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STRUCTURE-ORIENTED MULTI-SCALE SIMULATION OF TWO-PHASE FLOWS – METHODOLOGY AND APPLICATION

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ABSTRACT

Modelling the dynamic behaviour of heterogeneous structure in two-phase systems is a challenging problem facing scientists and engineers, though the well established computational fluid dynamics has found widespread applications in process industries. In recent years, multi-scale methodology has received more and more attention and its incorporation into CFD may promote significant advancement of our ability of simulating complex two-phase flows. This paper outlines the challenging problems in modelling two-phase flows from the perspective of complexity science. The strengths and weaknesses of various approaches are discussed and the energy-minimization multi-scale (EMMS) approach is incorporated into the two-fluid model, leading to a strategy of the so-called structure-oriented multi-scale simulation which is developed at IPE to cope with the spatial-temporal coupling and variation of hierarchical multi-scale structure in complex two-phase flows. It is found that besides the improvement in prediction of meso-scale structure and hydrodynamics, this strategy offers physical explanations for some critical issues like choking in gas-solid fluidization and necessary parameters for specifying the hydrodynamics of CFB risers. It is also extended to determine the bubble diameter for gas-liquid flows by analysing the compromise of dominant mechanisms for bubble break-up and coalescence. This paper is concluded by discussing some further extension of this promising approach.

NOMENCLATURE

a average acceleration for particles
C_D average drag coefficient
C_{Dc} drag coefficient for particles in dense phase
C_{Df} drag coefficient for particles in dilute phase
C_{Di} drag coefficient for clusters
d_{cl} cluster diameter
f dense phase fraction
G_s solids flow rate
I solid inventory
N_{st} volume-specific energy consumption for suspension and transportation of particles
U_c dense phase superficial gas velocity
U_{dc} dense phase superficial particle velocity
U_{df} dilute phase superficial particle velocity
U_f dilute phase superficial gas velocity
U_g superficial gas velocity
W_{st} mass-specific energy consumption for suspension and transportation of particles

β average drag coefficient for particles in an element
ε_c dense phase voidage
ε_f dilute phase voidage
ε average voidage

CHALLENGING PROBLEMS IN MODELING TWO-PHASE FLOWS

Flows involving more than one phase are often encountered in chemical and physical processes of industries. A physical understanding of these flows is of critical importance for design, scale-up, control and optimization of processes, yet offers problems of far greater complexity than encountered in single-phase flow. For example, three important phenomena are prevalent in most two-phase systems, namely, structure heterogeneity, state multiplicity and scaling-up effects. *Structure heterogeneity* is related to the discontinuities at the phase interfaces, usually involving meso-scale non-uniform structures such as particle-rich clusters, streamers or strands in gas-solid systems, and bubble plumes as well as liquid-rich vortices in gas-liquid systems. *State multiplicity* refers to the variation of macro-scale structures with operating conditions. An example is the so-called choking representing the jump change between the regime of dilute transport and fast fluidization due to a slight variation of operating conditions in gas-solid fluidization. *Scaling-up effects* reflect the phenomena of structural changes with the scale of reactor size, causing the difficulties in transferring the database and experiences obtained from lab-scale or even pilot-scale experiments to commercial-scale facilities.

Apparently, the common characteristic of all the above complicated phenomena is the occurrence and variation of the heterogeneous structure which has an important bearing on the transfer properties, as reviewed by Li & Kwauk (2003). These two-phase systems belong to complex systems which are non-linear and non-equilibrium with the hierarchical multi-scale structure as their common nature.

The multi-scale nature has brought about a series of key issues on the frontiers of physical modelling and numerical simulation, which attracted the attention of researchers from various disciplines (*Gas-solid flow*:

Enwald, Peirano, & Almstedt, 1996; Peirano & Leckner, 1998; Gidaspow, Jung, & Singh, 2004; Sinclair & Van Wachem, 2004; *Gas-liquid flow*: Jakobsen, Sannæs, Grevskott, & Svendsen, 1997; Joshi, 2001, 2002; Rafique, Chen, Duduković, 2004; *Multi-phase flow*: Kuipers & Van Swaaij, 1997; Sundaresan, 2000; Wachem & Almstedt, 2003; Hanratty et al., 2003; *Granular flow*: Campbell, 1990; Goldhirsch, 2003; among others). This article will not follow the general guidelines or roadmaps indicated in the literature of reviewing articles of two-phase flows, but try to highlight the issues from the perspective of complexity science.

The principal scientific issue in recent years may be the understanding of the occurrence of complicated meso-scale structures such as aforementioned clusters or bubbles. It is recognized that these meso-scale structures are germane to the transport properties between phases and therefore play a profound role in the macro-scale behaviours. For example, Li & Kwauk (1993, 2003) elucidated that the average drag coefficients C_D were quite different for different structures even with the same amount of particles and fluid flow rate in a given volume. Local meso-scale structures led to a decrease in C_D, though the average parameters were identical.

Since meso-scale structures are of crucial importance in the modelling of two-phase flows, another question is how to describe them. Apart from discrete simulations and direct numerical simulations for simple flows, it is possible to model the structures directly for each specific case in engineering. However, physical modelling needs to know the underlying physics associated with the meso-scale structures and perhaps to ascertain their origin, evolution and definitive characteristics, all of which are still far from being well understood at present. This is because the meso-scale structures spanning a wide range of length and time scales are usually dominated by many unclear mechanisms. Recently, Agrawal et al. (2001) reported that inertial instabilities can give rise to meso-scale structures when the relative motion between phases is large enough in gas-solid flow. A general theoretical framework is still lacking for analysing the coupling of complicated multiple dominant mechanisms, and we believe that there must exist some stability criteria in two-phase systems, which could reflect the compromise of multiple dominant mechanisms and be responsible for the formation of meso-scale structures (Li & Kwauk, 2003).

