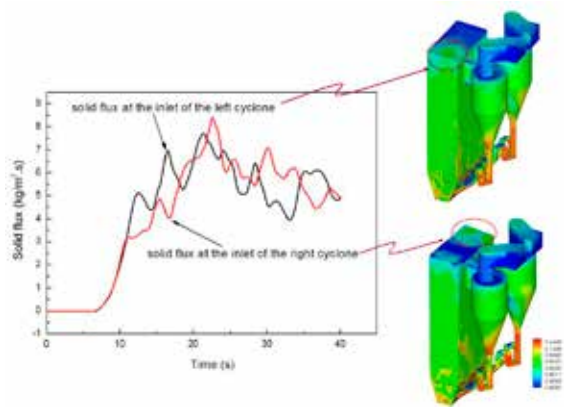

Fig. 5. Alternate peak flux of solids into two parallel cyclones of a 150MWe CFB boiler (Zhang et al., 2010).

It is worth noting that the reactive CFD simulation of a CFBB is far from reaching maturity. Apart from the consideration over intrinsic kinetics and long residence time of particles, the complex coupling between multiphase flow and reactions is always a hard topic that deserves more efforts on meso-scale modeling.

CONCLUSION AND PERSPECTIVES

Gas-solid fluidized bed is a typical dissipative system, featuring meso-scale structures with bimodal distribution of parameters. Traditional two-fluid model and relevant closures depend on local equilibrium and homogeneous distribution assumptions, and fail to predict the solid flux and flow regime transitions in circulating fluidized beds even with fine grid resolution. To solve this problem, recent years have witnessed a blossom of meso-scale modeling research from various aspects of the problems and angles of view. In particular, through structure-dependent analysis of mass, momentum and energy conservation, we can unify the hydrodynamic equations of two-fluid model and those of the EMMS model. Further, by extending

structure-dependent analysis to the extremum behavior of energy dissipation, we find that the minimum energy dissipation rate applies only to the uniform flow in gas-dominated regime, but fails in the particle-fluid compromising fluidization regime. In contrast, the EMMS stability condition, which is based on the principle of compromise in competition, can well describe the variational behavior of meso-scale structures, and hence the EMMS-based multi-scale CFD has found successful applications in both academic and industrial fields by greatly improving prediction in terms of multiphase flow and reactions as well as understanding of flow regime transitions.

We can expect the meso-scale modeling will remain to be a hot topic for a longer time, as the secrets of scale-dependent, nonequilirbrium multiphase flows are not fully understood. More in-depth investigation should be conducted by integrating experimental measurement, theoretical derivation and numerical simulations. In experiments, microscopic, noninvasive observation of velocity distribution, correlated density fluctuation or clustering will be helpful to quantify the dissipative behavior of fluidization under different energy driving conditions. With experimental quantification of meso-scale structures, statistical analysis based on nonequilibrium distribution may require novel mathematical skills to unravel the complex dependence of stress-strain relation on the mass exchange between phases. Structure-dependent energy dissipation analysis can help elucidate the dissipative nature of meso-scale structures, and further extend the application of EMMS-based meso-scale modeling. DNS is a powerful tool to investigate the dissipative behavior of fluidization. Due to its high demand in computing resources, current DNS is largely limited to simulations over static arrays of particles or small-sized, periodic flow domains, which are different from realistic fluidization systems.

Fig. 6. Version 1.0 of VPE: On the right is an experimental unit. A screen of the same height as that of the unit is shown in the middle. A computer controls both the experiment and simulation to allow online comparison (Li et al., 2016)

Recognizing the generality of multiscale structures in different systems, the EMMS principle of compromise in competition has been developed into a multiscale computational paradigm featuring scale-dependent computation, communication and storage (Ge et al., 2011; Li et al., 2016). Taking this advantage, as shown in Fig. 6, a supercomputer with a peak performance of 1.0 Pflops and a version 1.0 of virtual process engineering (VPE) platform (Liu et al., 2012; Li et al., 2016) has been constructed, which enables us larger-scale DNS and much faster CFD for commercial scale reactors, even to the level of quasi-real-time computation (Ge et al., 2011; Ge et al., 2015). Such a big jump of capability will radically modify our research mode, bring us to the new paradigm of virtual process engineering and help explore the meso-science on the horizon (Li et al., 2016).

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