MULTI-SCALE MODELING

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Summary

Complex systems and multi-scale structures are characteristic of many natural and

artificial processes. Multi-scale methodology is necessary for the faithful description of these processes. Three different kinds of multi-scale methods are discussed. The descriptive method lays a basis for the other two methods, but no correlation between scales is considered. The correlative method can describe the correlation between neighboring scales or levels, but has faced with closure problems within a level, which can be solved by incorporating the variational method that correlates different scales through stability conditions.

The variational method is more relevant to complexity science and is, therefore, discussed in more detail with the example of energy minimized multi-scale model (EMMS) which is originally developed for particle-fluid systems. Extension and generalization of the method to different systems and their applications in respective engineering practices are also included. It is indicated that the local compromise between different dominant mechanisms with respect to both time and space may lead to the formation of meso-scale structure which satisfies a variational criterion defined by the minimization of a lumped parameter. The discussion concludes with prospects on the future development of the methodology and its implications for chemical engineering.

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1. Introduction

From elementary particles to the whole universe, the world is characterized by multi-scale diversity, heterogeneity and complexity. Approaches based on linearity, average and reductionism are insufficient for understanding this hierarchical multi-scale structure. The so-called “multi-scale methods”, which can be traced back to the 1970’s, have thrived in the 1990’s as promising prediction tools and mechanism probes. The new term, “multi-scale science”, was proposed independently in different fields, including mathematics, physics, chemistry, astronomy, geology and biology, and in applied fields such as materials, mechanics, image analysis, computational methods and atmospheric science. Many prestigious scientific conferences have chosen multi-scale science as a major topic. However, few in-depth explorations have been made in the field of chemical engineering, though the development of product engineering and virtual processes is calling for a higher level of quantification, which requires significant progress in the study of multi-scale methods.

This chapter reviews the development of multi-scale methodology with particular emphasis on that in complex chemical engineering systems. Three kinds of multi-scale methodologies will be discussed: descriptive, for distinguishing the phenomenological difference among structures at different scales; correlative, for formulating phenomena at higher scales by analyzing the mechanisms at lower scales; and analytical, for revealing the dominant mechanisms of the structure and the relationship between the scales. In particular, the analytical methodology is detailed by taking the Energy Minimization Multi-Scale (EMMS) model as an example, which has been developed over 20 years at the Institute of Process Engineering (IPE).

The EMMS model stemmed from a rough idea that stability conditions must be incorporated into quantitative description of multi-scale structures, which is first demonstrated in establishing such a model for gas-solid systems. In elucidating the

physical mechanism underlying the stability conditions, it was recognized that identifying the extreme tendencies of the dominant mechanisms and expressing their "compromise" can serve as a general strategy for some other systems, such as turbulent flow and gas-solid-liquid flow. The research then extended to different aspects. The authenticated results are summarized in flow prediction softwares and applied to the optimal design of some industrial processes, and on the other hand, more systems such as granular flow, emulsions and reaction-diffusion systems are studied with the same strategy in the hope to find possibly generalized methodology for studying multi-phase complex systems. In addition, the detailed physical picture about how "compromise" leads to stabilities was revealed by computer experiments on gas-solid systems, which gave plain verification of the model. A comprehensive review of the model, both in retrospect and prospect, is given in this chapter in the background of analytical multi-scale methodology.

2. Multi-Scale Structures in Chemical Engineering

With the publication of some profound monographs, among which "Exploring complexity" by Nicolis and Prigogine and "Synergetics" by Haken should be cited, the 1980s witnessed a flourish of complexity science, and an institute devoted to complexity study was founded by Gell-Mann and his colleagues. Although the definitions of complexity and complex system are still in debate, self-organized multi-scale structures and nonlinear non-equilibrium interactions among them have been widely accepted as characteristic features of complex systems, as reflected by the focusing of publications in this area.

Broadly speaking, phenomena in nature are either equilibrium or non-equilibrium. Equilibrium systems obey the variational criteria of maximum entropy, while linear non-equilibrium systems follow minimum entropy production rate in limited cases. However, there is no single general criterion for non-linear and non-equilibrium systems, and from a different point of view, this can be construed as either a reason or a result of the complexity involved in such systems. In fact, studies have shown that complex systems usually involve a compromise of different variational criteria each presenting a dominant mechanism in shaping its behavior (J. Li & M. Kwauk, 2003. Chem. Eng. Sci. 58: 521-535; J. Li, J. Zhang, W. Ge & X. Liu, 2004. Chem. Eng. Sci. 59: 1687-1700). The multiplicity of dominant mechanisms is inherently related to the multiplicity of scales and the lack of a united criterion.