The next issue results from the inter-correlations between scales, usually involving implicit and two-way coupling in two-phase systems. This can be partially reflected by the concerns in literature as to how the cell-scale constitutive relations are developed for phase stresses and interfacial forces by using the micro-scale information. This concern belongs to the so-called correlative multi-scale methods which may be inadequate for the complete analysis of the complex two-phase systems, for it is generally difficult for common correlative multi-scale methods to achieve a systematic description of implicit and two-way coupling. These methods focus on explicit and one-way coupling at present (Li & Kwauk, 2003, Li et al., 2005).

Moreover, the concept of meso-scale structures can be extended to other types of heterogeneities like temporal and dynamical structures other than geometrical entity. However, the multi-scale temporal and dynamical structure thereby induced has not received as much attention as for spatial structures.

Last but not the least, complex two-phase systems may exhibit strong coupling between temporal and spatial variations. In order to model this coupling, a practical way is to combine the analysis of multi-scale spatial structures with current computational tools, which is though a rough description for temporal variations at present. This concept is practiced by the so-called structure-oriented multi-scale strategy developed in the Institute of Process Engineering (IPE) of the Chinese Academy of Sciences by incorporating the energy-minimization multi-scale (EMMS) approach into current commercial CFD packages.

CURRENT MODELING APPROACHES — AN OVERVIEW

Current modelling approaches for two-phase flows can fall into three general categories in terms of their ability of characterizing the heterogeneous structure, that is, *discrete* based on micro-mechanism, *average* without distinguishing structural differences at different scales, and *multi-scale* considering the disparity of behaviours at different scales, as illustrated in Fig. 1.

Discrete approach

Fig. 1(a) and 1(b) illustrate a global view of the particle distribution in a gas-solid fluidized bed and a local view of the structure inside an element, respectively. Approaches involving direct numerical simulations or discrete simulations are regarded to be fundamental and capable of precisely describing the physics on micro-scale. In the direct numerical simulations (Fig. 1(g)), the fluid phase and particle phase are described by conservation equations and Newton's second law of motion respectively, and the coupling of two phases are either treated from the calculated velocity field of the fluid using the unstructured grids surrounding particles (Hu, 1996), or determined by some front tracking methods in gas-liquid flow simulations. In discrete simulations such as the pseudo particle modelling (Fig. 1(f)), the continuous fluid phase is discretized into fictitious particles, and particle-fluid interactions are realized through the collision processes between pseudo particles (smaller one) and real particles (larger one) (Ge & Li, 2003). However, application of these approaches is restricted to the simulation of simple two-phase flows with fewer particles or smaller Reynolds numbers due to the prohibitive cost of computation or complicated techniques for grid generation or for interface tracking. The prospect of pseudo-particle modelling is promising in that the computation can be highly parallelized by virtue of its locally interactive nature. In fact, the exact flow field around each single particle illustrated in Fig. 1(b) was extracted from the parallel simulation implemented on 1024 CPUs with the so-called macro-scale pseudo-particle modelling (Ge & Li, 2001; Tang et al., 2004).

Average approach

The two-fluid model was proposed that both phases were assumed continuous and inter-penetrable, as shown in the shaded area in Fig. 1(c), and conservation equations were developed in an average sense. Although this approach has already been applied in commercial

computational fluid dynamic packages for engineering simulation, the average treatment of phases may discount

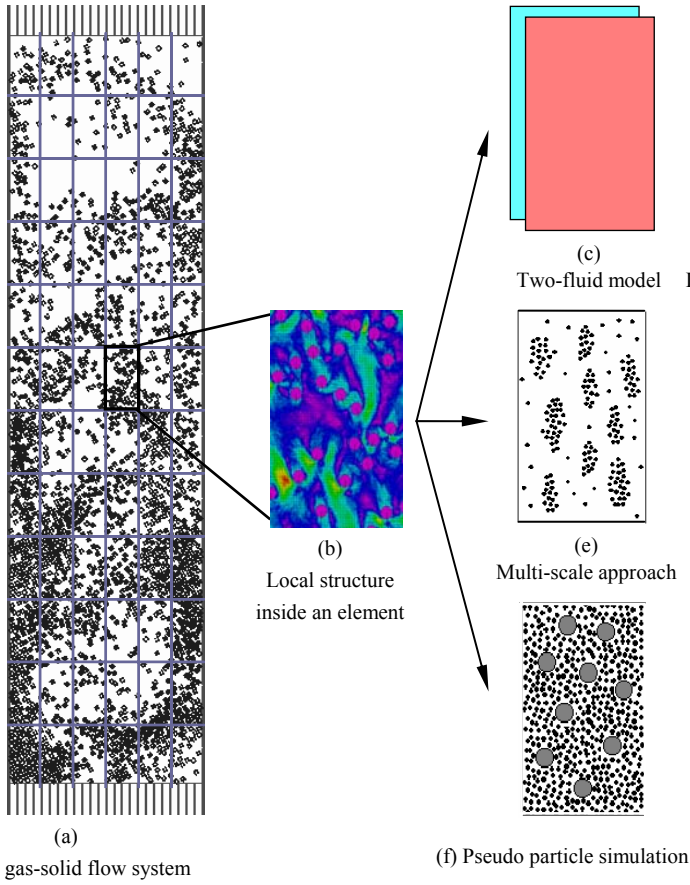


Figure 1: Comparison of various modelling approaches.

