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Scale-up and multiphase reaction engineering

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Successful scale-up of new multiphase reactions from the laboratory into practical processes is important to all sectors of the process industry. Business demands that process technologies involving molecular transformations maintain high profitability and operate safely within existing environmentally regulations. Current societal expectations and regulations require that all process technology should be environmentally responsible [1]. One key question to be answered is whether or not these expectations can be met in the foreseeable future with the current approaches to scale-up and technological workforce. In addition, advances in chemistry, physics, materials, and biology will continue to generate new potential reaction pathways for more efficient utilization of non-renewable and renewable resources. Another key question is whether the current methods for process scale-up incorporate the relevant scientific advances to ensure 'green technologies', or are they just extensions of previous largely empirical approaches having limited utility and reliability? Evidence suggests that only a science-based scale-up methodology can substantially reduce the risk of new process commercialization and provide reliable estimates of both profitability and environmental impact. We review briefly here the historical approach to scale-up and opine on the challenges of implementing improved approaches.

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Introduction

Multiphase chemistries involving reactions between gases, liquids, and solid reactants that are catalyzed by homogeneous organometallic complexes [2], heterogeneous inorganic solids [3] or biocatalysts [4–6] are the basis for nearly all processes used to manufacture organic and inorganic intermediates and end-use products, such as fuels and chemicals from petroleum feed-stocks [7], bulk commodity, specialty and fine chemicals [8], medicinal intermediates and pharmaceuticals [9,10], and various polymers [11–13]. End-of-pipe processes for environmental remediation also rely upon multiphase catalyzed chemistries for emissions control [14–16]. Various handbooks provide reviews of the science and technologies associated with heterogeneous catalysis [17], homogeneous catalysis [18], industrial biocatalysts [19] and multiphase polymers [20]. In addition, several monographs [21,22] also review the scope of industrial catalysts and processes, and consider their environmental footprint [1]. These collective works suggest that catalyst science and technology is a critical component of every industrial sector and also plays a major role in enabling existing global lifestyles. Hence, the practical catalytic reactor that converted crude raw materials into useful products should be given notable attention.

To maintain the lead over their competition, catalyst vendors must provide replacement catalysts having improved measures of performance, such as higher activity, better selectivity, extended life, lower pressure drop, better mechanical integrity, improved thermal stability, and reduced catalyst fines with competitive pricing. The approaches used for scale-up of catalyst recipes and the challenges encountered with evaluating their performance in commercial reactors are proprietary, although information is sometimes reported when a notable success or a disaster occurs. Anecdotal evidence suggests that old scale-up rules based on empiricism prevail in practice, since little or no investment has been made in adding more science to scale-up. In addition, utilization of an improved catalyst by various customers across various reactor configurations for a given technology allows the catalyst supplier to assemble a significant data base on reactor performance that can be used in look-up tables to make empirically-based suggestions on how to handle particular process situations. Most replacement catalysts in an existing process lead only to incremental improvement in practical reactor performance, so the risk is much smaller when compared to a new process. Invention of new or improved catalysts for more economical processes with a reduced environmental footprint [23] is a leading research topic. Examples of catalytic technologies that are receiving increased emphasis include those that: (1) produce cleaner energy sources from various feedstocks [24]; (2) create higher quality lubricants [25,26]; (3) capture, control, or utilize greenhouse gases [27,28]; (4) convert natural gas or bio-based methane gas to chemicals and fuels [29]; (5) minimize environmental impact or reduce the environmental footprint [30–32]; (6) transform bio-based feedstocks to either hydrogen or targeted organic chemicals [33–35]; (7) gasify biomass for production of either hydrogen [36], synthesis gas [37], chemicals and other products [38]; and (8) generate power using fuel-cells [39]. One conclusion that emerges is that the likelihood of successful translation and scale-up of these new catalytic technologies from laboratory research to commercial-scale processes is notably enhanced when reaction engineering principles are closely integrated with other ongoing science, engineering and business development activities [40•,41].

