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Among the trends for a modern chemical engineering: CAPE an efficient tool for process intensification and product design and engineering

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Abstract

To respond to the changing needs of the chemical and related industries in order both to meet the today's economy demands and to remain competitive in global trade, a modern chemical engineering is vital to satisfy both the market requirements for specific nano and-micro scale end-use properties of products, and the social and environmental constraints of industrial meso and-macro scale processes. Thus an integrated system approach of complex multidisciplinary, non-linear, non-equilibrium processes and phenomena occurring on different length and time scales of the supply chain, from molecular-scale to the production-scales, is required. A modern 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 and micro-engineering for micro structured equipment; (3) Extend chemical engineering methodology to product design and engineering using the "triplet molecular Processes-Product-Process Engineering (3PE)" approach; (4) Implement multiscale application of computational chemical engineering modelling and simulation to real-life situations from the molecular scale to the production scale, e.g., in order to understand how phenomena at a smaller length scale relate to properties and behaviour at a longer length scale.

The present publications will emphasis the multidisciplinary and multiscale approach of chemical engineering and the unique role of CAPE for investigations in the previous objectives**.**

Keywords

Future of chemical engineering, multidisciplinary and multiscale approach of chemical engineering, the triplet "molecular Processes-Product-Process Engineering", product design and engineering, end-use property, process intensification.

1. Current trends in chemistry and sustainable development

At the beginning of this new century, the chemical and related industries including petroleum, pharmaceuticals and health, agriculture and food, environment, textile, iron and steel, bitumous, building materials, glass, surfactants, cosmetics and perfume, and electronics, etc, are 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. The new keywords associated with modern chemistry in the 21st century are life sciences, information and communication sciences, and instrumentation.

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

There are two major demands:

- Knowledge of which products and processes will be competitive in the new global economy. Here the keywords are globalization of business, partnership, and innovation, mainly involving an acceleration of the speed of product innovation. For example, the half-life of product innovation (time to market) in the early 1970s was about 10 years. Currently, one year in often considered long, this is a result of the increased competitive pressure in the market. 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.
- Evolving market demands present 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 Analysis (from the cradle to the grave), see for examples the European REACH regulations.

To respond to such a required sustainable development and to offer a contribution to fight against the non-sustainable mankind of the to-day world production, chemistry and chemical engineering face the following challenges:

- 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. Innovative processes for the production of commodity and intermediate products, where patents usually do not concern the products, frequently need further research on the process itself. With such 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 loss and product / by-product recyclability must be considered. And the trend towards global-scale facilities may soon require a total change of technology, with the current technology no longer capable of being built "**just a bit bigger**" if one has to handle throughputs never seen before in the chemical industry. So we are face with a demand on **process intensification** leading to a possible change in technologies to scale up new processes reliably from the current semi-works scale to vast scale in which there is no previous experience.

New specialities, active material chemistry and related industries involve the chemistry/biology interface between 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 is driven by the today market objectives, where sales and competitiveness are dominated by the end-use property of a product as well as its quality features such as shape, colour, aesthetic, chemical and biological stability, degradability, therapeutic activity, rugosity, taste, succulence; and more generally sensory properties. The control of the end use property, expertise in the design of the process, continual adjustments to meet changing demands, and speed in reacting to market conditions are the dominant elements. These high-margin products involving customer-designed or perceived formulations for **product design and engineering** require process intensification with new plants, no longer optimized to produce one product at good quality and low cost. Instead the need is for multipurpose systems, easily switched over to other recipes (flexible production, small batches or continuous processes, modular set-ups and so on).

2. Today chemical engineering approach: The integrated multidisciplinary and multi time and length scales Process Engineering approach for Process Intensification and Product Design and Engineering

The purpose of teaching and basic research in chemical engineering is still the development of concepts, methods and techniques to better understand conceive and design processes to transform raw material and energy into useful products. This involves the synthesis of nano-and microstructures materials, design, scale-up or scale-down operation, control and optimization of industrial processes through physical-bio-chemical separations as well as through chemical, catalytic, biochemical, electrochemical, photochemical and agrochemical reactions. But the today emphasis on end-use properties requires also a wide variety of technologies including the new role of micro technology, i.e., the use of micro structured mixers and reactors for Process Intensification.

Moreover it is important to note that today 60% of all products sold by chemical and related companies are crystalline, polymeric, or amorphous solids. These materials must have a clearly defined shape in order to meet the designed and desired quality standards. This also applies to paste-like and emulsified products. Actual developments require increasingly specialized materials, active compound and special effects chemicals which are in fact much more complex in terms of molecular structure than traditional high bulk volume industrial chemicals.

Thus the modern chemical engineering is also concerned with understanding and developing systematic procedures for the design and optimal operation of chemical, petrochemical, pharmaceutical, food, cosmetics…process systems, ranging from the nano-and micro systems used for product analysis, tests or production to industrial-scale continuous and batch processes, all within the concept of the chemical supply chain.