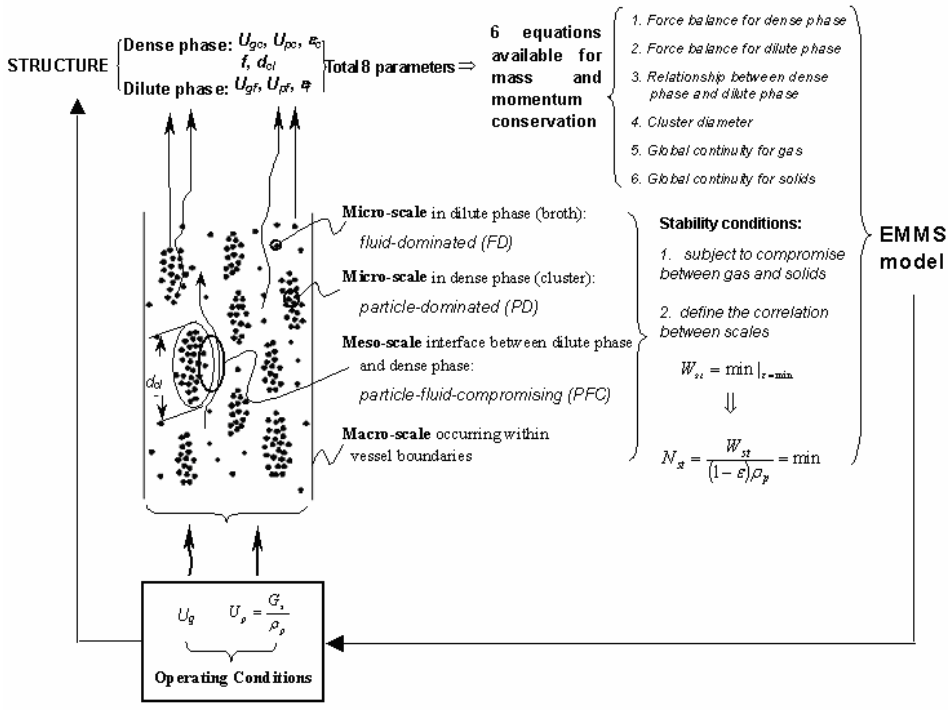


Figure 2: Dominant mechanisms and stability criteria in complex gas-solid flows (Li & Kwauk, 2003).

its prediction accuracy because the meso-scale structure heterogeneity are smoothed out and in reality multiple states of structure may exist in a local unit heterogeneity are smoothed out and in reality multiple states of structure may exist in a local unit. Then the structure-dependent transport properties and underlying dominant mechanisms can not be identified. Therefore, it is not surprising that the development of closure relations reflecting the underlying physics associated with structure heterogeneity has been recognized to be a central problem for the two-fluid modellers. Although the discrete particle model illustrated in Fig. 1(d) can trace the trajectory of each single particle, the fluid phase is calculated on the same scale as that of the two-fluid model and therefore the average treatment of the coupling of two phases cannot lead to an accurate calculation of particle trajectories.

Furthermore, the inability of the two-fluid model to simulate complex two-phase flow is not solely because of its inherent vice of average treatment of structure, but due to the incomplete understanding of the dominant mechanisms on different scales and of the ways of their coupling, which may provide the intrinsic drive to shape the multi-scale structure heterogeneity. This is further illustrated in Fig. 2 where the gas-solid system is decomposed into a solid-rich dense phase and a gas-rich dilute phase. The gas-solid interaction displays a multi-scale nature involving three totally different mechanisms (Li & Kwauk, 2003): the flow is "particle-dominated" in dense phases wherein the movement tendency of particles is realized by suppressing that of gas and accordingly the drag coefficient C_{DC} can be as high as 10^5 for a typical CFB riser in the FCC process; whereas the fluid is "gas-dominated" in dilute phases, that is, the movement tendency of gas is realized by suppressing that of particles, and the corresponding drag coefficient C_{Df} can be lower than 10^2. "Particle-gas-compromising" occurs between dilute phases and dense phases wherein the movement tendencies of neither gas nor particles can dominate the other, but has to compromise with each other, leading to the behaviour disparity between the dense phase and the dilute phase. The relevant drag coefficient C_{Di} between the dense phase and the dilute phase is even much lower than C_{Df}. The effect of heterogeneous structure on mass transfer coefficient has been demonstrated by Wang et al. (2005).

Obviously, for the average approach, these different mechanisms and corresponding drag coefficients are blurred into one another and the average drag coefficient over the specified volume can be distorted even in orders. In practice, the Wen & Yu correlation originally developed from the vessel-scale experiments of liquid-solid fluidized beds is often employed at present to calculate the drag force on cell-scale in the two-fluid modelling of heterogeneous gas-solid fast fluidized beds. This application has been questioned by researchers and is probably the key to understanding why current CFD fails to work well in simulating the dynamic behaviour of meso-scale structures such as particle clusters in the FCC/air systems, and why in many cases some parameters or correlations (say, the size of cluster or bubble, the drag coefficient) have to be adjusted empirically to fit the CFD calculation with experimental data.

Multi-scale approach

In recent years we can begin to benefit from the development of complexity science and multi-scale methodology, which assumes increasing importance in different fields and become promising approaches for characterizing complex systems of remarkable multi-scale structures. According to Li & Kwauk (2003), a general multi-scale methodology has not yet established and various methods available at present can be classified into three general categories: descriptive, correlative and variational. Compared to the other methods, the variational multi-scale method is not restricted to neighbouring scales in principle and considers the implicit interdependence between scales. The first step is to resolve the system into different scales and dominant mechanisms, each of which follows its own role and extremum tendency, though constrained by others. Then stability criteria are introduced by analysing the compromise between dominant mechanisms in the system. For the details of variational multi-scale method, the interested reader is referred to the publication of Li & Kwauk (2003), and Li et al. (2004).

However, direct application of the variational multi-scale method to complex two-phase systems is still difficult due to the following four aspects. First, the mathematical solution of the multi-object optimization problem in variational method is generally troublesome. Second, the stability criteria itself should be expressions of the new properties emerged and cannot be derived from common dynamic or statistic analysis, thereby increasing the difficulty in its formulation. For engineering problems of two-phase flows in gas-solid fluidization, these problems were overcome by using some simplified physical intuitive ways. A conceptual strategy was practiced in the energy-minimization multi-scale (EMMS) approach for the gas-solid two-phase flow in fluidization (Li & Kwauk, 1994), as illustrated in Fig. 2. The third question is how to verify the stability criteria in the EMMS model. Previously, computations were carried out for different gas-solid and liquid-solid systems by directly employing the EMMS approach without theoretical verification, and reasonable results were obtained by showing the variation of system heterogeneity and predicting the so-called choking in gas-solid fluidization (Li & Kwauk, 1994; Li et al., 1999). Recently the pseudo particle simulation was employed to provide some proofs in this regard since it has the capability of recurring the underlying mechanisms and phenomena of complex two-phase flows, which is hardly captured by experimental measurements or other numerical calculation (Li et al., 2004). The fourth difficulty is that the variational method at present describes only the multi-scale spatial structure for the steady state. To simulate the spatio-temporal evolution of multi-scale structure, a structure-oriented multi-scale simulation is developed by combining the EMMS model with traditional two-fluid models.

