CHINA PARTICUOLOGY Vol. 3, No. 3, 151–164, 2005

EXTENDING THE KNOWLEDGE BASE OF CHEMICAL ENGINEERING

Mooson Kwauk

Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100080, P. R. China
E-mail: mooson@home.ipe.ac.cn

Abstract The obvious current reversion to micro-scale investigations in basic chemical engineering, combined with the need, of a quite different nature, in the rapid growth of high added-value and small-lot functional materials, have been pointing to an area not yet sufficiently covered by the unit operations, transport phenomena and chemical reaction engineering. Although it is difficult to define accurately this area, a cursory scan of the activities already in progress has revealed a few common attributes: multi-phased (structured), multi-scaled, multi-disciplined, nonlinear, needs for resolution to reductionism-solvable subsystems, and pervasive in the process industry. From these activities, the present paper drafts a tentative scheme for studying the related problems: first to dissect a problem into various scales — spatial, temporal or otherwise as best suits the case in hand — in order to identify pertinent parameters which are then organized into model formulations. Together with inter-scale model formulations, a zoom-in/zoom-out process is carried out between the scales, by trial-and-error and through reasoning, to arrive at a global formulation of a quantitative solution, in order to derive, eventually, the general from the particular.

Keywords chemical engineering, basic knowledge, frontier, prospect, future, opportunity, challenge

1. A Knowledge Base of Successive Generalizations

The formation of the knowledge base unique to chemical engineering has resulted from repeated stages of discovering *the general from the particular*, as shown in Fig. 1 — first, the *unit operations* (UO) around the beginning of the 20th century, generalized from industries using similar types of operations; second, the principles of the *transport phenomena* (Transport), generalized from the unit operations, in mid-20th century, incorporating a great deal of physics and mathematics. The unit operations were accepted somewhat as the cornerstone of chemical engineering, but, unfortunately they are all physical in nature and do not encompass the very important chemical aspects of the chemical industry. Early attempts were made to organize these chemical aspects, in a manner similar to the UO, into the *unit processes,* which were, unfortunately, more taxonomic than heuristic for providing guidelines in the design, operation and innovative manipulation in the chemical industry. On the other hand, the principles of transport phenomena were made use of in combining with the chemistry involved in industrial processes to create the third-stage generalization in the emergence of *chemical reaction engineering* (CRE). Progressing with the stages, the science content of the ChE knowledge base (shown as the abscissa in Fig. 1) has been on the increase.

Rightfully the trio, UO-Transport-CRE, became the ensconced knowledge base for chemical engineering until, in the latter part of the 20th century, it was realized that this

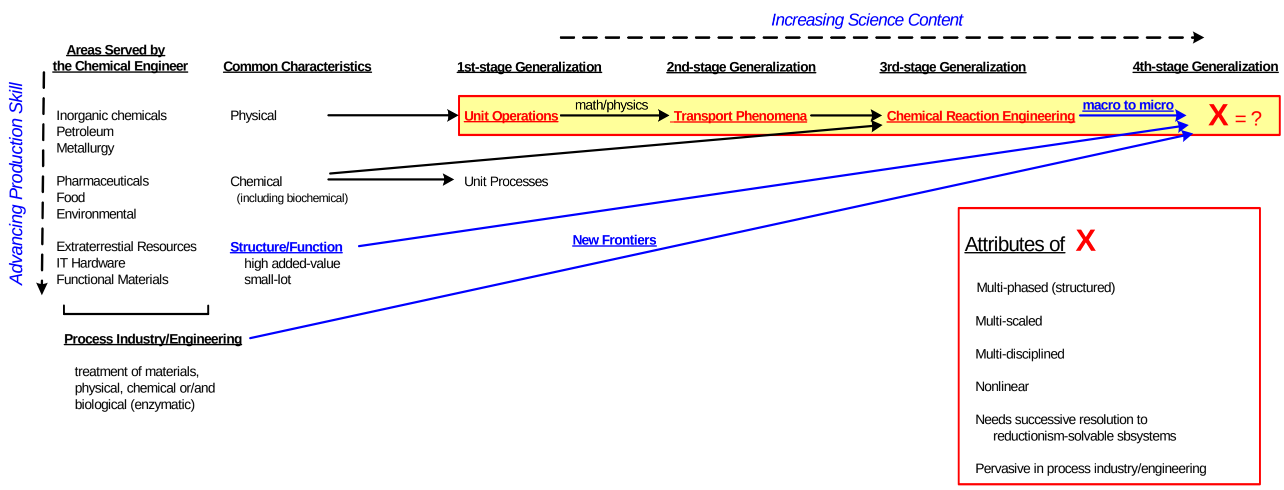

Fig. 1 Extending the knowledge base of chemical engineering.