This chain begins with chemical or other products that industry must synthesize and characterize at the molecular level. The molecules are then aggregated into clusters, particles, or thin films. These single or multiphase systems form microscopic mixtures of solid, paste-like, or emulsion products. The transition from chemistry and biology to engineering involves the design and analysis of production units, which are integrated into a process, which becomes part of a multi-process industrial site. Finally this site is part of the commercial enterprise driven by market considerations and demands the inclusion of the product quality.

In the supply chain, it should be emphasized that product quality is determined at the nano-and micro scales and that a product with a desired property must be investigated for both structure and function. Indeed the key to success is to obtain the desired end-use properties, and then to control product quality, by controlling the microstructure formation. So a thorough understanding of the structure/property relationship at both the molecular scale (e.g., surface physics

and chemistry) and the microscopic scale (e.g., coupling reaction mechanisms and fluid mechanics) is of primary importance to be able to design production processes. This will help to make the leap from the nano scale to the production process scales that ensure the customer quality requirements.
Moreover most of chemical processes are non-linear and non-equilibrium, belonging to the so-called complex systems for which multi-scale structure is the common nature.
This requires an integrated system approach for a multidisciplinary and multiscale modelling of complex, simultaneous and often coupled momentum, heat and mass transfer phenomena and kinetic processes taking place on different scales:

- different time scales (10^{-15} to10^{8}s) from femto and picosecond for the motion of atoms in a molecule during a chemical reaction, nanoseconds for molecular vibrations, hours for operating industrial processes, and centuries for the destruction of pollutants in the environment.
- different length scales (10^{-9} to10^{6}m) are encountered in industrial practice with approaches on the nanoscale (molecular processes, active sites), on the microscale (bubbles, droplets, particle wetting, and eddies); on the mesoscale for unit operation (reactors, exchangers, columns); on the macroscale for production units (plants, petrochemical complexes,..) and on the megascale(atmosphere, oceans and soils e.g., up to thousands of kilometres for dispersion of emissions into the atmosphere).

So organizing scales and complexity levels in process engineering is necessary in order to understand and describe the events at the nano and micro scales and to better convert molecules into useful and required products at the process scale i.e., organizing levels of complexity, by translating molecular processes into phenomenological macroscopic laws to create and control the required end-use properties and functionality of products manufactured by continuous or batch processes (transforming molecules into money).

I have defined this approach as “le Génie du triplet Processus-Produit-Procédé (G3P)” or “the molecular Processes-Product-Process Engineering (3PE)”: an integrated system approach of complex multidisciplinary non-linear and non-equilibrium phenomena occurring on different length and time scales, in order to understand how physical-bio-chemical phenomena at a smaller length-scale relate to properties and behaviour at a longer length-scale, e.g., organizing levels of complexity.
To illustrate, biology’s catalysts, enzymes, are protein molecules that substantially speed up the biochemical reaction in the cell, and understanding an enzyme at the molecular or nano scale level means that it may be tailored to produce a particular end-product at the product and process meso-and macro

scales (see Figure 1). This leads to considerable opportunities to apply genetic-level controls to make better biocatalysts and novel products, or develop new drugs and new therapies and biomimetic devices while responding to societal challenges. Moreover, advances in genomics mean that customised chemical products are likely to become more relevant, and very soon. And the ability to think across length scales makes chemical engineers particularly well poised to elucidate the mechanistic understanding of molecular and cell biology and its larger-scale manifestation, i.e., decoding communications between cells in the immune systems. So this multiscale approach has tremendous potential for linking marketing, modelling and optimisation tools to create the optimal chemical for every client or product.

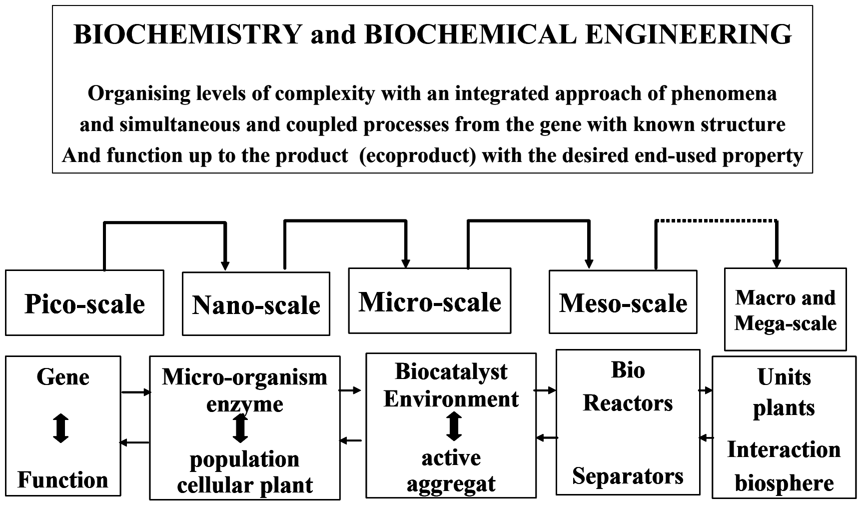

Figure 1: A view of modern multi length scales approach of biochemistry and biochemical approach