STRUCTURE-ORIENTED MULTI-SCALE SIMULATION

The step of structure-oriented multi-scale simulation can be constructed as follows.

Retrieving the lost structure information

As discussed previously, the heterogeneity under cell scale is neglected in current two-fluid models, so the first step is to establish a structure-oriented model to retrieve the

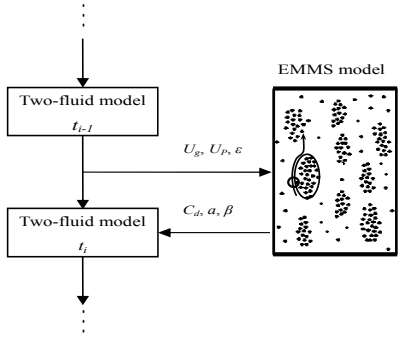
lost structure information. The physical basis of the EMMS model has been illustrated in Fig. 2, where a multi-scale analysis leads to the resolution of the structure into the gas-rich dilute phase and the particle-rich dense phase, and of the gas-solid interaction into what occurs inside dilute phase and dense phase at particle-scale respectively, as well as that between dense clusters and dilute broth at the interface of clusters. Each phase is characterized by the fluid and solids flow velocities (U_c, U_{dc}, U_f, U_{df}), and the voidage (ε_c, ε_f), while the heterogeneity is specified by the cluster diameter (d_{cl}) and dense phase fraction (f). Six dynamic constraints are found, that is, the momentum balance equations for both phases, the interphase pressure drop balance equations, the continuity equations for the fluid and the solids, and finally the cluster diameter correlation. A stability condition is introduced intuitively to close the model and correlates the dominant mechanisms and the variables from different scales. It is formulated as $N_{st}=W_{st}/\rho_p(1-\varepsilon)\rightarrow$min. which can be understood as the compromise of the two tendencies, that is, the tendency for the fluid to pass through the particle layer with least resistance ($W_{st}\rightarrow$min.) and the tendency for the solids to maintain least gravitational potential ($\varepsilon\rightarrow$min.), where N_{st} and W_{st} stand for the mass-specific and volume-specific energy consumption for suspending and transporting particles respectively, and ε represents the local average voidage. By solving this nonlinear optimization problem, the structure parameters neglected in the average approach and the corresponding gas-solid interaction at different scales can be obtained.

Calculation of the transfer parameters

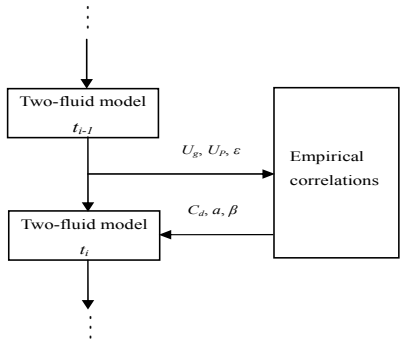
When retrieving the structure information, the transfer parameters between phases such as the average acceleration and the average drag coefficient for the particles of a cell can be calculated. The previous steady EMMS model was adapted by Yang et al. (2003, 2004) so that these transfer parameters were implicitly correlated with structure parameters through the coupling of non-linear equations and optimization process related to stability condition. In contrast to the empirical correlations employed in current two-fluid models, the transfer parameters obtained in this way embody the information of heterogeneous structure, and is therefore very important for the simulation of computational fluid dynamics. Wang & Li (2006) proposed a slightly different version of this model by differentiating the accelerations for different phases.

Spatial-temporal correlation

We are now in a position to realize the spatial-temporal correlation in the way illustrated in Fig. 3. At each time step, the local velocities and volume fraction of phases calculated from the two-fluid model are fed into the EMMS model to obtain the structure information, the average acceleration and the average drag coefficient, which are then fed back to the two-fluid model. This procedure is essentially a kind of correlative method so that a practicable way for implementation is to use an explicit coupling between different scales rather than to solve the optimization problem and non-linear equations considering the computational consumption for each cell, and hence some specific techniques have to be developed to transform the previous implicit coupling into the simplified explicit correlations without losing its physical essence. Fig. 3 compares two different couplings with the two-fluid model, that is, using the EMMS model (upper inset) and using the empirical correlations (lower inset). Since we retrieve the lost structure information by using the EMMS model, the interphase coupling can be calculated accurately compared to the empirical correlations, thereby leading to more reasonable predictions, as shown in the bottom of Fig. 4.

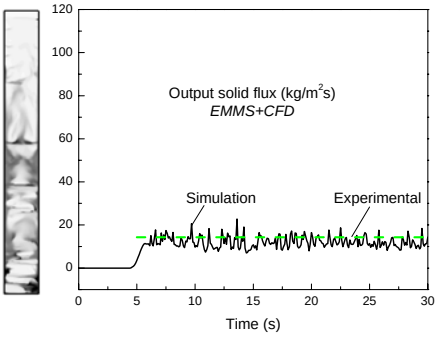


(a) Structure-oriented multi-scale simulation: EMMS+CFD



(b) Average approach: empirical correlations + CFD

Figure 3: Strategy for spatial-temporal correlation: comparison of structure-oriented multi-scale simulation with current two-fluid approach. (Yang, et al., 2003, 2004)



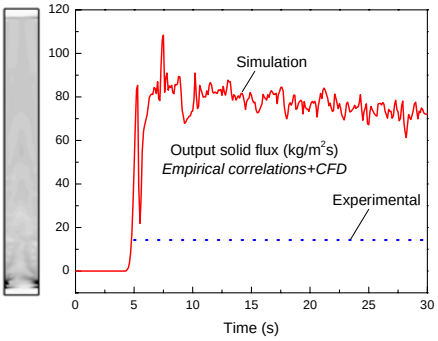


Figure 4: Comparison of results for solid distribution (left) and output solid flux (right). (Yang, et al., 2003, 2004)

It can be seen from Fig. 4 that the output solid flux predicted from the combination of the EMMS model with the two-fluid model is close to the experimental measurement, whereas the prediction from the CFX4.4 employing empirical correlations (Wen & Yu/Ergun equations) in the two-fluid model is far beyond the experimental data. Correspondingly, the meso-scale heterogeneity is clearly observed in the former approach, reflecting the unique feature of gas-solid flow. The latter approach generates only the homogeneous structure due to the overestimation of the drag coefficient (Yang et al., 2003, 2004).

