Structure heterogeneity, regime multiplicity and nonlinear behavior in particle-fluid systems

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STRUCTURE HETEROGENEITY, REGIME MULTIPLICITY AND NONLINEAR BEHAVIOR IN PARTICLE-FLUID SYSTEMS

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Abstract - This paper is devoted to the understanding of the structure heterogeneity, regime multiplicity and behavior nonlinearity of particle-fluid systems which give rise to predominant difficulties in their modeling and scale-up. Possible approaches are explored for dealing with these aspects of complexities. Two types of nonlinearity are recognized in particle-fluid systems — intrinsic, as related directly to particle-fluid interaction, and secondary, as related to particle geometric and system scale-up. It is indicated that multiple resolution with respect to energy, process, movement and structure may be a promising approach to coping with intrinsic nonlinearity, though understanding of secondary nonlinearity calls for more specific analysis of the effects of external factors on intrinsic nonlinearity.

INTRODUCTION

Particle-fluid two-phase flow is a common phenomenon in nature. In the past decades, much attention has been paid to the quantification of particle-fluid interaction and the predictive design of reactors. However, understanding of such a system is still limited due to its complexity, and reactor design is still based on trial and error approaches (Reh, 1995).

Complexity of particle-fluid systems mainly results from *structure heterogeneity* showing combinations of a particle-rich dense phase and a fluid-rich dilute phase, and *regime multiplicity* referring to a spectrum of inflective or jump changes of flow structure. In addition, it is far from easy to transfer research results in the laboratory to industry where particles are likely multisized and irregularly shaped, and system dimensions could be several orders of that of laboratory systems. All these difficulties are related to the nonlinearity of the system which forms the main barrier to understanding and quantifying particle-fluid systems. Such nonlinearity could be *intrinsic* or *secondary*. This paper focuses on exploring possible approaches to deal with such a complicated problem.

INTRINSIC NONLINEARITY

Intrinsic nonlinearity of particle-fluid two-phase flow is attributed to *particle-fluid interaction*, and provides the key to understanding structure heterogeneity and regime multiplicity.

Regime multiplicity and Bifurcations

Concurrent-up particle-fluid two-phase flow operates in the fixed bed when fluid velocity U_g is lower than minimum fluidization velocity U_{mf} . With increasing fluid velocity, the system approaches the state of the minimum fluidization at U_{mf} and expands homogeneously. Then, at somewhat higher fluid velocity U_{mb} , the system suddenly segregates into a dense phase (emulsion phase) and a dilute phase (bubble phase). The system continues to expand heterogeneously thereafter with further increase in fluid velocity until dilute transport occurs, also suddenly, at the so-called “choking” velocity U_{pt} . The occurrence of such fluidization regime transitions correspond to the bifurcation phenomenon in thermodynamics (Li et al., 1995).

In fact, the relationship between fluid velocity and the generated pressure gradient for homogeneous particle-fluid fluidization within the velocity range between U_{mf} and U_{mb} with fine particles ($Re_p < 2$) can be expressed as

$$U_g = \frac{d_p^2 \epsilon^{4.7}}{18(1 - \epsilon)\mu_f} \cdot \frac{\Delta P}{\Delta L} \quad (1)$$

indicating that $\frac{\Delta P}{\Delta L}$ responds to U_g nonlinearly due to the dependence of ε on U_g , unless the system operates in the fixed bed regime in which ε keeps constant. This feature is verified by experiments in Figure 1, showing the change of $\frac{\Delta P}{\Delta L}$ with increasing U_g for FCC/air system ($\rho_p = 930 \text{ kg/m}^3$, $d_p = 54 \mu\text{m}$) measured with a pressure transducer in a fluidized bed of 90 mm ID. In the fixed bed regime, $\frac{\Delta P}{\Delta L}$ is related to U_g linearly. Beyond the minimum fluidization velocity U_{mf} , bed voidage starts to increase, leading to nonlinearity in the system according to Equation (1). With increasing bed expansion, the effect of nonlinearity is intensified, and reaches a critical extent at minimum bubbling velocity U_{mb} , at which the uniform bed structure is disrupted due to the self-organization of particles and the fluid, resulting in the formation of a dissipative structure in the system characterized by ordered behavior as will be discussed below. This transition from uniform expansion to bubbling fluidization is physically referred to as a nonequilibrium phase transition or the first bifurcation. The dissipative structure in the bubbling regime stabilizes at maximum energy dissipation according to Li and Kwauk (1994), which is again suddenly destroyed at another higher critical

