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Approaching virtual process engineering with exploring mesoscience ☆

Jinghai Li *

State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China

HIGHLIGHTS

- Evolution of chemical engineering features the increasing generality of its knowledge base.
- Three mesoscales at material, reactor and system levels are currently the challenges of the field.
- All mesoscale phenomena are likely governed by the principle of compromise in competition.
- Breakthrough on mesoscience will enable the realization of virtual reality of chemical engineering.
- Resolution of three mesoscales will make a new age of chemical engineering.

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ABSTRACT

Different disciplines deal with mesoscale problems between the scales of element (micro) and system (macro) in different ways. Usually, coarse-graining or statistical approaches, which are averaging approaches, are used. However, averaging approaches tend to lack or ignore the governing principles ruling phenomena at mesoscales between elements and systems. Mesoscience will enable us to explore the principles common to all mesoscales to correlate parameters between micro- and macroscales.

In chemical engineering, understanding dynamic multiscale structures, which are critical to reaction and transport processes, remain a challenge because they are all complicated at mesoscales of three levels: material, reactor and system, making it difficult to solve problems at each level and to correlate these levels. This paper reviews three decades of work on mesoscale phenomena in chemical engineering from principles, modeling, and simulation, through to application and generalization. It is revealed that all mesoscale phenomena in these systems follow a common principle of compromise in competition between dominant mechanisms, and can be generally formulated as a multiobjective variational problem. This leads to recognition of the possibility of an interdisciplinary science, mesoscience, to encompass all mesoscale problems existing between elemental particles and the observable universe.

The possibility of realtime simulation of chemical processes based on mesoscale modeling is discussed, focusing on the structural and logical similarity between problem, model, software and hardware. Finally, this review is concluded with the prospects of the emerging mesoscience, the development of multiscale computation, and the possible realization of virtual reality. It is believed these advances will mark a new age of chemical engineering if materialized, subject to the resolution of three mesoscales and bridging of the two gaps between levels.

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* Fax: +86 10 6255 8065.
E-mail address: jhli@ipe.ac.cn

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1. Chemical engineering science is now in a transitional period with respect not only to new challenges in engineering practice, but also to its disciplinary knowledge base, as it progresses from empirical to quantitative and further towards virtual process engineering

Chemical engineering was established as an engineering discipline about one century ago. Its knowledge base has gradually evolved from specific knowledge of various unit operations [1,2] to general knowledge of common transport phenomena [3,4] for different unit operations, and is now progressing toward new developments such as product engineering [5] and virtual process engineering (VPE) [6,7]. These developments call for an upgraded knowledge base, probably featuring unified principles of common scientific problems associated with different phenomena [6,7], as summarized in Fig. 1 and discussed in details later.

Although a consensus on the contents that will form the new knowledge base of chemical engineering has not been reached in our community, and even what the research focus will be is still being debated, the objective or dream is clear; that is, to design materials according to required properties and functions, to develop and scale-up processes quantitatively to industrially produce large amounts of these materials, and to integrate and optimize these processes with respect to energy, resources, and environment to achieve competitive, sustainable and greener production of materials, energies, and other chemical products. This broad objective is termed "virtual reality (VR)" in process engineering or VPE for the complete process of "molecules into money" [8]. VR, sometimes referred to as immersive multimedia, is a computer-simulated environment that can simulate physical behavior in places in real or projected situations [9]. In chemical engineering, VR is used to simulate and visualize real industrial processes on computers by solving the mathematical equations of physical models with numerical methods. This allows chemical engineers to design, scale-up, optimize or control processes online and in real time (or if not in real time, at an acceptable rate) without the need to conduct numerous experiments in multiple stages involving trial and error [10,11]. Realization of VR in chemical engineering is currently a great challenge, but also hints that a golden age of chemical engineering science [12] is to come.

Realization of VR in chemical engineering immediately raises many questions: How can we enable the transition from its current status to a new age of chemical engineering? What or where is the key to open the door to this new age? Is the current knowledge base of chemical engineering sufficient or not? If not, what is missing and what should be the research focus? Is this disciplinary transition of the knowledge base of chemical engineering related to the global tendencies of science and technology? If yes, what is this relationship? To answer these questions is of course difficult, but ignoring them will certainly delay the progress toward achieving VR.