APPLICATIONS

The structure-oriented multi-scale simulation has been applied in some engineering design and optimization processes such as the calculation of the gas-solid flow for a FCC riser of PetroChina and the maximizing iso-paraffins process of SinoPEC. Moreover, this strategy is recently extended to the modelling of bubble diameter for gas-liquid flows. Some important issues regarding the modelling and control of gas-solid and gas-liquid flow systems can be explained physically through the structure-oriented multi-scale simulation, as exemplified below.

Choking prediction

The choking phenomenon representing the regime transition between dilute transport and fast fluidization is a remarkable characteristic for gas-solid two-phase flow in fluidization and still far from being physically interpreted under a unified approach. However, the stability criterion enables the EMMS model to predict the variation of system heterogeneity and non-linear behaviours, thus a physical mapping of fluidization regimes can be achieved by identifying the choking as a jump change between two branches of the stable solution of the EMMS model (Ge & Li, 2002). This model is further verified in the calculation of a FCC riser of PetroChina by comparing the prediction of this model with the experimental data, the empirical correlations proposed by Xu et al. (2001), and the simulation results from the incorporation of the EMMS model into the two-fluid model (Yang, et al., 2005). In the latter simulation approach, the solid flux out of the top outlet is instantaneously monitored and then fed back to the riser via the bottom inlet instead of specifying a solid circulation rate. Calculations showed a reasonable agreement among the results of above methods and experimental data, as shown in Fig. 5. In addition, due to the consideration of the compromise of dominant mechanisms via the stability condition, the EMMS model can obtain reasonable predictions within a relatively broader range of particle properties and reactor sizes compared to empirical correlations which shows the best accuracy for some circumstances but is only suitable for a limited range.

Necessary parameters for specifying hydrodynamics of CFB risers

In spite of the extensive experimental study on the hydrodynamics of CFB risers for several decades, there exists confusion in literature as to whether gas superficial velocity U_g and solids circulation rate G_s are enough for determining the hydrodynamics of circulating fluidized bed (CFB) risers. The experimental findings of Li et al. (1988, 1998) showed that the different axial voidage profiles might prevail in a riser even under the specified U_g and G_s, and the imposing pressure ΔP_{imp} has to be considered as an important factor. ΔP_{imp} reflects the driving force feeding particles from downcomer to riser and can be changed by adjusting the solids inventory (I) in the downcomer or the state of the opening or aeration of solid flow control valve. A recent critical review and reiteration on this issue was made by Xu & Gao (2003).

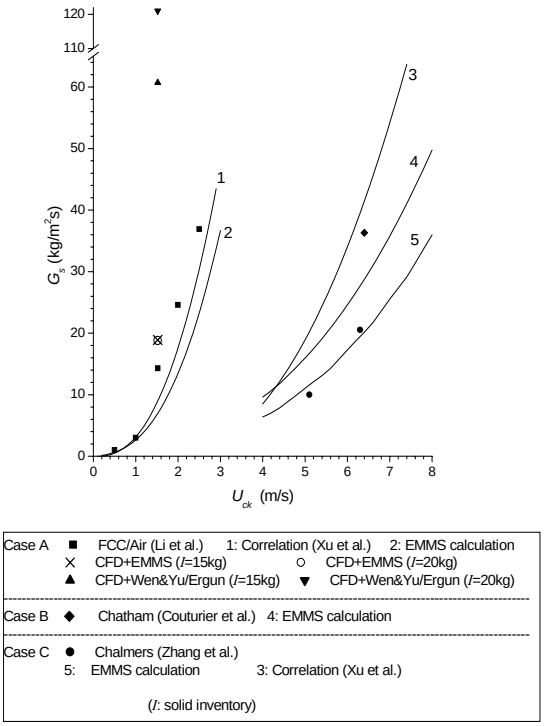


Figure 5: Comparisons of choking predictions with experiments (Ge & Li, 2002; Yang et al., 2005)

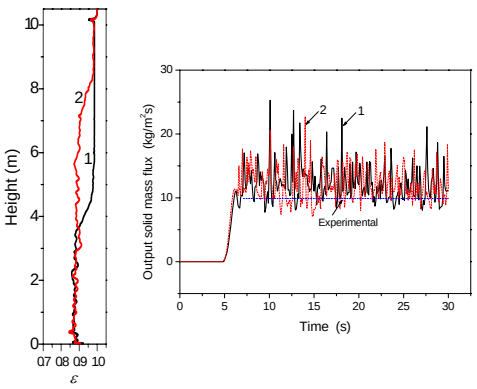


Figure 6: Simulation results of axial voidage profile (left) and output solid flux (right) (Yang et al., 2004).
1: U_g=1.52 m/s, I=15 kg; 2: U_g=1.52 m/s, I=20 kg

Apart from experimental investigation, computation based on the structure-oriented multi-scale simulation can also provide some clues in this regard, as shown in Fig. 6 (Yang et al., 2004). The hydrodynamics of a FCC riser with 10.5 m in height and 0.09 m in diameter was simulated by employing the structure-oriented multi-scale simulation. The solid flux entered into the bottom-inlet was

instantaneously updated by the monitored data of top-outlet. The different initial bed heights evaluated from the experimental solid hold-ups in the riser were preset to consider the effect of solid inventory.