Figure 1. Regimes and bifurcations of particle-fluid systems.

velocity U_{pt} , at which the fluid becomes capable of dominating the movement of particles, and the self-organization of particles is therefore suppressed, resulting in a uniform structure in the system, as indicated by voidage measurement with an optical probe shown in the subfigures. Such a jump change is called the second bifurcation in terms of thermodynamics, and "choking" in terms of engineering. This newly formed regime operates in dilute transport, stabilizing at minimum energy dissipation (Li and Kwauk, 1994).

In summary, regime multiplicity in a particle-fluid system may be physically attributed to bifurcations in the system each of which corresponds to a critical point at which the stability condition of the system changes suddenly. Further details are discussed by Li *et al.* (1995).

Structure Heterogeneity and Disordered Behavior

Flow structure in particle-fluid systems shows complicated changes in the whole regime spectrum as illustrated in Figure 2, which is based on measurements, by using an optical probe having linear response to particle concentration, in a circulating fluidized bed of 90 mm ID with FCC particles fluidized with air. This figure shows that the two-phase structure exists in the whole regime spectrum from bubbling to fast fluidization, resulting from the self-organization of both the fluid and the particles, that is, self-organization of the fluid leading to the formation of the dilute phase, while that of the particles, to the appearance of the dense phase. Bed voidages in these two distinct phases are essentially constant, and tend to extreme values of unity for the dilute phase and minimum fluidization voidage ε_{mf} for the dense phase.

This type of behavior can also be demonstrated by the bifurcation diagram of voidage ε versus fluid velocity U_g , as shown in Figure 3. This figure indicates that the flow structure of the system is characterized not only by such extreme behavior, showing the highest probabilities of the occurrence of the dense phase with voidage ε_{mf} and the dilute phase with voidage 1.0, but also by highly irregular behavior indicated by the

Figure 2. Time series of voidage changes in different regimes of particle-fluid systems.

Figure 3. Bifurcation diagram of local voidage measured by an optical probe.

voidages covering the intermediate range between ϵ_{mf} and 1.0. In the fixed bed regime, bed voidage is consistently equal to ϵ_{mf} . With the occurrence of the first bifurcation, an ordered two-phase structure appears, resulting in the alternating occurrence of the two extreme voidages, ϵ_{mf} and 1.0. With increasing fluid velocity, irregular disturbances show up, and are gradually intensified, as indicated by increasing probability of voidages between these two extreme values. As soon as the second bifurcation occurs at the critical velocity U_{pt} , corresponding to the saturation carrying capacity, this extremum behavior no longer persists, and a narrowing of the distribution of voidages to a very limited range is found. It might well be possible that the dynamic behavior in each of these regimes can be further resolved into a relatively regular component with low frequency and big magnitude corresponding to meso-scale fluctuations of flow structure (e.g. bubbles and clusters) and a more irregular component with high frequency and small magnitude corresponding to micro-scale changes of flow structure. Such a resolution of dynamic behavior is an important subject to be studied, which is expected to contribute to the quantification of dynamic behavior.

Multi-Scale Structure and Behavior

Because of the two-phase heterogeneous structure in particle-fluid systems, particle-fluid interactions are not identical for individual particles, resulting in different behavior at different scales. Therefore, analysis based on average parameters, as is commonly done, is not sufficient for characterizing such a complicated phenomenon. Figure 4 shows different patterns of particle concentration at different scales which were simultaneously measured. Figure 4a shows the time series of particle concentration measured by using a Phase-Doppler Particle Analyzer (PDPA) system with a measurement volume of micro-meter scale, Figure 4b using an optical probe with a measurement volume of milli-meter scale, and Figure 4c using a pressure transducer across a measurement section of centi-meter scale. It is observed that significantly different dynamic characteristics prevail on different scales and therefore multi-scale analysis is necessary. Visual observation already reveals a clear difference

between the time series in Figure 4. Further analysis is needed for quantifying such a difference.

