CHEMICAL ENGINEERING in 2010, *QUO VAMUS*?

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Keywords: Future of process and chemical engineering, the length and time multiscale approach, the triplet “molecular Processes-Product-Process Engineering” approach, process intensification, product design and engineering, CAPE, green and sustainable chemical engineering.

Contents

Summary

In order both to respond the today’s economic demands and to remain competitive in global trade, the chemical and related industries have to satisfy the market requirements for high-volume low-price bulk intermediate chemicals or for specific nano- and micro-scale end-use properties of low-volume high-price specialty and functional chemical products, as well as the social and environmental constraints of industrial meso- and macro scale processes. This requires chemical engineering to follow a scientific approach that involves a multidisciplinary and multiscale time and length integrated system approach to the complex simultaneous and, often, coupled transfer phenomena and nonlinear, non-equilibrium molecular processes that occur on different length and time scales of the supply chain. That is, a good understanding of how phenomena at a smaller length scale relates to properties and behavior at a longer length scale is necessary (from the molecular- scale to the production-scales). This has been defined as the triplet "molecular Processes-Product-Process (3PE)" integrated multiscale approach of chemical engineering. Thus a modern sustainable and green chemical engineering can be summarized by four main objectives:

(1) Increase productivity and selectivity through intensification of intelligent operations and a multi scale approach to processes control: nano and micro-tailoring of materials with controlled structure;

(2) Design novel equipment based on scientific principles and new production methods: process intensification using multifunctional reactors or micro-engineering for micro structured equipment;

(3) Manufacturing end-use properties to synthesize structured products, combining several functions required by the customer with a special emphasis on complex fluids and solid technology, necessitating molecular modeling, polymorph prediction and sensor development,

(4) Implement multiscale application of computational chemical engineering modeling and simulation to real-life situations from the molecular scale to the production scale involving process control and safety, e.g. the computation of some desired information on a fine scale to pass a coarser scale or vice versa.

This chapter will emphasize the previous objectives that characterize the modern chemical engineering: a sustainable chemical engineering which is concerned by the development of the sciences and technologies encountered in the integrated multidisciplinary and the time and length multiscale 3PE approach to answer to the society demand of the couple green product design/green process engineering.

1. Introduction

Chemical and related process industries are at the heart of a great number of scientific and technological challenges posed to chemical engineers.

The chemical and related industries including oil and gas, oil shale, petrochemicals, pharmaceuticals and health, agriculture and food, environment, pulp and paper, textile and leather, iron and steel, bitumen, building materials, glass, surfactants, cosmetics and perfume, and electronics, etc, are today in a phase of rapid evolution. This development is due to unprecedented demands and constraints, stemming from public concern over environmental and safety issues. Chemical knowledge is also growing rapidly, and the rate of discovery increases every day. Over 14 million different molecular compounds could be synthesized in 2005. About 100,000 can be found today on the market, but only a small fraction of them are found in nature and most of them are deliberately conceived, designed, synthesized and manufactured to meet a human need, to test an idea or to satisfy our quest for knowledge. The development of combinatory chemical synthesis with the use of nano-and micro technology is a current example. Already chemistry plays an essential role in man’s attempt to feed the population of the planet, to tap new sources of energy, to cloth and house humankind, to improve health and eliminate sickness, to provide substitutes for rare raw materials, to design necessary materials for the ever growing new information and communication technologies and to monitor and to protect our environment, to cite but a few. But clearly today a great number of the demands concern the development of the biomaterials, the preparation of nanoparticles, controlled release of pharmaceutics, bio nanotechnologies, biomass conversion, use of ionic liquids and aqueous biphasic systems, the relaxation dynamics of complex molecular compounds, fabrication of polyphase microreactors for selective reactions, etc... All these demands are clearly focused on societal demands such as CO2 sequestration, chemical looping combustion, Methane CPO and reforming, biofuel synthesis or Hydrogen production. Most of these topics are listed in roadmaps published in the last decade, i.e., 12 principles of green chemistry (Anastas 1998) and of green engineering (Anastas, 2003), the UK IChemE 21st Century Chemical Engineering roadmap, 2007, the 12 great challenges listed by the American National Academy of Engineering (NAE USA 2008) or the European process intensification roadmap (ERPI 2008, www.creative-energy.org). These roadmaps insist on the planetary global anxiety where chemical and process engineering will play a crucial role: sustainability, health, security and environment, energy, water, food and drinks, biosystems engineering, solar energy, nuclear fusion, etc…. And these roadmaps militate for an evolution of chemical engineering towards a modern process engineering voluntarily concerned by sustainability: green engineering (Garcia-Serna et al., 2007).The existing processes and the new processes will have to be progressively adapted to the principles of the “green chemistry”.