Fig. 6 indicates that when the solid inventory I is increased from 15 kg (curve 1) to 20 kg (curve 2), the only difference between the two curves of axial voidage profile is the position of the inflection points, whereas both the cross-sectional voidage at the top-dilute region (ε^*) and the bottom-dense region (ε_a) are invariable. In addition, the time-averaged output solid fluxes illustrated in the right inset of Fig. 6 are almost identical, implying that the system may reach the state of the so-called saturation entrainment: the gas cannot entrain more particles out of the riser though the solid inventory (I) is increased from 15 kg to 20 kg. The riser itself seems to have the capacity of adjusting the height of its bottom-dense region to accommodate the increased solid inventory rather than to blow them off. This simulation is evidently consistent with the experimental findings of Li et al. (1988, 1998) that when the solids inventory is increased within a certain range at a given superficial gas velocity U_g, the solid circulation rate G_s remains essentially constant, and the only variation of the S-shaped voidage profile is the movement of the inflection point. In this sense, this structure-oriented multi-scale simulation furnishes another proof for the conclusion that it is inadequate to determine the hydrodynamics of CFB risers by specifying only U_g and G_s.

Wang & Li (2006) attempted to reiterate this simulation by employing their model and provided more results for this matter. Fig. 7(a) shows the existence of three kinds of flow patterns, that is, dilute transport, and axially non-uniform flow and dense transport, as designated by Li et al. (1988, 1998, 1999) and Xu & Gao (2003). The axially non-uniform flow occurring at I=15 kg exhibits an S-shaped voidage profile and the corresponding solid flux is 14.3 kg/m^{3}s measured in experiment and 12.6 kg/m^{3}s monitored in simulation, whereas the dense transport flow pattern occurring at I=35 kg and the dilute transport pattern occurring at I=7.6 kg indicate two almost vertical profiles for axial voidage. In these cases, the solid flux G_s increases to 26.6 kg/m^{3}s in experiment and 26.9 kg/m^{3}s in simulation for the dense transport, or decreases to 10.0 kg/m^{3}s in simulation for the dilute transport.

Summarizing the results in Fig. 6 and Fig. 7 (a), we can arrive at a conclusion that when the solid inventory (I) falls within a certain range, the G_s is invariable with the variation of the solid inventory and therefore cannot be treated as an independent parameter for the determination of hydrodynamics of a CFB riser. In this case, the solid inventory (I) or imposing pressure ΔP_{imp} should be considered as another necessary parameter. On the other hand, G_s can be varied when the solid inventory is outside this range, and hence becomes an independent variable.

Wang & Li (2006) also tries to simulate the ability of the system to tolerate the variation of solid inventory within a certain range while holding a constant value of G_s, as shown in Fig. 7(b). Compared to the dense transport flow occurring at I=35 kg, if the initial bed height H_0 is deliberately decreased from 2.8m to 1.2m (corresponding to the decrease of the solid inventory from 35 kg to 18.16 kg) and holding the original G_s (26.6 kg/m^{2}s) of the dense transport flow through the EMMS-based drag model, the

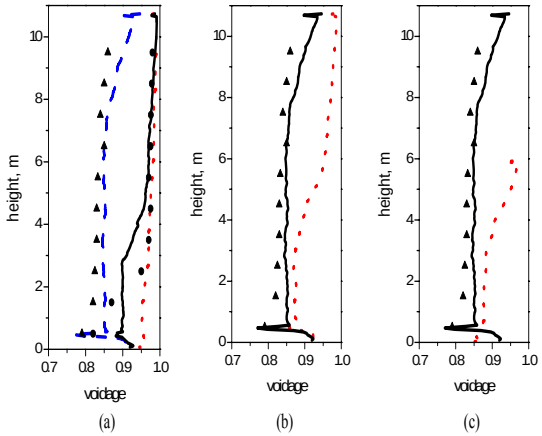
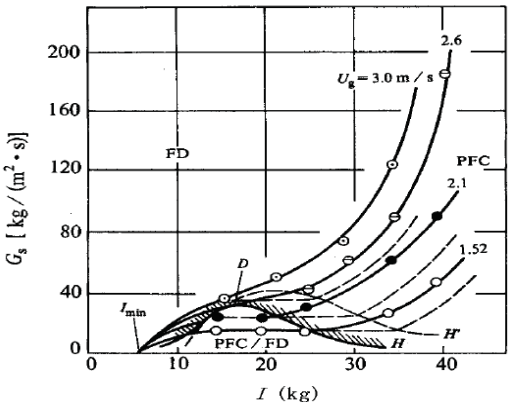


Figure 7: Computed axial profile of voidage under different conditions and U_{g0} =1.52m/s. (Wang & Li, 2006)
(a): solid line and • : H_0=0.9 m (I=15 kg);
dash line and ▲: H_0=2.8m (I=35 kg)
dot line: H_0=0.2m (I=7.6 kg)
(b): solid line: H_0=2.8m (I=35 kg)
dot line: H_0=1.2m (I=18.16 kg)
(c): solid line: 10.5m high riser; dot line: 6.0m high riser; ▲: exp. Data

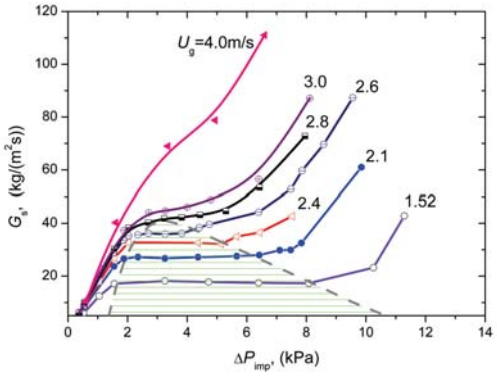
monitored time-averaged output solid flux falls to 12.5 kg/m^{2}s and the axial voidage profile shifts to an S-shaped curve, implying that the axially non-uniform flow prevails in this case.