Chemical engineering is a diverse and evolving discipline dealing with dynamic structures, typically nonlinear, non-equilibrium and hierarchically multi-scale in nature. Therefore, complexity is routinely encountered in chemical engineering and has been the bottleneck for its development. For chemical reactors ranging from micro-reactors through bench-scale and pilot-reactors, to commercial reactors, the scaling-up process is not only a major challenge for chemical engineers and scientists but also crucial to the survival of the chemical companies in the world of commercialization and globalization. On the other hand, novel concepts and methods, such as molecular self-assembly, nanotechnology and supermolecular chemistry, are needed to develop processes for products with specific end-use properties, which are pushing the frontiers of complex science even further.

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As an expression of its complexity, typical scales involved in chemical engineering are shown in Figure 1. Starting from the molecular level that includes scales of atoms, molecules and assemblies, the domain of chemical engineering enters gradually from that of chemistry or biochemistry, to focus on the reactor level consisting of particle (or droplet or bubble) scale, aggregate scale and apparatus scale, which is the central stage for traditional chemical engineering. Product engineering correlates the molecular level with reactor level in designing and manufacturing customized and functional chemicals. On the ecological level involving process apparatus, factories and the environment, chemical engineers are now working with ecologists on process system engineering for less consumption and better environment, as well as higher efficiency and profits.

Besides the vast span of spatial scales, the time scales involved in chemical engineering also range from 10^{-15} to 10^{8} s. For the motion of atoms in a molecule during a chemical reaction, the typical time scale is of the order of femto- and picoseconds, and for molecular vibrations, the typical period is in nanoseconds. The characteristic time scale of industrial processes is up to hours and that for the destruction of pollutants in the environment may last for centuries.

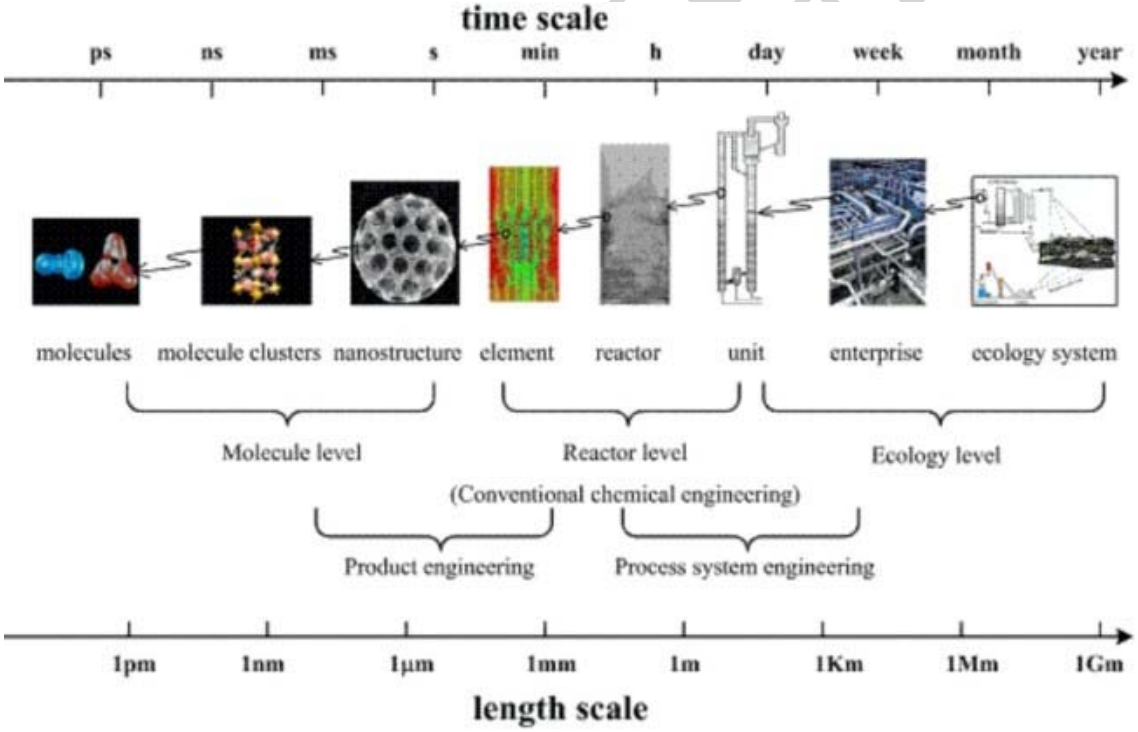

Figure 1: Spatio-temporal multi-scale structure in chemical engineering (J. Li, W. Ge, J. Zhang & M. Kwauk, 2005. Chem. Eng. Res. & Des. 83(A6): 574-582).

