

# In the Framework of Global Trade, Sustainability and Industry Demand for Innovative Process and Technologies, what kind of Modern “Green” Chemical Engineering is Required for the Design of “the Factory of the Future”?

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**Abstract:** The chemical, petroleum, gas, energy and related industries are today confronted with the globalization of the markets, acceleration of partnerships and demand for innovative process and technologies for economic growth, and they are required to offer a contribution to the fight against environmental destruction and not always sustainable behavior of the today world production. This militates for the evolution of chemical engineering in favor of a modern green process engineering voluntarily concerned by sustainability that will face new challenges and stakes bearing on complex length and time multiscale systems at the molecular scale, at the product scale and at the process scale.

Indeed, the existing and the future industry processes are progressively adapted to the principles of the « green (bio) chemistry ». This involves a modern approach of chemical engineering that satisfies both the market requirements for specific nano and microscale end-use properties of competitive targeted green (sustainable) products, and the social and environmental constraints of sustainable industrial meso and macroscale production processes at the scales of the units and sites of production.

These multiscale constraints require an integrated 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 means a good understanding of how phenomena at a smaller length-scale relates to properties and behavior at a longer length-scale, from the molecular and active aggregates-scales up to the production-scales (*i.e.* the design of a refinery from the Schrödinger's equations...).

It will be seen that the success of this integrated multiscale approach for process innovation (the 3<sup>rd</sup> paradigm of chemical engineering) is mainly due to the considerable developments in the analytical scientific techniques coupled with image processing, in the powerful computational tools and capabilities (clusters, supercomputers, cloud computers, graphic processing units, numerical codes parallelization etc.) and in the development and application of descriptive models of steady state and dynamic behavior of the objects at the scale of interest.

This modern scientific multiscale approach of chemical engineering « the green approach of process engineering » that combines both market pull and technology push is strongly oriented on process intensification and on the couple green products/green processes “to produce much more and better in using much less”, *i.e.* to sustainably produce molecules and products responding to environmental and economic challenges.

It will be pointed out that process intensification due to innovative continuous flow process processes (novel process windows) and innovative technologies and new equipment construction technologies (additive manufacturing) 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 in a mobile banana container platform for small-scale production of specialty chemicals, or more generally modular plants leading to flexible chemical production by modularization and standardization in the pharmaceutical and specialty chemical industries and in a great number of other fields such as materials, petroleum and gas, water treatment and desalination and environmental management, among others.

**Keywords:** Green chemical and process engineering, Multiscale modeling, Sustainable product design and engineering, Novel process windows, Factory of the future, Modular plants, Additive manufacturing.

## 1. INTRODUCTION: CURRENT TRENDS AND DEMANDS IN CHEMICAL AND RELATED INDUSTRIES: NEEDS OF PROCESS INNOVATION LINKING MARKET PULL WITH THE CUSTOMER'S REQUIREMENTS TO TECHNOLOGY PUSH WITH SUSTAINABLE ENGINEERING AND TECHNOLOGY SOLUTIONS

Globalization, sustainability and necessary technological advancement and evolution are today

connecting industries, firms, and countries like never before, providing ample opportunity to improve or refine supply chain design. In this framework the chemical and related industries including oil and energy production, bitumous, pharmaceuticals and health, agriculture and food, phosphoric industry, environment, textile, iron and steel, 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, and fast-rising energy

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demand which will require the US \$45 trillion for new infrastructure investment by 2030 [1].

More precisely, a great number of the today demands concern the development of biomaterials, the preparation of nanoparticle, the controlled release of drugs, the bio nanotechnologies, the conversion of biomass, the use of ionic liquids and biphasic aqueous systems, the dynamic of relaxation of complex molecular compounds, the design of polyphasique micro structured reactors for selective reactions, to cite but a few. Most of these demands are clearly focused on societal requirements such as the CO<sub>2</sub> sequestration or its utilization as a feedstock, the chemical looping combustion, the synthesis of biodiesel, the production of hydrogen, the steam and dry methane reforming or the catalytic partial oxidation of methane to produce syngas (mixture of H<sub>2</sub> and CO) that is the feedstock for the natural gas-to-liquid processes, which increases the options for the transport and marketability of the remote gas resources. Moreover, increased opportunities to utilize methane as a feedstock for fuels and chemicals are now resulting from the “shale gas” revolution. A great number of these topics are listed in the European and North American « roadmaps » published in the last decade, which have pointed out a planetary global anxiety and concern where chemical engineering shall play a crucial role: sustainability, health, safety and environment, energy, water, food and drinks, biosystems engineering, solar energy, nuclear fusion, etc. So the existing processes and the future processes will be progressively adapted to the principles of the « green chemistry » [2]. And the roadmaps, proposed to respond to the changing needs of the chemical and related industries in order both to meet the previous today's economy demands and to remain competitive in global trade, militate for the evolution of chemical engineering in favour of a modern process engineering voluntarily concerned by sustainability (the green process engineering) that will face new challenges bearing on complex systems at the molecular scale, at the product scale and at the process scale, for the design of the factory of future in the framework of industry 4.0 [3, 4].

