The need of strong Innovation for advances in "green" and sustainable chemical engineering which is required for the design of "the factory of the future"

Jean-Claude Charpentier, Olivier Potier

Laboratoire Réactions et Génie des Procédés, UMR 7274, Université de Lorraine, Nancy
jean-claude.charpentier@univ-lorraine.fr olivier.potier@univ-lorraine.fr

In the framework of circular economy, global trade, sustainability, water scarcity, climate change, and economic growth or crisis, the chemicals, pharmaceuticals, food, water and waste, oil and gas, energy and related industries are today confronted with the strong demand for the innovative process and sustainable technologies required for the design of the factory of the future. This involves the use of industry 4.0 technologies to improve manufacturing operations by reducing resources and energy usage and improved production efficiencies, thus leading to the design of sustainable technologies, which satisfies in fact the circular couple economy-engineering concept. This has militated for today trends and evolution of chemical engineering in favor of a modern green process engineering which is voluntarily concerned by sustainability and that faces new challenges and stakes bearing on complex length and time multiscale systems at the molecular, product and process scales. This involves a multiscale approach that satisfies both the market requirements for specific nano and microscale end-use properties of competitive targeted green products, and the social and environmental constraints of sustainable industrial meso and macroscale green production processes at the scales of the units, sites of production and international distribution networks.

More precisely, these multiscale constraints for product design and engineering require an integrated multiscale system approach of complex multidisciplinary, non-linear, non-equilibrium processes and transport phenomena occurring on the different time and length scales of the chemical supply chain. This approach encompasses the traditional areas of chemistry and biochemistry (product design area), of chemical engineering (single and multiphase systems, process unit and plant area), and of process system engineering area (process control, optimization, and management). This means a good understanding of how phenomena at a smaller length-scale relates to properties and behavior at a longer length-scale, from the subatomic, molecular and active aggregates-scales up to the production-scales and commercial practice.

The success of this integrated approach of chemical engineering, which is necessary for process innovation (the 3rd paradigm of chemical engineering), will be more and more mainly due to (i) the considerable developments in the analytical scientific techniques coupled with signal and image processing, (ii) the powerful computational tools and capabilities (i.e., clusters, supercomputers, cloud computers, graphic processing units, numerical codes parallelization etc..), (iii) the development and application of fine descriptive models of steady state and dynamic behavior of the objects at the scale of interest, and (iv) the opportunity due to the Big Data movement (i.e., involvement of big data obtained by artificial intelligence and machine learning): this helps to structure and reduce the voluminous amount of digital figures (Big Data) obtained from multiscale theoretical analysis, modeling and numerical simulation into concise formulation for more facile application.

Complementarily, the Multiscale Compartmental Modeling allows such multiscale modeling with low computational time/power compared to Reactive Computational Fluid Dynamics simulations, while integrating much more details than the systemic approach (see Figure 1 for the different modeling approaches to a flue gas desulfurization unit, from Jourdan et al. C.E.S. 210 (2019) 115196).

In this multiscale framework, the trends in chemical engineering will be more and more oriented on both "product design and engineering" (focusing investigations on the couple green products/green processes) and "process intensification" (focusing investigations to produce much more and better in using much less raw materials and energies): the aim is to sustainably produce molecules and products with end-use properties responding to environmental and economic challenges at process scale, and aiming to economic growth, i.e. in reducing time-to-market. Such today trends future advances in

chemical engineering will help to answer to the required novelty, innovation, creativity, and continuous flow of sustainable technologies_leading to efficient mass and energy utilization, lower costs, process safety and to better quality of life.

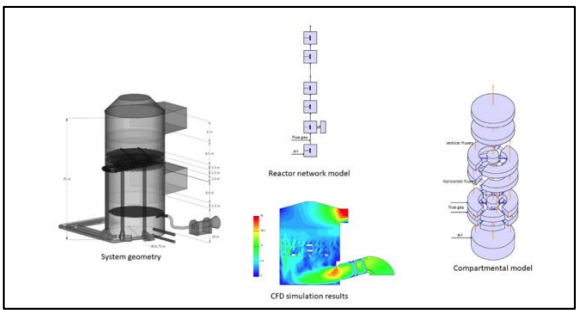

Figure 1

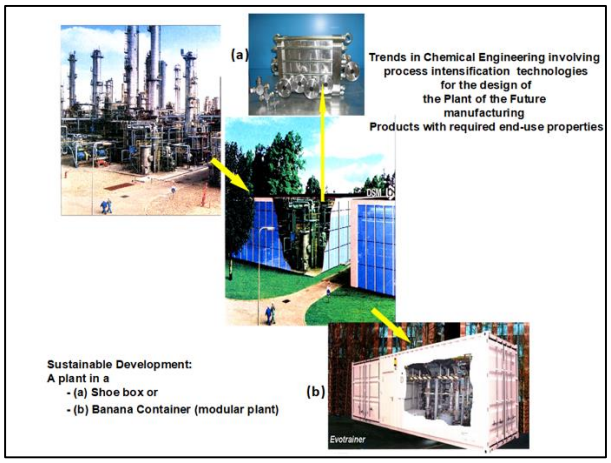

Figure 2

Figure 1: Example of different modeling approaches applied to a flue gas desulfurization unit
Figure 2: Examples of the utilization of the technologies of process intensification: schematic vision of how the eco-efficient "factory of the future" for the manufacturing of targeted customized products may look versus a conventional plant (top left), i.e., a plant in a shoe box for polymer production (a) or in a mobile banana container platform for small-scale production of specialties (b)

Actually, this multiscale approach of chemical engineering, "the green approach of process engineering" combines Innovative Design Sciences such as the C-K Theory that helps to find new processes and development ways while using and developing the knowledge basis of chemical engineering.

Moreover, it should be pointed out that present and future trends for investigations in process intensification will led to innovative continuous flow processes (i.e., novel process windows) and to innovative new equipment construction technologies (additive manufacturing, i.e., 3D printing of devices such as micromixers, microexchangers or micro structured reactors for chemical synthesis and analysis). These trends will contribute to the design of the eco-efficient "factory of the future": i.e., a plant in a "shoe box" for polymer production or a modular plant inside a mobile "banana container" platform for small-scale production of specialty chemicals (see schematic presentation on figure 2).

This compact manufacturing unit design is already and will be more and more driven by the advantages of continuous processing and efforts made in continuous manufacturing, ranging from the replacement of individual batch synthesis steps to complete end-to-end (chemicals to formulated products) continuous manufacturing, i.e., integration of synthesis, purification, and formulation in the same container (figure 2b). Actually, this trend in chemical engineering investigations emphasizes today process intensification with a continued development of compact manufacturing units promising localized, on-demand production of a wide range of products, including pharmaceutical, flavors, and specialty polymers. Moreover, this trend in chemical engineering will also contribute to the evolution in the manufacturing environment cointed as industry 4.0 which provides tools such as Artificial Intelligence, Machine Learning, Big Data, Augmented reality and Metaverse. Such tools could potentially contribute to a better understanding of phenomena that are difficult to explain within the framework of current available theoretical models and that consequently may contribute to a better understanding of consumer preference and market behaviour. They may lead to new modes of production and to the factory of the future that involves the concept of platforms and modular plants or container format approach to achieve faster product development (i.e., reducing time-to-market by some 50%) and address the growing trend of individual and customized products.

Finally, the previous today and future trends for the required advances in chemical engineering involve or require more and more innovation. This will be discussed and emphasized in the presentation.