3. Approaches to Analyze Multi-Scale Structures

Since multi-scale structure is intrinsic to most complex systems, its modeling and analysis plays a key role in understanding the essence of complex systems. Such analysis is also crucial to the design and control of the facilities, processes and products

in chemical engineering. For physical analysis of spatio-temporal structures, the approaches can be classified into three categories in general.

3.1. Averaging Method

The averaging method uses lumped parameters for a certain spatio-temporal volume by assuming the system to be uniform all over the volume. That is, it does not distinguish the scales below the volume or the different mechanisms involved in shaping the structures within that volume. Therefore, the averaging method is, in principle, insufficient for formulating the interactions in complex systems. As exemplified in Figure 2 for gas-solid two-phase systems, the drag coefficient in the dense phase is as high as 10^5 for a typical Circulating Fluidized Bed (CFB) riser in the Fluid Catalytic Cracking (FCC) process, whereas that in the dilute-phase is less than 10^2. The relevant drag coefficient between the dilute broth and the dense clusters is even much lower. If the averaging method is used, these three different regimes will be obscured and the corresponding drag coefficients will be identical. This explains why currently Computational Fluid Dynamics (CFD) software seldom fits experimental data well, and why adjusted parameters have to be used for multi-phase systems.

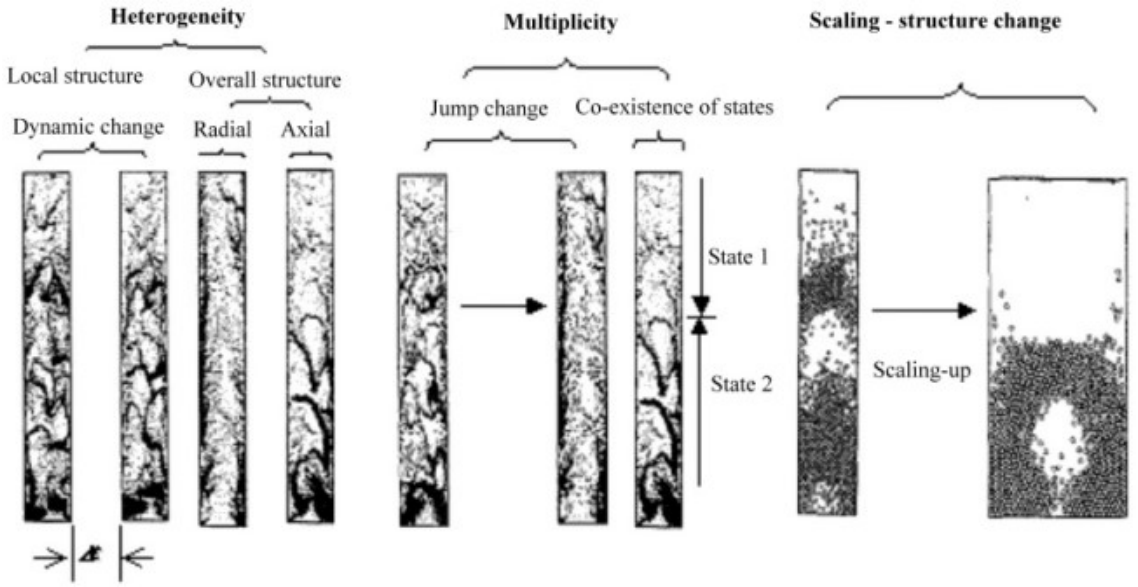

Figure 2: Complex structural changes in particle-fluid chemical reactors (J. Li & M. Kwauk, 2003. Chem. Eng. Sci. 58: 521-535).

