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# Among the trends for a modern chemical engineering, the third paradigm: The time and length multiscale approach as 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 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 microscale end-use properties of products, and the social and environmental constraints of industrial meso and macroscale 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 is required. That is, a good understanding of how phenomena at a smaller length-scale relates to properties and behaviour 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. Indeed a modern chemical engineering can be summarized by four main objectives: (1) Increase productivity and selectivity through intensification of intelligent operations and a multiscale 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) 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, e.g., in order to understand how phenomena at a smaller length-scale relate to properties and behaviour at a longer length-scale. The presentation will emphasize the 3PE multiscale approach of chemical engineering for investigations in the previous objectives and on its success due to the today's considerable progress in the use of scientific instrumentation, in modeling, simulation and computer-aided tools, and in the systematic design methods.

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**Keywords:** Future of chemical engineering; The third paradigm: The multiscale methodology; The triplet "molecular Processes-Product-Process Engineering" approach; Product design and engineering; Process intensification; CAPE

## 1. Introduction: current trends in chemistry and sustainable development

The chemical and related industries including petroleum, pharmaceuticals and health, agriculture and food, environ-

ment, textile, iron and steel, bitumous, building materials, glass, surfactants, cosmetics and perfume, 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

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issues. Chemical knowledge is also growing rapidly, and the rate of discovery increases every day. The development of combinatorial 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 today's global economy. Here the keywords are globalization of business, partnership, and innovation, mainly involving an acceleration of the speed of product innovation. Currently, as a result of the increased competitive pressure in the market, 1 year for the half-life of product innovation (time to market) 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.
- Evolving 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 stakeholders analysis, indicators and LCA (from the cradle to the grave), e.g., the European REgistration, Evaluation, Authorization, of Chemicals (REACH) regulations for chemical products.

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, the following challenges are faced by chemical and process industries, involving complex systems at the process scale, at the product scale, and at the molecular-scale.

- For the production of commodity and intermediate products where patents usually do not concern 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 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 recyclability), 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 controlled and safe, which 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 technologies no longer capable of being built “just a bit

bigger”, if one has to handle throughputs never seen before in chemical and related industries. Indeed worldwide plant capacity must increase by a six-fold by 2050 if a growth rate of 4% is assumed. So we are faced with a demand on process intensification 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 where there is no previous experience. And large-scale production units can be created by integration and interconnection of diverse, small-scale locally structured elements into large-scale macro-production units (Jenck et al., 2004; Hasebe, 2004; Bayer et al., 2005).

- New specialities, 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 today's market objectives, where sales and competitiveness are dominated by the end-use property of a product as well as its quality features and functions including performance and convenience. 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 (cleansing, adhesion, etc.). 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 paint or in a coating. And these high-margin products which involve customer-designed or perceived formulations require new plants, which are no longer optimized to produce one product at good quality and low cost. Actually, for these short-lifetime and high-margin products, the client buys the product that is the most efficient and the first on the market, but pays high prices and expects a large benefit (Hill, 2004, 2009; Costa et al., 2006; Seider et al., 2009). The need is for multipurpose systems and generic equipments, which will not be optimized but that can be easily cleaned and easily switched over to other recipes (flexible production, small batches modular set-ups and so on). Also, it may happen that these products are not made in dedicated equipment but rather in whatever equipment that is available at the specific time.

The aforementioned considerations about required product design and associated process engineering 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 current complementary approach for chemical engineering, which involves the organization of scales and complexity levels and the application of multiscale and multidisciplinary computational chemical engineering modeling and simulation to real-life situations, from the molecular-scale to the overall complex production-scale for commercialization, i.e., CAPE.

## 2. A today's complementary approach in 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 (Mills et al., 2007; Hessel et al., 2008). 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-volume bulk 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 (Grossmann, 2004).

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 for inclusion of the product quality.

In the supply chain, it should be emphasized that product quality is determined at the nano- and microscales 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 nano- and/or 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 helps to make the leap from the nanoscale 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 multiscale structure is the common nature.

This requires an integrated system approach for a multidisciplinary and multiscale modeling of complex, simultaneous and often coupled momentum, heat and mass transfer phenomena and kinetic processes taking place on different scales:

- Different time scales ( $10^{-15}$  to  $10^8$  s) from femtoseconds and picoseconds 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 ( $10^{-9}$  to  $10^6$  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).