Approaches to Deal with Intrinsic Nonlinearity

All the complexities mentioned above are related to intrinsic nonlinearity, as a result of the mutually *compromising/constraining* actions between particles and fluid, which are unique for particle-fluid two-phase systems as distinguished from single-phase flow, and therefore should be the focus in this field.

Particle-fluid systems can be considered to consist of two interpenetrating media with different dimensions and densities, each of which possesses its own tendency of individual movement, that is, particles tend to look for the lowest potential energy, while the fluid always seeks paths with the lowest resistance to flow. With increasing dominance of the

fluid over particles, a particle-fluid system can operate in *particle-dominating*, in *particle-fluid-compromising*, and in *fluid-dominating regime* in sequence (Li et al., 1992). When neither the fluid nor the particles can dominate the system alone, they have not only to compromise with each other in realizing their respective movement tendencies, leading to ordered and extremum behavior, but also to constrain each other in responding to conservation conditions, resulting in disordered and irregular behavior.

The above analysis indicates the feasibility of system resolution with respect to process, movement and structure. In addition, resolution of energy consumption in particle-fluid systems is also essential (Li et al., 1988). The total energy consumption with respect to unit mass of particles in unit cross-sectional area normal to the direction of flow can be expressed as

Figure 4. Different dynamic behavior at different scales.

$$N_T = U_g g \left(\frac{\rho_p - \rho_f}{\rho_p} \right) \quad (2)$$

in which the reversible portion for transporting particles is

$$N_t = \frac{G_s g}{(1 - \epsilon) \rho_p} \quad (3)$$

Therefore, the total dissipated energy is

$$N_{dis} = N_T - N_t \quad (4)$$

It was elucidated that $N_t \rightarrow \text{extrema}$: *maximum* in the dilute transport regime and *minimum* in the fluidization regime (Li, et al., 1993). From the constancy of N_T at specified U_g , extremum of N_{dis} can be deduced. That is, the nonextremal total energy is resolved into its extremal reversible and irreversible components. Therefore, it can be envisaged that multiple resolution will be a promising approach to understanding the intrinsic nonlinearity in particle-fluid systems.

SECONDARY NONLINEARITY

Intrinsic nonlinearity complicates the understanding of particle-fluid interactions, which is the basis for modeling particle-fluid systems. However, there is another aspect of nonlinearity related to external factors, here called secondary nonlinearity, giving rise to difficulties in employing established models in engineering practice. This paper is intended to pay attention to two aspects of secondary nonlinearity caused by particle geometric properties and scale-up effect.

Particle Size Distribution

Particles in particle-fluid two-phase flow are usually multi-sized. Mean diameters are often used for defining the dimension of such multisized particles, among which the so-called surface to volume mean diameter

$$\bar{d}_s = \left[\sum_{i=1}^M (x_i / d_i) \right]^{-1} \quad (5)$$

is most common. This is however based only on geometric factors, and is inadequate to characterize the dimension of multisized particles due to the nonlinear response of particle-fluid interaction to particle diameter. Particle-fluid interaction must be included in the definition of mean diameter.

In principle, the mean diameter of multisized particles should satisfy the equivalence between multisized particles and monosized particles, that is, a reasonable mean diameter has to be deduced from the equivalence involved. For instance, mean diameter for calculating the drag force in multisized particle-fluid system must be subject to the following equivalence

$$\bar{C}_D \bar{n} \frac{\pi \bar{d}^2}{4} \frac{\rho_f U_g^2}{2} = \sum_{i=1}^M C_{Di} n_i \frac{\pi d_i^2}{4} \frac{\rho_f U_g^2}{2} \quad (6)$$

from which we can deduce

$$\bar{d} = \bar{C}_D / \sum_{i=1}^M C_{Di} \cdot x_i / d_i \quad (7)$$

where $\bar{C}_D$ is the drag coefficient based on $\bar{d}$. It is indicated that the mean diameter of multisized particles for calculating the drag force is related not only to the size distribution of particles, but also to parameters defining the drag coefficient. Obviously, the mean diameter defined above satisfies only the equivalence of drag force. For calculating other processes such as heat transfer, chemical reaction etc., different mean diameters have to be defined. Unfortunately, such a problem has not received sufficient study.