Moreover, chemical knowledge is also growing rapidly, and the rate of discovery increases every day. The development of combinatory chemical synthesis with the use of nano-and micro technology is a current example. Another one is the use of the so-called Big Data and the analytical strategies in the chemical supply chain design and optimization moving forward.

So, what can be expected from a modern chemical and process engineering to face the previous challenges, what kind of process engineering for technology innovation?

In fact, there are two major demands in order to assure development, competitiveness and employment in process industries [3, 5, 6]:

- How to answer to the rapid growth in consumer demands (market pull) for products with targeted end use properties, together with process constraints stemming from public and media concerns over environmental and safety issues, in combination with tools like stakeholders analysis, indicators such as Life Cycle Exergy Analysis (LCEA) which clarifies quantification of resource depletion, waste emission and process losses when comparing different substances, or 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”, e. g. the European Registration, Evaluation, Authorization of Chemicals regulations for chemical products (REACH, [http://ec.europa.eu/environment/chemicals/reach/reach\\_intro.htm](http://ec.europa.eu/environment/chemicals/reach/reach_intro.htm)) or the European Road Map for Process Intensification, Creative Energy-Energy transition (ERPI, <http://www.creative-energy.org>).
- How to product and with the help of which processes and technologies (technology push) in order to compete in the today's 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. 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 in several industry segments. This means that it is increasingly difficult to be first on the market with an innovative product, and thus speeding up the product / process sustainable development is of paramount importance.

So, to answer these two different demands for sustainable products with sustainable processes and involving 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), this requires that chemical and process engineering has to be more and more in charge of process innovation with the research of innovative processes and technologies.

## 2. WHAT KIND OF CHEMICAL ENGINEERING IS REQUIRED FOR PROCESS INNOVATION? NEEDS OF MULTISCALE APPROACH FOR TARGETED PRODUCT DESIGN AND ASSOCIATED SUSTAINABLE PROCESS ENGINEERING

In fact, chemical and process engineering together with chemical sciences 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 (ethylene, ammonia, calcium carbonate, sulfuric acid, methanol, ethanol, etc.), 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. Optimizing with traditional monetary objective is rarely adequate for finding sustainable solutions because of the presence of market externalities which are not reflected in the prices. Rather, the compensation resulting from increased selectivity and savings linked to the process itself must be considered, and the issue is who can produce large quantities at the lowest possible price with non-polluting technologies, reduction of raw materials and energy losses and product / by-product recyclability. For such high-volume bulk chemicals that still today 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. This requires new innovative approaches for process intensification and process control at the process plant-scale by using process system engineering (PSE) and computer-aided process engineering (CAPE) methodologies and tools [7, 55], including adaptive management and risk management. 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 innovation 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. 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 followed by an appropriate integration of these intensified devices into complete production units. 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 trend and challenge in the design of the factory of future is to involve the use of microtechnologies to design microstructured heat exchangers, mixers or reactors (F3 FACTORY, <http://www.f3factory.com>) [113].

- For the production of new specialties, active material chemistry and related fine chemistry industries (e.g., the fast moving consumer goods - FMCG), the chemistry/biology interface of the agriculture, food and health industries are involved. Similarly, the production of new specialties involves upgrading and conversion of petroleum feedstock and intermediates, conversion of coal-derived chemicals or synthesis gas into fuels, hydrocarbons or oxygenates. These productions are driven by today's market objectives, where sales and competitiveness are dominated not only by the technical or compositional specification of a product but rather by the end-use property of this product as well as its quality features, such as sensory properties, and functions, such as performance and convenience. This control of the end-use property at the molecular-scale, expertise in the design of the process, continual adjustments to meet the changing demands of the customers, and speed in reacting to market conditions are the dominant elements. Indeed, 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 an oil additive, in paint, in ink, in a cleaner, in a coating or in a food. More generally for the 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. The production of these high-margin products requires new plants, which are no longer optimized to produce one product at good quality and low cost. Here the need in process innovation requires multipurpose technologies and generic equipments, (flexible production, small-scale batches or continuous set-ups, modular setups and so on [109]).