We may expect that this issue could be further clarified in this way. First the simulation is carried out by using the cycling configuration for solid circulation flux and an initial bed height corresponding to the solid inventory for axially non-uniform flow. An S-shaped axial voidage profile with an inflection point should be obtained in this case. Then during the simulation, the G_s at inlet is deliberately increased to a value which corresponds to the dense transport or decreased to a value corresponding to the dilute transport (this can be achieved by adjusting the opening of the solid control valve connecting the riser and downcomer in experiments). Hold this changed G_s at inlet for a certain time interval and then recover the previous cycling configuration for solid flux. Under such a circumstance, the old pressure balance between riser and downcomer should be destroyed and one may well suppose that the flow pattern would shift to the dense transport or the dilute transport. However, in reality, we could find, as described by Li and Kwauk (1994), that the output solid flux is still equal to the previous solid saturation carrying rate K^* of the axially non-uniform flow, whereas the inflection point and the height of the bottom-dense region may increase or decrease to adapt the new situation due to the external variation of solid flux. Meanwhile, corresponding to the variation of solid inventory in the riser, the solid inventory in downcomer will decrease or increase. This will then recover G_s at inlet to the original value of the axially non-uniform flow. At last, the inflection point move to a new position and a new pressure balance be established between the riser and the downcomer.

Fig. 7(c) shows the influence of riser height on the occurrence of S-shaped profile. A non-cycling case is set, namely, specifying G_s directly at the bottom-inlet, other than the cycling configuration in previous simulations. Compared to the vodage profile of the dense transport flow for the riser of 10.5 m height, an S-shaped profile is observed for the riser of 6.0 m height but with different asymptotic voidage in the top and bottom regions than the previous axially non-uniform flow.



(a)



(b)

Figure 8: Relationship among U_g, G_s and ΔP_{imp} for FCC/air system.
(a). Experimental data by Li & Kwauk (1994).
(b). Simulation by Wang & Li (2006).

Fig. 8 compares the diagram of simulated flow regime with that obtained from experimental measurements of Li & Kwauk (1994). Both figures show the existence of three different operating modes of the CFB riser in terms of the relationship among U_g, G_s and ΔP_{imp}. The zone termed FD (fluid-dominated) toward the left denotes the dilute transport regime where $G_s < K^*$, whereas the zone termed PFC (particle-fluid-compromising) toward the right represents the dense regime with $G_s > K^*$. The saddle area between them stands for the transition regime characterized by the coexistence of a dense bottom and dilute top, or in other words an S-shaped voidage profile, as illustrated in Fig. 6 and Fig. 7. The solid flux G_s in this regime is almost invariable and equal to the saturation carrying rate K^*. It is noticed that the range of ΔP_{imp} or I for holding a constant G_s decreases with the increase of gas velocity U_g. At last, beyond the summit (point D) of the saddle area, the transition between the dilute transport and dense transport is smooth without the middle plateau, implying that the two regimes are indistinguishable in the sense of the solid axial concentration profile.

Based on these discussions, we can conclude that U_g and G_s are insufficient to determine the hydrodynamics of CFB risers both for experiments and simulation. It should be noticed that Xu & Gao (2003) provided an analysis to explain the confusion on this matter in literature. In addition, the effect of the imposing pressure ΔP_{imp} or solid inventory I in current simulation is realized through the preset of initial bed height evaluated from the experimental solid hold-up in the riser. This configuration can be further improved by directly specifying the imposing pressure ΔP_{imp} near the bottom-inlet of the riser, say, evaluating ΔP_{imp} from the solid inventory in the whole CFB system and the pressure drop of solid control valve in some way.

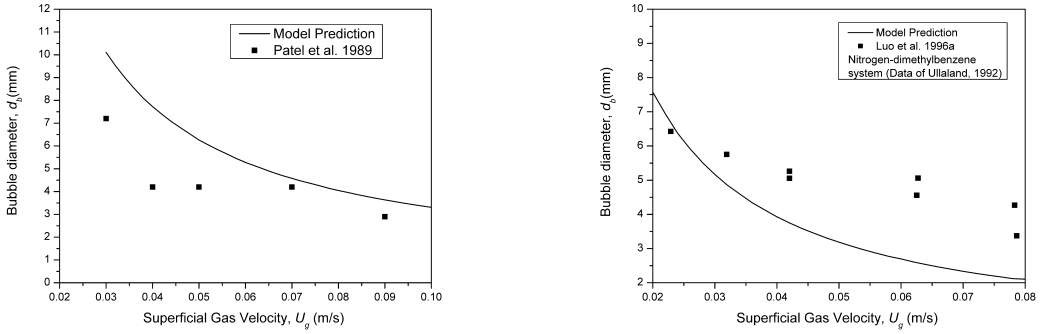
Recently, the coexistence of bottom dense and top dilute regions was also simulated by Gidaspow and coworkers (Jiradilok, et al., 2006).

DETERMINATION OF BUBBLE SIZES FOR GAS-LIQUID BUBBLY FLOWS

Bubble size is a key factor affecting the hydrodynamics and transport characteristics of bubble column reactors. However, the mean bubble diameter has to be assumed a priori in current CFD simulation by employing some empirical correlations, or adjusted by a trial-and-error procedure to fit the CFD model prediction with experimental data as pointed out by Chen et al. (2005). Incorporating the population balance model (PBM) into the CFD model may provide another choice to consider the effect of the size distribution of bubbles. Nevertheless, besides the increase of computation consumption, how to describe the multiple mechanisms for bubble breakup and coalescence is still a formidable problem for this strategy. Based on the similarity between gas-liquid bubbly flow and gas-solid fluidized bed systems identified by some researchers (Bi & Grace, 1996; Ellenberger & Krishna, 1994), the EMMS model is recently extended to determine the size of bubbles for gas-liquid flows (Zhao et al., 2006). Bubble diameter is regarded as the characteristic size of meso-scale structure which results from the compromising between the dominant mechanisms in the gas-liquid system. A multi-scale analysis of interactions between eddies and bubbles are performed, and the energy dissipated through viscous dissipation in turbulent liquid phase and that through bubble oscillation are found to be the competing mechanisms determining the bubble diameter. Each of these two mechanisms can be characterized as the minimization of an energy dissipation term to achieve a steady state. As a result, a stability criterion based on their joint effects is proposed to delineate their compromise.