Presented at 10th Anniversary Celebration of CENG at HKUST, August 28, 2004, in a symposium themed "Chemical Engineering in Asia: Education, Research & Development".

knowledge base was essentially macroscopic and did not suffice to address problems such as underlie the mechanisms of many processes, physical as well as chemical. This realization promoted a sudden interest in exploring the micro-scale phenomena ranging from bubbles, droplets and solid particles down to the molecular/atomic dimension. At the same time, the need for the expertise of the chemical engineer greatly expanded with advancing production skills (shown as the ordinate in Fig. 1) — from commodity chemicals through pharmaceuticals, food processing, environmental protection, to extraterrestrial resource conservation and utilization, especially the provision of functional materials, for instance, for the IT industry including device-making, e.g., via CVD — thus providing additional impetus for extending the ChE knowledge base. (See Kwauk, 2004)

2. The 4th-Stage Generalization — Ready Applicants

Thus the motivating forces — the need for macro-to-micro studies in the established ChE knowledge base, the variety of high added-value and small-lot functional materials, and the anticipated needs in the ever advancing production skills in the future process industry/engineering — are pointing to a *terra incognito “X”* in the ever developing ChE knowledge base. More than a mirage in the distant offing, this “X” is to be turned into a *terra firma* with fresh science input through the toils of dedicated applicants. Let us examine a few.

2.1 Fluidization — dynamic structure for multiphase flow

Large-scale industrial application of fluidization began with the Winkler coal gasifier in the 1920’s, followed by, two decades later, fluidized catalytic cracking whose design and operation were much supported by laboratory studies by the then engineering scientists. The phenomenon of gas bubbling through a moving matrix of particles is fascinating enough to arouse the interest of engineers to study and speculate on the dynamics of bubbling fluidization. Between the micro-scale of the particles and the macro-scale of the equipment, the bubbles actually constitute a meso-scale of great significance. However, all these predated the recognition as of the 1980’s of the macro-scale limitation of UO and Transport, and neither was the generic importance of scale much appreciated in those early days.

It remained for another two decades until the emergence of the circulating fluidized bed (CFB) pioneered in Germany, or fast fluidization (FF) in USA, that outperformed the classical bubbling fluidized bed in many ways (Squires et al., 1985), that people began to deal with another type of gas-solid contacting, that is, instead of gas bypassing a matrix of solid particles in the form of bubbles, the solid particles form transient clusters suspended in a dilute broth of discrete particles. Here, particle clusters are as much a meso-scale phenomenon as bubbles were the meso-scale feature of bubbling fluidization. This recognition of the significance of scale brought about immediate returns in treating the new gas-solid system.

Altogether eight parameters could be specified to describe the FF/CFB, as shown in Fig. 2, including the meso-scale clusters together with their assigned symbols. Unfortunately only six conditions could be identified, that is, one less than necessary for solution. The search for the missing condition was more conceptual than mathematical. Among the multitude of candidates, finally *energy* was found to satisfy the vacancy, that is, the energy involved in suspending and/or transporting the solid particles per unit mass of solid particles and/or per unit volume of the system, needs to be either maximized or minimized.

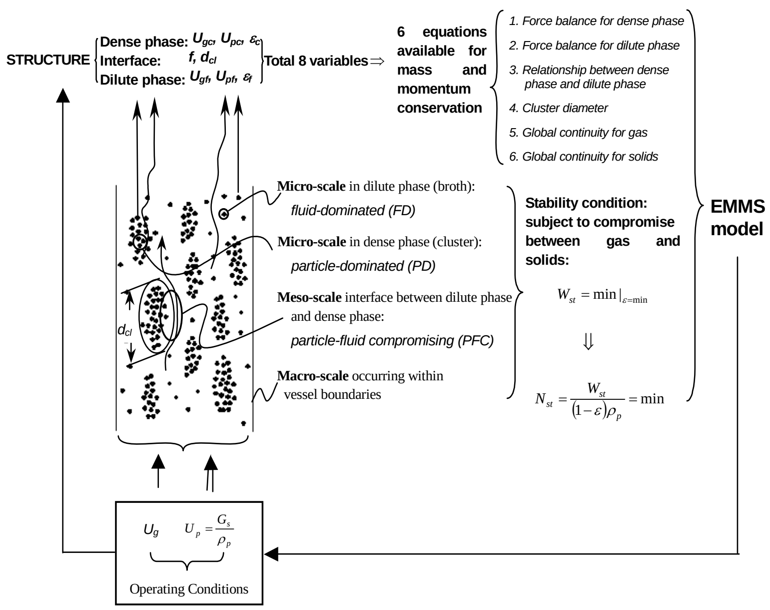

Fig. 2 Physical basis of the EMMS model (Li & Kwauk, 2003).