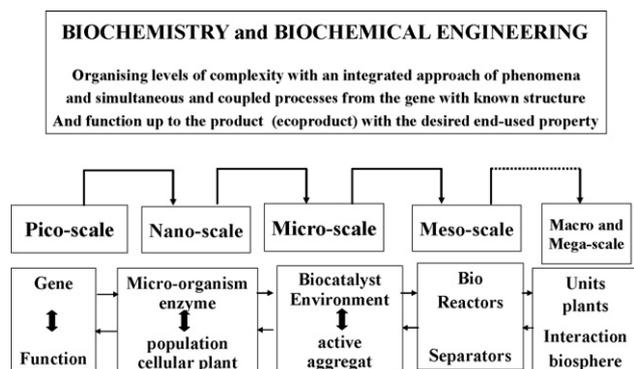
So organizing scales and complexity levels in process engineering is necessary to understand and describe the events at the nano and microscales and to better convert molecules into useful and required products at the process scale, i.e., organizing levels of complexity, by translating molecular processes 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) approach”: 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 (Charpentier, 2002). The associated idea of multiscale modeling is the computation of some desired information on a fine scale to pass a coarser scale or vice versa.

This multiscale approach is encountered in biotechnology and bioprocess engineering to better understand and control biological tools such as enzymes and microorganisms and to manufacture structured products. In such cases, it is necessary to organize the levels in terms of increasing complexity, from the gene with known properties and structure, up to the product-process couple, by through modeling of coupled mechanisms and processes that occur at different scales, as shown in Fig. 1 (Charpentier, 2004).

As highlighted in this figure, this approach covers the nanoscale (molecular and genomic processes, and metabolic transformations), the microscale (respectively, enzymes in integrated enzymatic systems, biocatalyst environment, and active aggregates), the mesoscale for unit operations (bioreactors, fermenters, exchangers, separators, etc.), and macroscales and megascales (respectively, for units and plants, and for the interaction with the biosphere).

Thus organizing levels of complexity at different length-scales, associated with an integrated approach to phenomena



**Fig. 1 – A view of modern multi length-scales approach of biochemistry and biochemical approach (Charpentier, 2004).**

and simultaneous and coupled processes, are at the heart of a new view of biochemical engineering.

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 nanoscale level means that it may be tailored to produce a particular end-product at the product and process meso- and macroscales (see Fig. 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 customized 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) using principles of chemical engineering (Chakraborty, 2003). Furthermore modeling and simulation of the human body on multiple scales provides the information necessary to develop highly efficient therapy strategies which aim at providing agent in the desired level of concentration right at the biological target such as a tumor by appropriate dosing strategies. And successful therapeutical strategies require multiscale modeling of the metabolism at the level of the cell, the organs and the complete human body on one hand and the drug delivery and dosing systems on the other hand (Klatt and Marquardt, 2007). So the multiscale approach has tremendous potential for linking marketing, modeling and optimization tools to create the optimal chemical for every client or product.

Another illustration of this multidisciplinary and multi-scale approach is met in the design of artificial membranes, functionalized and tailored membranes and more generally membrane 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 modeling for design at molecular and nanoscale levels becomes essential for a high-level control of process performances and advanced knowledge of membrane functions, i.e., for process intensification. In other words, how, with the limited available information, do we reliably link the macroscale process performance to local phenomena at the microscale (the membrane pore) or the nanoscale (solute–solute or solute–barrier inter-

actions)? This has supported the creation of the European Network of Excellence “NanoMemPro” whose title, “Expanding Membrane Macroscale Applications by Exploring Nanoscale Material Properties” ([www.nanomempro.com](http://www.nanomempro.com)) is quite comprehensive (Rios et al., 2007).

The above examples underline the importance of the integrated multidisciplinary and multiscale approach for product design and engineering (Charpentier, 2009). And it is clear that the rise in interest in multiscale modeling approaches and the integration and solution of composite models built from several partial models is driven primarily by product design where the nano and microscales characteristics are seen as vital to “designer” products. Combined with the meso and macroscale (which are typical issues at the equipment and plant levels), the emphasis on multiscale representation will continue to grow.

So, in addition to the basic and irreplaceable notions of unit operations, coupled heat, mass and momentum transfers, the traditional tools of chemical engineering, as well as the fundamentals of chemical and process engineering (separation engineering, catalysis, thermodynamics, process control, economic considerations, etc.), this integrated multidisciplinary and multiscale approach is beneficial and has considerable advantages for the development and success of this engineering science in terms of concept and paradigms for product design and engineering, especially in case of market-driven approach (Ng et al., 2005).