Figure 5. Change of mean diameter of multisized particles.

From Eq. (6), the mean diameter for a specified size distribution for glass beads in air ($d_1=7.26\text{mm}$, $d_2=4.26\text{mm}$, $d_3=1.48\text{mm}$, and $x_1=22\%$, $x_2=33\%$, $x_3=45\%$) has been calculated, as shown in Figure 5. It is shown that the mean diameter is not constant, as usually considered, but changes from a minimum value equal to

$$\bar{d}_{min} = \left(\sum_{i=1}^M x_i / d_i^2 \right)^{-1/2} \quad (8)$$

for $Re_p < 2$ to a maximum value

$$\bar{d}_{max} = \left(\sum_{i=1}^M x_i / d_i \right)^{-1} \quad (9)$$

for $Re_p > 1000$. For these two extreme cases, the drag force is proportional to particle diameter and to its square, respectively, while in the range between these two cases, drag force responds to particle diameter nonlinearly, giving rise to a challenging problem in this field.

Irregular shape of particles causes even more complicated nonlinearity in particle-fluid systems, which also calls for study.

Scale-up

Because of the prevailing nonlinearity in particle-fluid systems, the traditional Buckingham π -Theorem based on superficial parameters alone is not sufficient for defining the similarity of particle-fluid systems. Figure 6 shows such an insufficiency. In addition to geometric similarity, dimensionless groups can be deduced from

Figure 6. Insufficiency of the π -Theorem due to bifurcations.

the π -Theorem, that is, Re_p for fixed bed; $Re_p, Fr, \rho_p / \rho_f$ and $U_g \rho_f / G_s$ for particle-fluid suspension including fluidization and transport. However, stability conditions ($N_{dis} = max$ for fluidization; $N_{dis} = min$ for transport) and bifurcations (at U_{mf} and U_{pt}) are not included in these groups, which also dominate the similarity rule of systems.

Recent study (Li et al., 1995) indicated that stability condition $N_{dis} = max$ affects significantly the similarity rule since it leads to a two-phase structure with an emulsion phase in which Re_p and Fr become almost constant, and can therefore be eliminated from the similarity rule. On the other hand, minimum fluidization velocity U_{mf} must be considered, resulting in the inclusion of U_{mf} / U_g in the similarity rule. After the second bifurcation, Re_p and Fr are re-involved in the similarity rule, and the two reference parameters U_{pt} and K^*

(saturation carrying capacity) must be considered due to the switch of stability condition from $N_{dis} = \max$ to $N_{dis} = \min$. It can therefore be concluded that bifurcations are of paramount significance to the similarity of particle-fluid systems. On the other hand, the change of system dimension may also cause nonlinearity and bifurcation, which is another challenging problem in scaling-up chemical reactors. Due to the nonlinear response of reactor performance to scale of the unit, the performance of a commercial unit cannot be fully predicted from laboratory and pilot experimental results. Such a prediction becomes absolutely impossible when bifurcation occurs. Therefore, we can conclude that the underlying solution to scale-up of chemical reactors calls for understanding of nonlinear behavior in particle-fluid two-phase systems (see also Schouten *et al.*, 1996).

NOTATION

C_D	particle drag coefficient
$\bar{C}_D$	mean C_D with respect to $\bar{d}$
d_p	particle diameter
$\bar{d}_s$	volume to surface mean diameter
$\bar{d}$	mean diameter defined by Eq. (6)
Fr	Froude number
g	gravity acceleration
G_s	solid flow rate
K^*	saturation carrying capacity
n	number density of particles
$\bar{n}$	mean value of n
N_T	total energy consumption with respect to unit mass of particles
N_t	energy consumption for transport with respect to unit mass of particles
N_{dis}	total dissipated energy with respect to unit mass of particles
Re_p	Reynolds number of particles
t	time
U_g	superficial fluid velocity
U_t	terminal velocity of particles
U_{mf}	minimum fluidization velocity
U_{pt}	minimum transport velocity corresponding to K^*
x_i	mass fraction of particles with diameter d_i
ρ_p	particle density
ρ_f	fluid density
ε_{mf}	voidage at minimum fluidization
ε	bed voidage

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