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Focusing on the meso-scales of multi-scale phenomena—In search for a new paradigm in chemical engineering

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ABSTRACT

To celebrate the 90th birthday of Professor Mooson Kwauk, who supervised the multi-scale research at this Institute in the last three decades, we dedicate this paper outlining our thoughts on this subject accumulated from our previous studies. In the process of developing, improving and extending the energy-minimization multi-scale (EMMS) method, we have gradually recognized that meso-scales are critical to the understanding of the different kinds of multi-scale structures and systems. It is a common challenge not only for chemical engineering but also for almost all disciplines of science and engineering, due to its importance in bridging micro- and macro-behaviors and in displaying complexity and diversity. It is believed that there may exist a common law behind meso-scales of different problems, possibly even in different fields. Therefore, a breakthrough in the understanding of meso-scales will help materialize a revolutionary progress, with respect to modeling, computation and application.

1. Meso-scales are a common challenge for understanding various multi-scale phenomena. Micro-mechanisms and macro-behavior can be correlated only when the meso-scales are physically understood.

For instance, turbulence is one of the few unsolved problems in classical physics (Feynman, Leighton, & Sands, 1963), which by itself is a typical meso-scale problem. At the micro-scale, we know very well the behaviors of fluid molecules and their interactions from statistical physics; at the macro-scale, fluid properties such as viscosity, density and average velocity are easy to measure. However, we do not have much knowledge on what happens at the meso-scale where turbulence is triggered from laminar flow. In fact, better understanding of many problems in both science and technology is more often than not blocked at the respective meso-scales (Li & Kwauk, 2003; Ge, Wang, Ren, & Li, 2008).

Both physical and life systems feature a multi-level hierarchy, showing multi-scale natures at each level, as shown in Fig. 1. Although the scientific problems faced in these systems are totally different, and have been studied within different fields, there is a common recognition that all boundary scales (both micro and macro) are known quite well, except the meso-scale, which has been a challenge to all respective fields (Li, Ge, & Kwauk, 2009). In fact, the compromise between dominant mechanisms at this scale leads to the so-called "complexity" and "diversity", and is believed to be the source of dynamic heterogeneity, coexistence of order and disorder and non-linearity.

Take hydroxyapatite for instance at the material level, as shown in Fig. 2a. It is a kind of material with the same well-known molecular composition and structure which is self-assembled in both human teeth and bones, and many more morphologies at meso-scale can be observed under different conditions. However, we do not know how to manipulate these meso-scale structures to produce different functional materials for different applications.

At the reactor level, as shown in Fig. 2b, chemical engineers have obtained knowledge about the global behaviors of a reactor and micro-phenomena around a single particle (available even from a textbook). However, we have learned very little about the meso-scale clustering phenomena, which are critical for mass transfer and reactions, as well as for determining the performance of reactor to a large extent.

2. Recent progresses in different fields have indicated that a common mechanism dominating meso-scale structures may exist for different systems, as being said, the compromise among the dominant mechanisms in complex systems has led to the emergence of meso-scale structures and defined the stability conditions of complex systems.

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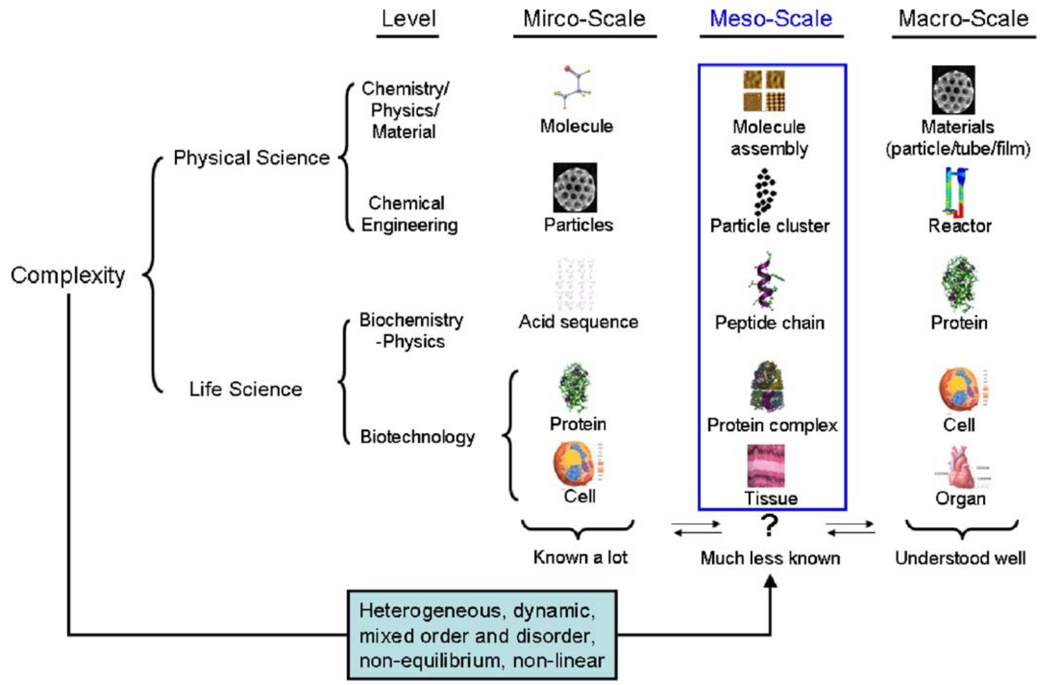