3.2. Discrete Method

The discrete method has found wide applications in computational mechanics and chemistry, especially for complex flows. These methods reconstruct continuum behavior from the movement and interactions of numerous particles with discrete attributes. Actually, different particles have been invented on different scales. On the micro-scale, the particles possess mainly molecular features with strong thermal movement and conservatively simple interactions. Continuum properties such as pressure and viscosity are expressed as the statistics on many particles. Molecular

dynamics (MD) may be considered a prototype on this scale. On the macro-scale, the particles are roughly treated as material elements with stress and energy dissipation between individual particles correlated to their state variables. Typical examples are smoothed particle hydrodynamics (SPH) and partially the moving particle semi-implicit (MPS) methods. On the meso-scale in between, dissipative particle dynamics (DPD) and its extensions are used, where both thermal fluctuation and energy dissipation are considered to describe the collective behavior of a cluster of molecules.

The most obvious virtue of discrete methods for simulating complex systems is their numerical simplicity and parallelism in dealing with a variety of challenges for continuum approaches, such as discontinuities, large deformation, fractures, and non-linear behaviors. Of course, discrete methods are computationally more expensive, but for the description of micro-scale and sometimes meso-scale structures and behaviors, they are the only choice because no continuum model actually exists in nature. Besides the traditional examples, such as reaction and transport processes on particle, droplet or bubble surfaces, micro- and meso-scale features are increasingly used in chemical engineering with the wider use of nano-materials and the advent of micro-chemical reactors. In a sense, the discrete method is a counterpart of quantum methods in chemistry. For the levels of description concerned, they are both direct simulation methods based on first principle.

3.3. Multi-Scale Method

The multi-scale method considers directly the disparity of behaviors and interactions on different scales, and is therefore a promising approach to identify the prevailing mechanisms in complex systems. Generally speaking, there are three kinds of multi-scale methodology: descriptive, correlative and analytical. The descriptive multi-scale methodology describes the appearance of various structures on different scales without analyzing the mechanisms behind their formation and the relationship between these scales. The correlative multi-scale methodology elucidates the behaviors on higher scales by analyzing the mechanisms on the next lower scales. The analytical multi-scale methodology reveals the relationship between scales by formulating stability criteria, dominant mechanisms and compromise between sub-mechanisms. The respective features of these three kinds of multi-scale methods will be discussed in the following sections in detail.

4. Descriptive Multi-Scale Methodology

Presently, most literature and websites on “multi-scale” are related to the descriptive method, shown in Figure 3(a). It is used not only for stationary structures, but also for those dynamic structures that change very slowly, such as the multi-scale structure of plants and the human body. However, it is only useful for distinguishing the various structures at different scales without revealing the physical relationships between the different scales and the underlying mechanisms. For instance, in the area of material science (Maroudas, 2000), molecular dynamics or density functional theory is used to accurately describe the material properties and dynamics on the micro-scale (time scales less than 1ps and length scales less than 1nm). Semi-empirical Hamiltonian or lattice dynamics is used to model the statistical mechanics on the meso-scale (time scales less

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than 10 ns and length scales less than 10^{-7} m). Finite element methods, finite difference methods or boundary integral methods are adopted to model macroscopic process to get the continuum properties on the macro-scale (time scales less than 1 hour and length scales less than 0.1 m). In addition, as Xi et al. (2000) have pointed out, material parameters should be studied on the basis of dominant physical mechanisms and formulated separately, that is, to separate the problem into various scale ranges, each covering the mechanisms acting at one of the scale ranges. The information obtained at a lower scale is not as a rule even passed to the higher scale so that the modeling results at higher scale could not be benefited or influenced by those at lower scales. Though this kind of descriptive multi-scale method follows the inherent logic of the physical phenomena of every scale, the relationship between different scales and hence the general intrinsic mechanisms may be ignored.

5. Correlative Multi-Scale Methodology

The shortcomings of the descriptive multi-scale methodology lead to the alternate usage of the correlative multi-scale methodology, illustrated in Figure 3(b). There are four strategies, discussed by Ingram et al. (2004), to establish such models.

The first is the "bottom-up" strategy for model construction: complex systems can be understood on the higher scale by analyzing lower-scale mechanisms. For instance, the Darcy's law on the macro-scale could be formulated from the Navier-Stokes equations on the meso-scale, which could again be derived from the Boltzmann equation on the micro-scale. As another example, mass transfer rate between gas and clusters on the meso-scale could be derived from that between gas and single particles on the micro-scale. It is reasonable to expect that if the lowest-scale mechanisms were not well understood, any deviation on lower scales would be magnified on higher scales. On the other hand, such deviation could be ignored when the lower-scale interactions do not contribute much to the behavior on the higher scales. For example, one could calculate gas-solid two-phase flow behavior without knowing the molecular structure of the solid particles involved. However, there is a lack of methods and tools currently for constructing bottom-up models efficiently in process engineering.