Another illustration of this approach is met in the design of artificial membranes, functionalized membranes and more generally membranes reactors, whose applications are found in water treatment, food and beverage, pharmaceutical and biotechnology, and biomedical, analytical and diagnostic applications. Indeed a deeper material analysis and characterization of structure and properties as well as modelling in design in molecular and nano scale levels becomes essential for a high control of process performances and advanced knowledge of membrane functions, i.e., for process intensification. This has justified the recent creation of the European Network of Excellence entitled "NanoMemPro" (www.nanomempro.com) whose project goal is "expanding membrane macro scale applications by exploring nano scale material properties". This underlines again the importance of the integrated multidisciplinary and multiscale approach.

So in addition to the basic and irreplaceable notions of unit operations, coupled heat, mass and momentum transfer, and the traditional tools of chemical engineering (separation engineering, catalysis, thermodynamics, process control), this integrated multidisciplinary and multiscale approach is a considerable advantage for the development and success of this engineering science in terms of concept and paradigms for both Process Intensification and Process Design and Engineering.

And it should be underlined that the 3PE approach is now possible thanks to significant simultaneous breakthroughs in three areas: molecular modelling in chemistry (both theory and computer simulation); scientific instrumentation and non-invasive measurement techniques coupled with image processing; and powerful computational tools and capabilities, especially involved and of great help for **modelling in CAPE new horizons.**

3. CAPE: Application of multiscale and multidisciplinary computational chemical engineering modelling and simulation to real-life situations: from the molecular scale to the overall complex production scale into the entire production site, including optimal process control, safety analysis and environmental impact

Computers have opened the way for the modelling of molecular and physical properties at **the nano-and microscopic scales**. Computer-aided molecular/mixture design (CAMD) is a promising topic in this area. It addresses the optimisation-based solution of the inverse problem of finding a compound or mixture of compounds, stemming from the very large number of degrees of freedom (that is, from the interactions). As a result, the computational requirements become excessive. And connecting design with reality, the consensus seems to be that simulation and computer-aid methods and tools for product design are useful in initial screening, but that experimental measurements are still essential for final design And through the interplay of molecular theory, simulation, and the experimental measurements a better quantitative understanding of structure-property relationships evolves, which, when coupled with macroscopic chemical engineering science forms the basis for the today required materials and process design.

Turning to the macroscopic scale, dynamic process modelling and process syntheses are increasingly being developed. To be competitive in the production of targeted products, just in time for delivery to the consumer whose needs are constantly evolving, requires analysis and optimization of the supply chains and the times taken by individual process stages. These also have to be simulated and evaluated in terms of costs. Indeed in the production site of the chemical and related process industries, the location of a particular component in the supply chain at a given time is not always well defined, i.e. a batch can be found in a stirred tank, a filter, a dryer, a pump, a mill and a storage container simultaneously. Event-driven simulation tools help solve these problems by simulating both material flows and states within the individual pieces of equipment, and by showing which alternative plant and storage strategies provide the greatest cost benefit. In certain occasions it has been shown that this dynamic simulation may enable to see in a matter of seconds whether bottle-necks may occur in the plant over the course of days, months or years. These can be eliminated by using additional pieces of equipment or by making additional resources available such as energy or manpower.

In the future, more effective CAPE is required to be competitive in the process industry, especially in expanding and developing interface specification standards to ensure interoperability of CAPE OPEN software components that will sustain growth and competitiveness. And challenges and opportunities still exist for the Process System Engineering PSE/CAPE community concerning several classes of chemical products, their design with respect to the important sustainable issues together with the need for appropriate tools.

Attention should be also focused on the systemic analytical models based on the multi-scale integrated approach previously referred that considers the global behaviour of complex systems as a whole, instead of looking at more and more mathematical details. Novel principles of the analytical models in chemical and process engineering should be sought at the highest level of integration. This approach is also required for a good understanding of the behaviour of the interactions in the optimal process control and operation. And it should be reminded that automation in world-scale plants provides high work force productivity, while in high margin multi-purpose plants it provides the capability to reach quality specifications and required throughputs quickly when restarting the process.

In conclusion it is interesting to underline the increasing part of the academic and industrial investigations in modelling, simulation, optimization, control and safety. But it should be emphasized that in order to help for process intensification and product design and engineering at any scale, modelling and simulation should be oriented towards the understanding of the physics, chemistry and biology of interactions rather than the refinement of numerical codes whose sophistication is not at all concerned with real life problems met in chemical pilot and production plants and in industrial practice for sustainable development.

Indeed never forget that in chemical engineering investigations on/in modelling and simulation, **what is needed in models is less anatomy and more physiology!**