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Views & Comments

Toward Greener and Smarter Process Industries

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1. Introduction

The main mission of the process industries is to process resources and energies into a form that can be utilized in other industries and throughout society. In this sense, process industries cover a vast territory, encompassing the chemical/biochemical, material, mining, metallurgical, power, food, and even pharmaceutical industries; in addition, they are closely related to mechanical, civil, electrical, and electronic industries, as well as to emerging fields such as biotechnology, nanotechnology, and information technologies.

Despite the global trend of the service and information industries taking up increasing shares of the economy, the fundamental role of the process industries should never be underestimated. In fact, this role is becoming more critical, in that society is becoming more and more sensitive to any malfunction of the process industries. The process industries are facing great challenges in supporting the fast and sustainable development of the global economy and society. These industries are required to adapt to consumer demands more quickly and in a more flexible way in our increasingly diverse and vibrant modern society; for example, e-commerce and greener processes need precise control in order to minimize their environmental impact, which is a major current concern.

However, the process industries traditionally rely heavily on stepwise experiments and on long-term experience for process development and operation. The high cost, low efficiency, and low effectiveness of this research and development (R&D) mode are increasingly incompatible with the requirements discussed above. Consolidation and extension of the theoretical foundations of process engineering and the application of new technologies from other fields and disciplines are urgently needed. We briefly discuss the most important aspects of this new mode, in our opinion, in the following article, which is based on our previous studies.

2. Multi-scale modeling and simulation

Computer simulation and optimization has long been expected to revolutionize process engineering. Accurate quantification of processes is, therefore, key to the upgrading of the process industries. The multi-scale nature of most processes should be considered in order to develop either coarse-grained discrete methods or continuum-based statistical averaging methods, with mesoscales at the center of each new method.

Most processes in the process industries involve atomic or molecular scales, at which the elemental processes of material and energy transformations actually take place, and equipment scales, at which industrial productions are operated. The typical scale difference between these two ends of the spectrum is roughly 10 orders of magnitude in both space and time. An intermediate scale, or the so-called particle scale (which includes bubbles, droplets, or simple elements in a broader sense), is usually involved as well. Between the intermediate scale and the two ends of the spectrum exist two mesoscales [1–3], which typically encompass molecular clusters and particle clusters, respectively. Although models can be established at each of these scales according to the distinctive mechanisms involved, no such model is complete or fully mature. This is particularly true for models at the mesoscales. However, bridging the scale differences across mesoscales is both theoretically and numerically infeasible. As a result, numerical simulations based on such models suffer from low accuracy and/or high computational cost in many cases.

A central problem in the modeling of mesoscale structures is the closure of dynamic equations for an expanded set of variables, as compared with the equations in simple averaging models. Semi-empirical phenomenological correlations are most commonly used in engineering practice; however, they typically suffer from low accuracy and limited application ranges, due to the lack of general and reliable physical backgrounds. Stability-constrained models may present an effective alternative, as demonstrated in multiphase systems [4–10] and turbulent flow [1,11]. This strategy can be applied both in statistical averaging in continuum methods [12,13] to develop sub-grid scale models, and in coarse-graining in discrete methods [14,15].

3. Virtual reality on the horizon

Virtual reality will become a revolutionary technology for process engineering. However, in addition to the general capabilities of virtual reality, physical phenomenological reality should be pursued in process engineering.

With the development of high-definition displays, graphics processing, and human-machine interfaces, virtual reality [16,17] has recently become a hot topic in information technology. However, its primary applications are currently in consumer products, entertainment, training, and education. With the development of simulation methods, software, and supercomputing, virtual reality will bring

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revolutionary changes to process engineering—once real processes can be reproduced in physically reliable computer simulations to an accuracy and resolution that are sufficient for engineering purposes, in contrast to the phenomenological descriptions that are most practiced in computer games. In a strict sense, a simulation should be fast and efficient enough to operate a process virtually through visualization and the user interface, and to preferably do so in an immersed environment.

Although the specific requirements for virtual reality in the process industries may differ significantly in various applications, they are far beyond the capacity of the simulation systems that are now available in process system engineering, which are mainly based on an overall mass and energy balance and on predefined dynamics rules. They are also far beyond the capacity of the computer-aided design and computer-aided engineering systems that are widely used in industries, which are mainly for geometrical design and static structural analysis, rather than for understanding the dynamics and mechanisms behind the processes.

To reach the necessarily high standard of accuracy and speed, computational models, software, and hardware should be developed consistently in terms of logic and configuration. As discussed above, mesoscale models are also at the core of this development. As we have explored in our own research on multiphase systems in recent years [1,2,15,18–20], the strategies of "from global to local" and "from distribution to evolution" seem to work favorably toward this goal.

The impact of virtual reality is profound, and its benefits are highly desirable. Since it provides a reliable digital counterpart with no physical construction or operation, virtual reality can be used to experiment with, observe, and measure real processes easily and thoroughly, and to optimize such systems extensively at a much lower cost and higher efficiency than before. Along with the physical reality provided by multi-scale modeling and supercomputing, the wide adoption of virtual reality will surely become a revolution in process engineering and in the process industries.

4. Analysis of big data

The analysis of the huge amounts of computational and measurement data from future technologies, such as virtual reality, also requires new science and technologies. *In situ* visualization, data mining, deep learning, artificial intelligence, and so forth, are promising candidates for this role. However, the physical structures of the data, especially at the mesoscales, should also be addressed.

The size of the data produced by the simulations and measurements that power virtual reality is huge by any standard. Sizes in the range of terabytes to petabytes per second may not be too extreme in the near future. On the one hand, visualization is important in order to obtain an intuitive understanding of the information contained in a process; on the other hand, visualization is insufficient for getting the most out of the data, since further analysis may reveal structure and dynamic mechanisms behind the data. For visualization, highly coupled processing and computation or *in situ* visualization will be necessary; otherwise, severe performance drops due to data transfer will be inevitable.

For extensive analysis of such data, methods in computer science that are currently being developed, such as data mining, deep learning, and artificial intelligence, are helpful. However, a pre-acquired knowledge of the "structures" (not formats) of the data is critical in order for these methods to obtain physically meaningful results and run more efficiently [3]. Otherwise, the same data may be interpreted in totally different ways and the results may be qualitatively unreasonable. Methods for the analysis of large and complex networks [21], such as the identification of their topological structures, may provide general mathematical tools for this purpose, when coupled with physical models on multi-scale structures. Investigations into reaction pathways using detailed reactive molecular dynamics simulations [22–24], and similar investigations on the optimization of logistic networks for crude oils and refined oil products, may benefit significantly from the studies in this field.

In conclusion, greener and smarter process industries require a deeper understanding of the multi-scale structures that are involved in processes; with this understanding at its core, virtual reality powered by supercomputing and big data analysis will bring about a revolutionary R&D mode in the process industries, and will ensure their fundamental role in future society.

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