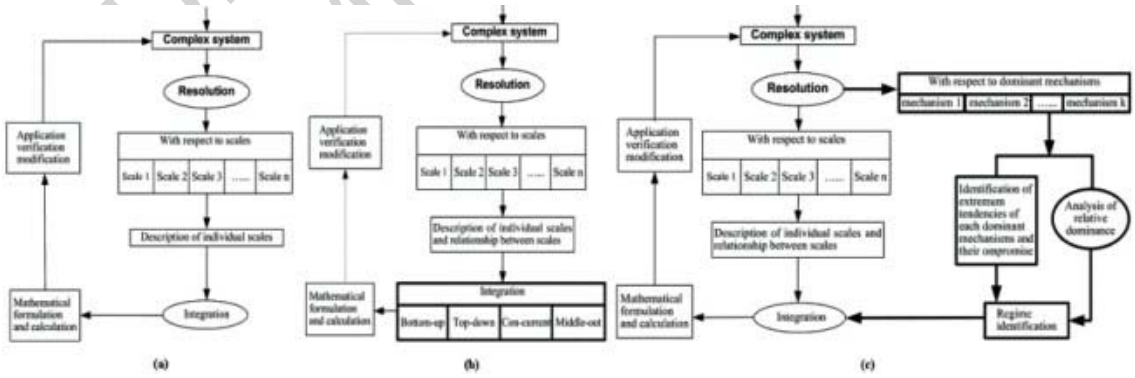

Figure 3: Comparison of three kinds of multi-scale methodology (modified from J. Li, W. Ge, J. Zhang & M. Kwauk, 2005. Chem. Eng. Res. & Des. 83(A6): 574-582; J. Li, M. Kwauk, 2003. Chem. Eng. Sci. 58: 521-535). (a): descriptive multi-scale methodology — only scale resolution is considered; (b): correlative multi-scale

methodology — on basis of scale resolution, interaction of elements is emphasized; (c): analytical multi-scale methodology — in addition to scale resolution, resolution with respect to mechanism is also carried out.

In contrast, the second, or the "top-down" strategy can be used to establish multi-scale models: a large scale model is constructed and refined by successively adding smaller scale models until detail and accuracy goals are satisfied. Plant designers prefer this method because of its efficiency. In establishing a plant, commercial requirement demands modeling at the plant scale as the crucial first step, which is then modified and refined by modeling at reactor scales: pilot plant and production reactors, transport, catalyst design, computational chemistry, etc. Further, modeling results at laboratory reactors scale can be used to fix the unified model. However, as Ingram et al. (2004) have noted, it is hard to keep track of process knowledge and model evolution over the process lifetime in top-down modeling strategy.

The other two strategies, "con-current" modeling as described by Lerou & Ng (1996) and "middle-out" method favored by Noble, have also found applications. But all these four strategies still focus on one-way coupling and the relationship between neighboring scales. In fact, a systematic inclusion of two-way coupling is only possible when the so-called analytical multi-scale method is incorporated, to consider the implicit interdependence between scales.

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Biographical Sketch

Li Jinghai, a chemical engineer, was born in Jingle County, Shanxi Province in October 1956. He graduated from the Department of Thermal Engineering of the Harbin Institute of Technology in 1982. He entered a master's degree program at his *alma mater* in the same year, obtained his Ph.D. in 1987 from the Institute of Process Engineering (IPE) of Chinese Academy of Sciences (CAS) in Beijing. He conducted his post-doctoral research at the City University of New York and the Swiss Federal Institute of Technology. After returning to China in 1990, he served as assistant professor, associate professor, professor, vice director and director of IPE in succession. In February 2004, he was appointed a vice president of CAS. He holds memberships of *Chinese Academy of Sciences*, *the Academy of Sciences for the Developing World* and *the Swiss Academy of Engineering Sciences*, and has duties at editorial or advisory boards of international journals such as *Chemical Engineering Science* (Elsevier), *Powder*

Technology (Elsevier) and *Advanced Powder Technology* (Elsevier). He is the president of Chinese Society of Particuology.

His research is focused on the establishment of Multi-Scale Methodology for multi-phase complex systems and application of computer simulation in scaling-up chemical reactors.

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