Fig. 9 shows the simulated bubble diameters for different systems. The prediction is in qualitative agreement with some experiment measurements in literature though it is not necessarily better. It should be noticed that the trends of the variation of bubble diameters are found to be variable

in experimental reports; therefore, we cannot expect an exact



(a) (b)

Figure 9: The influence of superficial gas velocity on bubble diameter (Zhao et al., 2006)
(a) air-water system (b) nitrogen-dimethylbenzene system

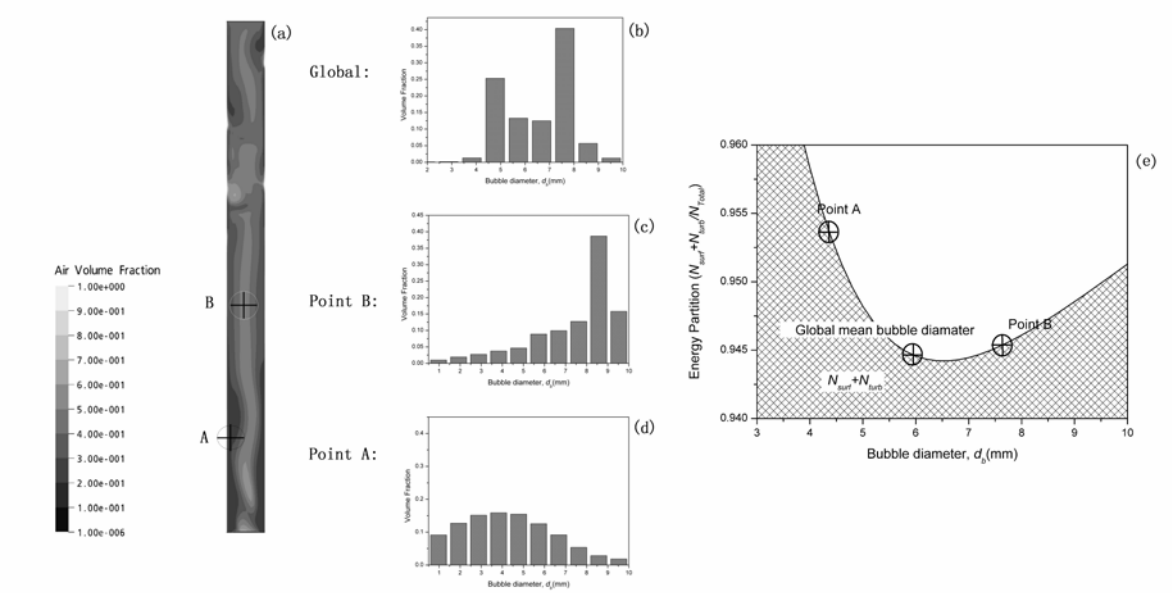


Figure 10: Bubble size distribution in a bubble column and related energy dissipation (Zhao et al., 2006)

coincidence of simulation with experimental reports since this model does not consider the size distribution in the axial and the radial directions. Nonetheless, the "mean bubble diameter" is essentially an intermediate parameter which is of critical importance for calculating the interphase momentum transfer in CFD models. The bubble diameter calculated from this model embodies the information of the multi-scale interaction of eddies and bubbles together with the compromise of dominant mechanisms for bubble break-up and coalescence. Therefore it provides a useful closure for the term of interphase momentum transfer in CFD models.

The stability criterion of the model is further demonstrated by a CFD simulation incorporating with a population balance model for a bubble column reactor. According to the results of this model, the smaller bubbles are mainly spherical and dominated by surface tension to achieve lower N_{surf} (Rate of energy dissipation per unit mass due to bubble oscillation), while the larger bubbles can interact with the turbulent flow to achieve lower N_{turb} (Rate of energy dissipation per unit mass in turbulent liquid phase). The bi-modal bubble size distribution displayed in inset "b" supplies an evidence of the alternative dominance of the two mechanisms for the global system. On the other hand, we may notice from inset "c" and inset "d" that points B and A are mainly composed of small and large bubbles, respectively and hence the local flow at points B and A is dominated by surface tension and turbulence, respectively. This spatio-temporal alternating can provide the way of compromise on a much larger scale. Fig. 10(e) indicates that a minimum of N_{st}, which represents the summation of N_{surf} and N_{turb}, can be reached in the whole bubble column reactor. In summary, the fact that a similar stability condition can also be found in gas-liquid systems and give some reasonable predictions is of significance to the fundamentals of multi-phase flow in that the stability criterion presented in the EMMS model may be a general relevance.

CONCLUSIONS AND PROSPECTS

Three different kinds of approaches can be employed to simulate the complex two-phase flow in process

engineering, viz., discrete approach, average approach and multi-scale approach. The chief advantages of the multi-scale approach over the average approach are the multi-scale resolution of the heterogeneous structure and of the interaction between phases together with the establishment of the stability criteria reflecting the compromise between dominant mechanisms. Incorporation of energy-minimization multi-scale (EMMS) approach with traditional CFD models leads to the structure-oriented multi-scale simulation, which has the ability of describing the spatial-temporal coupling and variation of multi-scale structure. Though this modelling strategy is at its preliminary stage, computations for gas-solid flows in fluidization indicates the improvement in predicting the solids entrainment rate and the meso-scale structure involving clusters or strands in contrast to the homogeneous structure simulated from the average approach. Furthermore, this modelling strategy can well predict the choking phenomena and clarify the issue concerning the necessary parameters for specifying the hydrodynamics of CFB risers. It is also extended to determine the bubble size for bubble column reactors.

We may expect some further extension for the structure-oriented multi-scale simulation in future. First, one of the advantages of the energy-minimization multi-scale (EMMS) approach is its ability to describe the sub-grid structure and interaction for different phases. But only the cell-averaged parameters are required in current two-fluid models, which may offset this advantage to some extent. Separation of meso-scale conservation equations may be a practicable scheme for further improvement on this matter. Second, as we discussed previously, the current structure-oriented multi-scale simulation involves the incorporation of the EMMS model with the two-fluid model, which is in essence a kind of correlative method. Therefore some specific techniques have to be developed to transform the previous implicit coupling into some simplified explicit correlations for efficiency and technical considerations. A more essential way may lies in the direct incorporation of the stability criteria into the phase-specific conservation equations in some way.

Anyway, with the development of the structure-oriented multi-scale simulation, it would attract more and more attentions and contribute substantially to the progress of process engineering and complexity science.

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