Thus to imagine reactions that will convert chemical substances we find around us into substances or products that serve the consumer’s needs, such is the business of chemists and such are the problems and challenges posed to and by chemical and related process industries. So:

2. Expectations from Modern Chemical Engineering in the Face of Challenges.

What do we expect from a modern chemical and process engineering to assure competitiveness, employment and sustainability in the chemical and related process industries?

In fact there are two major demands associated with the previous challenges in order to assure development, competitiveness and employment in such process industries:

- How to product and with the help of which processes in order to compete in the global economy where the keywords are globalization of business, partnership, and innovation, mainly involving an acceleration of the speed of product innovation (innovation means discovery + development). This involves that the speed of product innovation is accelerating. For example in the fast moving consumer goods business to which the majority of the food business belongs, the half-life of product innovation (time to market) has decreased from 10 years in 1970 to an estimated 2-3 years in the year 2000 and currently, as a result of the increased competitive pressure in the market, one year for the half-life of product innovation is today often considered long. This means that it is increasingly difficult to be first on the market with an innovative product, and thus speeding up the product / process development is of paramount importance.
- How to answer to the evolution of market demands presenting a double challenge: in developing countries, manpower costs are low and there are less constraining local production regulations. In industrialized countries, there is rapid growth in consumer demand for targeted end-use properties, together with constraints stemming from public and media concerns over environmental and safety issues, in combination with tools like Life Cycle Exergy Analysis (LCEA) which clarifies quantification of resource depletion, waste emission and process losses when comparing different substances, and also Life Cycle Inventories (LCI) and Life Cycle Assessment (LCA) that are important tools which determine all environment impacts respectively “from cradle to factory gate” or “from cradle to grave”, see for

examples the European Registration, Evaluation, Authorization of CHemicals regulations (REACH http//ec.europa.eu/environment/chemicals/reach/reach_intro.htm) for chemical products.

To answer these two different demands and to respond to such a required development for sustainable products and processes and to offer a contribution to fight against the most often non-sustainable mankind of the today world production (remember that only 25 wt% of mother earth's extracted resources is used for the production of goods and services, the other 75% is lost due to pollution, waste and environment disturbances), *chemical engineering is already engaged but will be more and more in charge to research innovative processes for the production of commodity and intermediate products, and also to progress from traditional intermediate high bulk chemistry to new specialties and active material chemistry and related industry*. Henceforth chemical sciences and chemical and process engineering are confronted with challenges concerning complex systems especially at the molecular scale, at the product scale and at the process scale.

Indeed:

- **For the production of commodity and intermediate products** (ammonia, calcium carbonate, sulfuric acid, ethylene, methanol, ethanol), where patents usually do not concern the product but rather the process, the processes can no longer be selected on a basis of economical exploitation alone. Rather, the compensation resulting from increased selectivity and savings linked to the process itself must be considered, which frequently needs further research on the process itself. The issue is who can produce large quantities at the lowest possible price. And the economic constraint will no longer be defined as sale price minus capital plus operating plus raw material and energy costs. Indeed with high-volume bulk chemicals, the problem becomes complex, as factors such as safety, healthy, environmental aspects (including non-polluting technologies, reduction of raw materials and energy losses and product / by-product recycling), must be considered. For such high-volume bulk chemicals that still remain a major sector of the economy (40% of the market), the client will buy a process that is not polluting and perfectly safe and controlled. This requires the use of process system engineering (PSE) and computer-aided process engineering (CAPE) methodologies and tools. Furthermore it has to be added that the trend towards global-scale facilities may soon require a total or more probably a partial change of technology, with the current technology no longer be capable of being built "just a bit bigger" if one has to handle throughputs never seen before in chemical and related industries. Indeed it is scheduled that worldwide plant must increase by a six-fold by 2050 if a growth rate of 4% is assumed.