And it should be underlined that the 3PE integrated approach is now receiving more and more attention thanks to the considerable developments in the analytical scientific instrumentation and non-invasive instrumentation techniques coupled with image processing, and in the development and application of descriptive models of steady state and dynamic behaviour of the objects at the scale of interest: molecules, structure of the catalyst, sites and local fluid dynamics, catalyst particle, process unit, process plant, and supply chain (Charpentier, 2007a).

Let us now consider the multiscale computational chemical engineering modeling and simulation.

### 3. CAPE: application of multiscale and multidisciplinary computational chemical engineering modeling 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 chemical and process engineering in the modeling of molecular and physical properties at the nano- and microscopic scales.

There is no doubt that molecular modeling now has an increasingly important role in future product design and engineering research and practices (Gani, 2004a, 2004b; Ungerer et al., 2007; Gerbaud and Joulia, 2006; Eckl et al., 2008, to list a few).

To illustrate, if we take the case of chemical product design where the molecular design problem is transformed into a computer-aided molecular design (CAMD) problem, the solution of the molecular and mixture/blend design involves various approaches. For solvent design involving relatively small molecules, target properties relate to the macroscopic-

scale while for drug design involving relatively large and very large molecules, target properties relate to microscopic and/or mesoscopic scales. And in this last case, as well as in the case of very complex molecules where a high level of molecular structural information need to be considered, the CAMD methods employ problem specific models based on property–molecular structural relationships. The molecular structure plays an important role in the estimation of end-use properties related to the design of these large and/or complex molecules, and when microscopic and/or mesoscopic scales have been employed for their molecular structural representation, it is necessary to estimate properties through parameters obtained from, for example, molecular simulation (Gani, 2004b). However, there are still many challenges to be met, stemming from the very large numbers of degrees of freedom that needs to be satisfied for the molecular-level description of real-life systems (that is, from the interatomic interactions). As a result, the computational requirements may become excessive. Anyway, in regard to connecting design with reality and its complexity, the consensus seems to be that computer-aided methods and tools for chemical product design are useful with regard to initial screening, but that experimental data are still essential for final design. The current methods are able to contribute by solving some of the problems during the early stages of chemical product design and thereby contribute to chemical product design by reducing the time and effort to solve them.

And less expensive and more rapid than new measurements, molecular simulation nonetheless allows often an improved determination of the parameters of routine models. And through the interplay of molecular theory, simulation, and experimental measurements a better quantitative understanding of structure–property relations then evolves, which, when coupled with macroscopic chemical engineering science, can form the basis for materials and process design. The principle challenge, however, is still often to be able to combine computer models of these different scales, in order to understand how phenomena at a smaller length scale relate to properties and/or behaviour at a larger length scale. In this respect, a long-term challenge is often to combine the thermodynamics and physics of local structure-forming processes like network formation, phase separation, agglomeration, nucleation, crystallization, sintering, etc., with multiphase computer fluid dynamics (CFD).

Turning to the macroscopic scale, dynamic process modeling 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 general, the integration and opening of modeling and event-driven simulation environments, in response to the current demand for diverse and more complex models in process engineering, is currently occupying a more important place. The Computer Aided Process Engineering European program CAPE-OPEN “Next generation computer aided process engineering open simulation environment,” should be mentioned at this point. CAPE-OPEN is a set of standards that defines interfaces to allow the integration of process modeling software components from diverse pre-processor, solver and post-solver environments simulator sellers, European clients and academic researchers in computing and simulation. It aims to promote the adoption of a standard of communication between simulation systems at any time and length-scale level (property models, unit operations, numerical utilities for dynamic, static, batch simulations) to simulate processes and allow the customers to integrate the information from any simulation package into another (CAPE-OPEN Laboratories Network-CO-LaN Consortium, [www.colan.org](http://www.colan.org)).

And in the future, it is clear that 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 in order to insure that the CAPE-OPEN idea is applicable to recent technical changes, an overview of the CAPE-OPEN-specific interoperability guidelines has been prepared by CO-LaN that provides developers of process simulation environments (PMEs), with insight into how to implement various CAPE-OPEN functionality using .NET development tools (Barrett et al., 2007).