The aforementioned considerations emphasize the today requirement of a chemical engineering that involves the integration of product systems engineering with the process plant scale because naturally the processing conditions will ultimately determine the product properties. So to-day process innovation is concerned by the multiscale phenomena encountered in the green product design and associated green process engineering, *i.e.*, fusing green chemistry and green engineering [8, 9]. And in the required modern chemical engineering for process innovation, this multiscale integration of the phenomena must be taken into account. But how and with which approach?

One answer is in presenting successively (i) the today's complementary approach for green chemical engineering, which involves the organization of scales and complexity levels and the application of the integrated multiscale and multidisciplinary computational modeling and simulation to real-life situations, from the molecular scale to the overall complex production scale into the entire production site of the supply chain for commercialization, including optimal process control, safety analysis and environmental impact, then (ii) the current models and simulation tools for the success of this multiscale modelling approach and (iii) the challenges and opportunities of this approach with integration of simulation codes.

### **3. THE TODAY'S APPROACH IN CHEMICAL ENGINEERING FOR PROCESS INNOVATION: THE INTEGRATED MULTIDISCIPLINARY AND TIME AND LENGTH MULTISCALE APPROACH IN THE CHEMICAL SUPPLY CHAIN**

The goal of basic research in chemical engineering is still the development of concepts, methods and

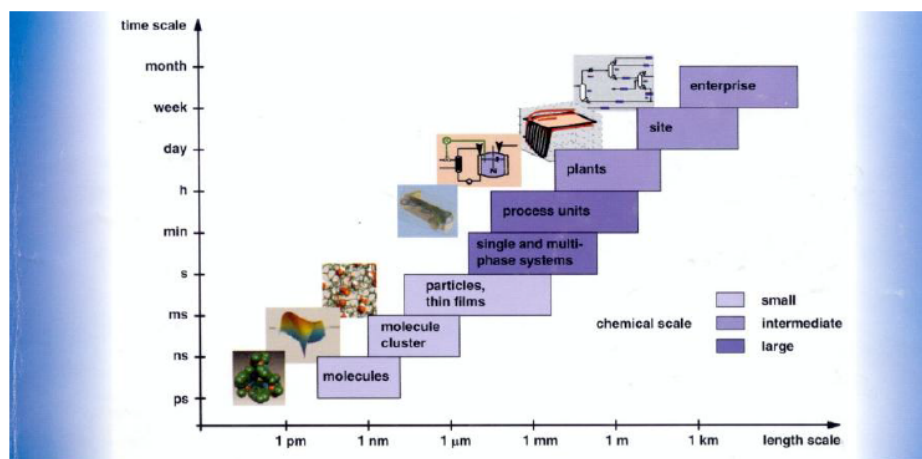
techniques to better understand conceive and design processes to transform raw material and energies into useful products. For illustration, this involves the synthesis of nano- and microstructured materials, design, scale-up or scale-down operation, control and optimization of industrial processes through physical-bio-chemical separations as well as through chemical, catalytic, biochemical, electrochemical, photochemical and agrochemical reactions.

But 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 catalytic reactors for process intensification [10]. Moreover it is important to note that today 60% of all products sold by chemical, oil and related companies are crystalline, polymeric, or amorphous solids. These materials must have a clearly defined shape at the product scale in order to meet the designed and desired quality standards. This also applies to paste-like and emulsified products. We have mentioned that actual developments require also 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 and related process systems, ranging from the nano- and micro systems used for product analysis, tests or production up to industrial-scale continuous and batch processes, all within the concept of the chemical supply chain (Figure 1 [11, 12]).

#### **3.1. The Chemical Supply Chain**

This chain begins with the set of chemicals or other products that industry must discover or synthesize and characterize at the molecular scale. The molecules are then aggregated into molecular clusters, microscopic particles and thin films as single or multiphase systems that finally take the form of macroscopic mixtures of solid, paste-like, or emulsion products. Through scale-up, the transition from chemistry and biology to engineering involves the design and analysis of the production units, which are integrated into a chemical process (*e.g.*, in a process flow sheet). Finally, that process becomes part of a site with multiple processes or several plants that are connected through suppliers, warehouses and distribution centres, which ultimately defines a commercial enterprise driven by business



Green Chemistry and Green Chemical Engineering are now concerned with the understanding and development of systematic procedures for the design and operation of chemical process systems, ranging: FROM Nano and microsystems-scales where chemicals have to be synthesized and characterized at the molecular-scale TO industrial-scale continuous and batch processes.