Fig. 1. Multi-level hierarchy and multi-scale natures of physical and life systems.

In gas–solids fluidization, for example, the meso-scale structures in forms of bubbles or clusters reflect the compromise between the gas-flow domination and solids-flow domination (Li & Kwauk, 1994). As shown in Fig. 3a, when a gas–solid fluidized bed is dominated by gas flow, as can be observed at high gas velocity beyond the transport velocity, the solids shall be subject to flow distribution and shall be pneumatically transported without distinct aggregation (i.e., $W_{st} \to \min$, W_{st} denotes volume-specific energy consumption for suspending and transporting particles (W/m^3)). When the gas flow is weak such that the solid particles cannot be suspended by the gas flow drag, the packed state of solid particles dominates the bed (i.e., $\varepsilon \to \min$, ε denotes voidage). Between the flow patterns at these two extremes, the tendency of gas passing through particles with least resistance (i.e., $W_{st} \to \min$) compromises with the tendency of the particles maintaining least gravitational potential (i.e., $\varepsilon \to \min$), thus resulting in $N_{st} \to \min$. The meso-scale structures originate, accordingly, from this compromise by satisfying gas dominance and solids dominance alternately with respect to space and time (here N_{st} denotes mass-specific energy consumption for suspending and transporting particles (W/kg), and $N_{st} = W_{st}/\rho_p(1-\varepsilon)$). Such compromise featuring the EMMS model (Li & Kwauk, 1994, 2003) has been verified in micro-scale simulations using pseudo-particle modeling (Li, Zhang, Ge, & Liu, 2004). At the micro-scale, the dominant mechanisms are presented alternately, and the stability criterion N_{st} is fluctuating, displaying no extremum tendency. At the meso-scale, the compromise between the dominant mechanisms gives the stability condition ($N_{st} \to \min$), though still with certain fluctuations. Finally, at the macro- (global) scale, a clear and smooth extremum tendency is observed. It was also identified that the choking transition from the fluidization state to the dilute pneumatic transport can be well explained with the transformation from gas–solids compromise to gas dominance (Li & Kwauk, 1994).

Further, the interphase drag between the meso-scale structure (particle clusters) and its surrounding fluid was found to be quite different from that inside the particle clusters and that in the dilute

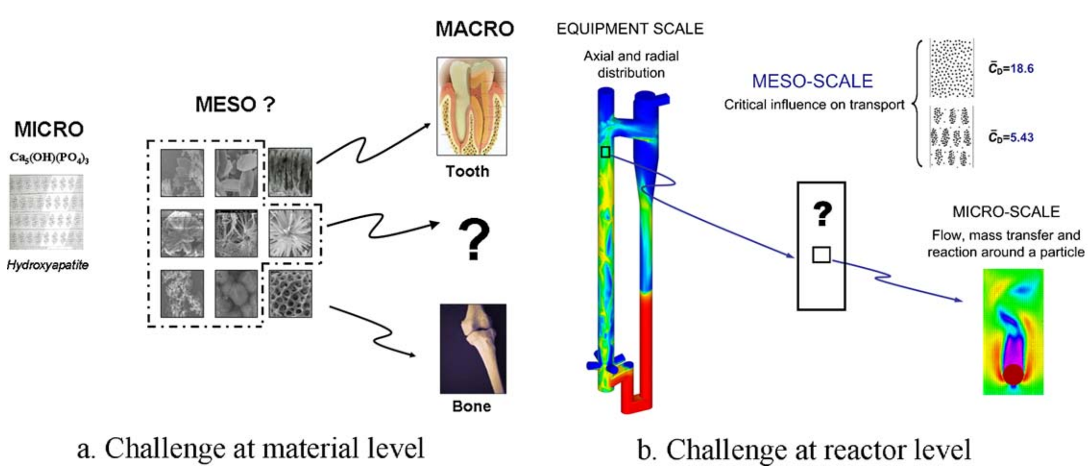

Fig. 2. Meso-scales—challenges in multi-scale modeling and simulation in chemical engineering.