So, chemical engineers are faced with the need for a change in technologies to scale-up the reliability of new processes from the current semi-work scale to a vast scale in which there is no previous experience.

This may involve an integrated multiscale design in the principles of chemical process design, i.e. rather than adapting the operating conditions and chemistry to available equipment, the process structure, architecture and equipment are adapted to physical-chemical transformations. Indeed large scale production units can be created by integration and interconnection of diverse, small-scale locally structured elements into large-scale macro-production units. A to-day challenge is to involve the use of microtechnologies to design microstructured heat exchangers, mixers or reactors. An illustration has been the creation of the European industrial-academic research consortium on structured design, IMPULSE (Integrated Multiscale Process Units with Locally Structured Elements) (www.impulse-project.net). This consortium has developed during the period 2006-2009, concerted research actions that encourage the development of the necessary methodological tools required for the future industrial implementation of the approach i.e., to design the process around the chemistry with the use of intensified devices designed to do what the chemistry needs, and appropriate integration of these intensified devices into complete production units. This has required designing demonstrator units to prove the concept of feasibility and superiority of multiscale process technology (Jenck et al., 2004, Matlosz, 2009).

- **New specialties, active material chemistry and related industries** involve the chemistry/biology interface of the agriculture, food and health industries. Similarly, they involve upgrading and conversion of petroleum feedstock and intermediates, conversion of coal-derived chemicals or synthesis gas into fuels, hydrocarbons or oxygenates. This progression is driven by the today new market objectives, where sales and competitiveness are dominated by the end-use property of a product as well as its quality features and functions. Indeed, end consumers generally do not judge products according to technical specifications, but rather according to quality features, such as size, shape, colour, aesthetic, chemical and biological stability, degradability, therapeutic activity, handling, cohesion, friability, rugosity, taste, succulence, and, more generally sensory properties, and also according to their functions. For example the quality features such as sensorial, mechanical, rheological, and physicochemical are related to the material properties such as viscosity, dielectric constant, and so on, as well as to how the constituents are assembled to form the micro or nanostructure of the product, as characterized by structural attributes such as particle, bubble or droplet size distribution, phase volume fraction, and particle shape. An understanding of the relationships between product performance, and material properties and structural attributes enables the designer to select the proper ingredients and design the manufacturing process to obtain a product with the desired performance. So this control of the end use property, expertise in the design of the process, continual adjustments to meet the changing demands, and speed in reacting to market conditions are the dominant elements. The key to the production of pharmaceuticals or cosmetics is not their cost, but their time to market, i.e, the speed of their discovery and production. Moreover for products where the value is added by a specific nanostructure, the customer will pay a premium for such a function, be it in a food, in a cleaner, in a paint or in a coating. **These high-margin products** which involve customer-designed or perceived formulations **require for chemical engineers to design new plants, which are no longer optimized to produce one product at good quality and low cost.** Actually the client buys the product that is the most efficient and the first on the market and he will have to pay high prices and expect a large benefit from these short-lifetime and high-margin products. The need is for multipurpose systems and small size and generic equipment which will not be optimized but that can be easily cleaned and disinfected and easily switched over to other recipes (flexible production, small batches modular set-ups and so on).

The aforementioned considerations presenting issues and challenges about required process and product design in the framework of globalization, sustainability and demands on technological innovation, must be taken into account in the modern "green" chemical and process engineering of today. But how?

We shall try to answer this question in presenting, successively, the complementary to-day approach for a modern chemical engineering, which involves the organization of time and length scales and complexity levels, and then the 4 parallel tracks met for the education and investigations in the topic, for driving sustainable social and economic development.

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