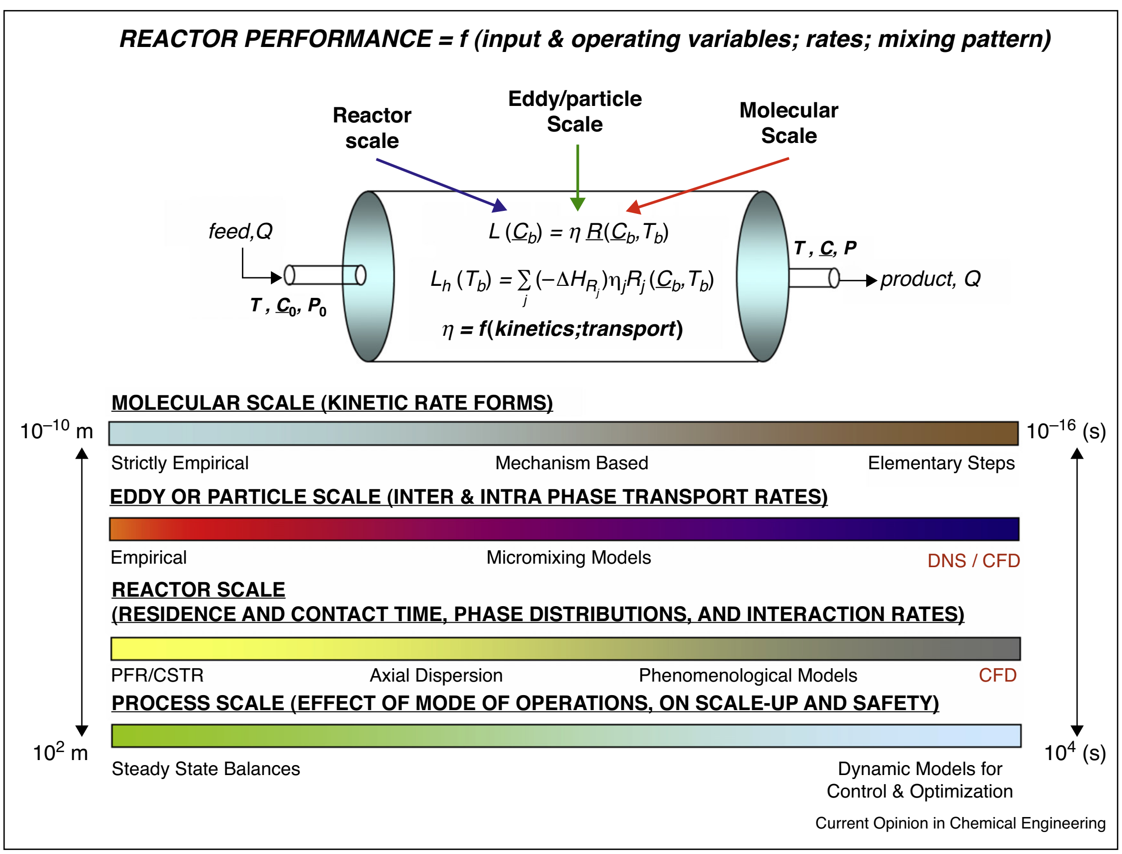
Reactor scale-up: current status

The state-of-the-art of multiphase reaction engineering (MRE) has been the subject of various reviews over the past 30 or so years [40•,42•,43,44•,45•,46–51,52•,53,54]. Although the installed cost of catalytic process reactors typically account for about 5–15% of the total capital, reactor performance always dictates the cost of downstream product refining as well as the flow rates and composition of recycle streams. A successful commercial catalytic process will retain favorable performance metrics as the catalytic chemistry upon which it was based is translated from laboratory reactors to commercial practice [55]. Classic monographs on chemical process scale-up [56,57•] describe customary practices, which are based on both heuristics and engineering-based models. We focus here on the evolution of reactor scale-up practices that allow increased incorporation of sound scientific and engineering principles.

The key phenomena that affect multiphase reactor performance occur on a large range of length and temporal scales and are illustrated in Figure 1 [6]. These include molecular-scale transport-kinetic interactions, eddy or particle-scale transport processes, and fluid flow patterns, hydrodynamics and transport on the reactor scale. These phenomena are subject to events that occur on the process scale, such as disturbances in reactor inlet flow rates, specie compositions, temperatures, pressures, and reactor heat transfer systems, to name a few.

The rates for these phenomena can be quantitatively described at the indicated length and temporal scales using models that start from an intuitive basic level, such as empirical power-law reaction kinetic models, and then evolve to a more sophisticated level based on fundamental

Figure 1



Key phenomena that affect reactor performance.