Currently, chemists and material scientists produce a huge number of publications on materials with various structures, most of which cannot be produced industrially. Chemical engineers typically design and scale-up chemical reactors using empirical approaches that are expensive, high risk, and difficult to optimize, leading to long development time, poor competitive capability and compromised efficiency. Although computer simulation has been widely used to speed up the development of various chemical processes, its reliability and scalability are still very limited, and far from the standard of VR. The multiscale approach is believed to be promising, but it seems that something is still missing in our ability to correlate different scales to comprehensively understand the coupling between reaction, hydrodynamics and transport behavior in chemical systems [6,7]. It is even more difficult to correlate these physical and chemical processes with economic and environmental factors. In fact, our understanding of complexity in complex systems is currently very limited [13].

At the same time, new challenges in engineering practice are also presented to chemical engineers because of depleting natural resources, particularly fossil fuel. Simultaneously, climate change is an even greater challenge we face that may require us to collect dozens of billions of tons of released CO_2 and store it safely. In addition, new materials have to be developed to replace ones traditionally extracted from natural resources, and efficient renewable energy technologies are needed for a sustainable supply of

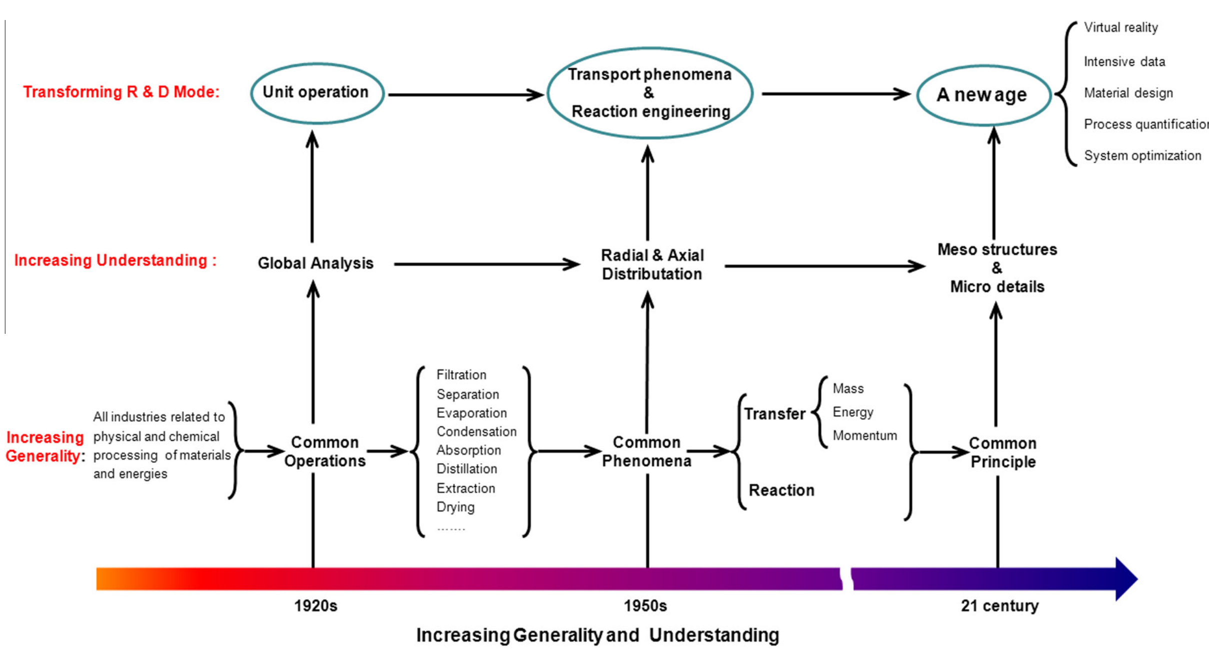

Fig. 1. The evolution of chemical engineering science features increasing generality of its knowledge base.