Anyway challenges and opportunities still exist for the Process System Engineering PSE/CAPE community concerning several classes of chemical products, their design and their corresponding processes (with respect to the important energy, environmental constraints and sustainable issues), together with the need for appropriate tools (Gani and Grossmann, 2007). Indeed in all cases, integration of the product and process design problem is achieved by solving simultaneously some aspects of the individual product and process design. And there still exist a need for a framework for this integrated multiscale product–process design by employing computer-aid methods and tools. Several authors have even emphasized the perspective, challenges, issues, needs, and have proposed future directions with respects to CAPE/PSE related research in this area in terms of environmental impact, LCA and/or sustainability (Grossmann, 2004; Gani, 2006; Gani and Grossmann, 2007). It is shown that many opportunities exist for the CAPE/PSE community to develop systematic model-based solution approaches that can be applied to a wide range of products and their corresponding processes, and that can help to find a solution, especially in terms of getting the product faster and cheaper to the market. It can be added that the widening span of the scales of the supply chain and the increasing diversity of processing methods call for a joint effort with the process intensification (PI) methodology, which aims at better utilization of physical resources and an associated reduction in numbers and sizes of process equipment (Becht et al., 2007; Charpentier, 2007b; Hessel et al., 2008; Moulijn et al., 2008).

#### 4. One remark concerning modeling and simulation for the integrated multiscale 3PE approach

One of the most important issues and needs related to the development of systematic computer-aided solution for product design and engineering methodologies are the models. For this integrated product–process design approach, in addition to the traditional process and equipment model, product models and product–process performance models, which simulate the function of the product during a specific application, are also needed. Constitutive (phenomena) models usually have a central role in all models types (Gani, 2006). Complementarily modeling should not be confused with numerical simulation. In contrast modeling must be an activity that requires knowledge and comprehension of scientific facts, experience, skills and judgment. More precisely the bottleneck for good models in the case of multiphase and complex systems is the understanding of the physics, chemistry and biology of the interactions rather than the refinement of numerical codes, whose sophistication is not at all concerned with real-life problems in laboratories, on pilot plants and production plants. One should not forget that in chemical engineering work related to product design and engineering, what is needed in models at the different levels of the supply chain is less anatomy and more physiology. This means that the models need to be developed through a systematic data collection and analysis effort, before any model-based integrated product–process tool of wide application range can be developed.

After this, attention should be also focused on the development of systemic analytical models, based on the multiscale 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 for integrated product–process design 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 process to be controlled, for control-oriented design, or for system diagnosis and management of the supply chain. Indeed remember that automation in world-scale plants provides high work force productivity, whereas in high-margin multi-purpose plants, it provides the capability to reach quality specifications and required throughputs quickly when restarting the process.

#### 5. Conclusions: the application of the multiscale methodology for a green chemical product design and engineering, and for process intensification, the third paradigm of chemical engineering?

The increased ability to monitor phenomena on the molecular and nanoscale has brought a fascination with molecular and nanoscale research, especially applied for chemical product design. While undoubtedly many important discoveries await us at these scales, the previously mentioned pressing challenges for product type and market segments relative to different types of industries require further development and implementation of rational methodologies for the transfer of molecular and nanoscale research and discoveries to production scale and commercial practice.

This is done by focusing simultaneously on process development and scale-up, and on developing techniques, and

simulation and modeling tools for multiscale analysis that will reduce scale-up risks. *And a process designed and engineered based on green chemistry principles for the customized product design, will commercially be “green” only if scaled up correctly, which will led to the development of cleaner new green processes, including process intensification (Charpentier, 2007b).* Clearly, a green chemical engineering involves sustainable products and processes.

So to satisfy the customer needs and market trends to obtain the desired products with innovative green processes, it has been shown that it is necessary to organize the levels of complexity that occur at the different levels of the supply chain, i.e., organizing levels of complexity, in order to understand how physical-bio-chemical phenomena at a smaller length-scale relate to properties and behaviour at a longer length-scale. This requires this “green” product–process design to follow a scientific approach – the 3PE approach – that includes a multidisciplinary and time and length multiscale integrated approach to the complex simultaneous and often coupled transport phenomena and molecular processes taking place on the different scales of the chemical supply chain. The associated idea of multiscale modeling is the computation of some desired information on a fine scale to pass a coarser scale or vice versa.

And in multiscale modeling, simulation, optimization, control and safety, it should be strongly mentioned that modeling 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 relevant with real-life problems met in laboratory, in plants and in industrial practice (“make models as simple as possible, but not simpler”, Einstein). Moreover it is recommended that the models should be developed through a systematic data collection and analysis effort, before any model-based integrated product–process tool of wide application range can be developed.

Finally in an era of globalization where the keywords concerning the paths for the future of chemical and process engineering are “process intensification” and “chemical product design and engineering”, *why not consider the integrated multiscale approach as the third paradigm of chemical engineering, if there is one?* Indeed this integrated approach is currently possible, thanks to considerable progress in the use of scientific instrumentation and powerful computational tools and capabilities, needed for modeling and simulation at different scales, and for systematic data collection and experimental verifications.

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