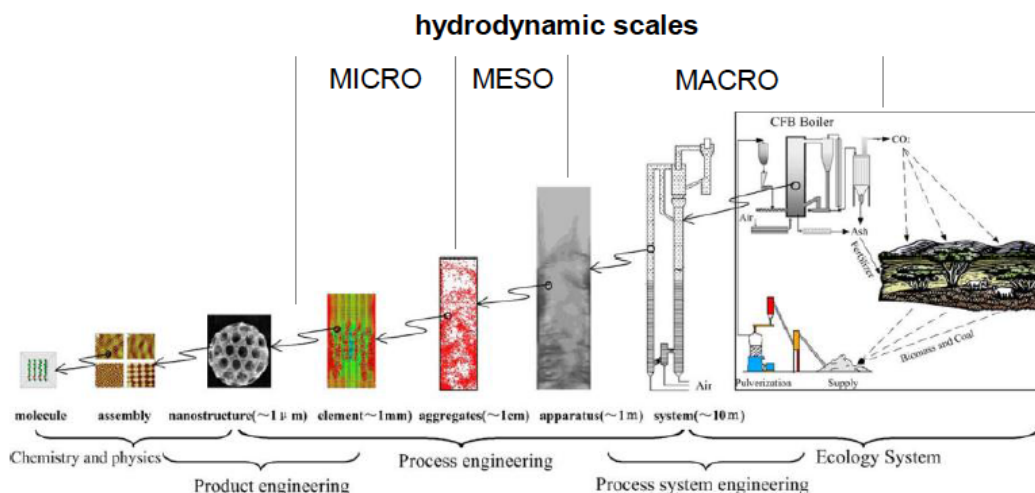
**Figure 1:** The time and length multi scales of the chemical supply chain.

considerations and market demands for inclusion of the product quality.

In the supply chain, it should be emphasized again that product quality is determined at the molecular nano- and/ or 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 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 macroscale that ensure the customer quality requirements at the product scale. And the ultimate aim is the translation of phenomenological laws and models, expressed by property, process and usage function, into commercial product technology. This requires the understanding of relationship between macroscopic performances and microscopic properties, and the ability to synthesize problems over length and time scales spanning many orders of magnitude.

To illustrate the Figure 2 [3, 13] shows a schematic vision of a catalytic multiscale fluidized-bed process with the localization of the different hydrodynamics

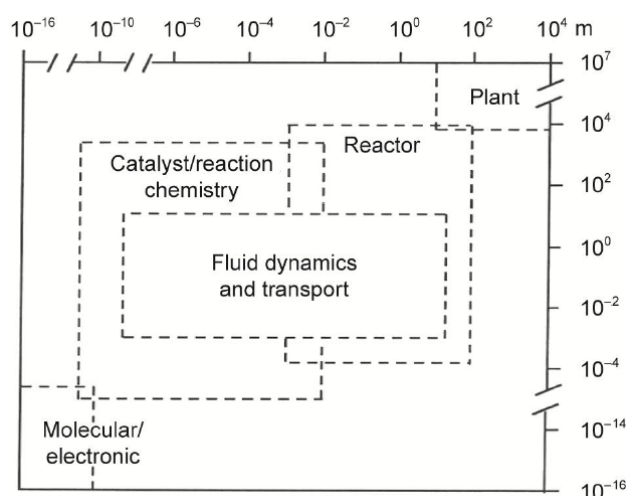


**Figure 2:** Different hydrodynamic length-scales of a catalytic fluidized-bed process.

length-scales with the links between phenomena involving physical-chemistry, product design and process engineering, process systems engineering and even the megascale ecological cycle.

Actually, most of chemical processes are non-linear and non-equilibrium. They belong 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 take place on different time and length scales encountered in industrial practise (Figure 3 [14]):

- different time scales ( $10^{-15}$  to  $10^8$ s) from femtoseconds and picoseconds for the oscillation of a hydrogen atom on the surface of catalyst nano particle or for the motion of atoms in a molecule during a chemical reaction, nanoseconds for molecular vibrations, up to hours and days for operating industrial processes and operational planning or months and years for tactical and strategic planning, and centuries for the destruction of pollutants in the environment.
- different length scales ( $10^{-9}$  to  $10^6$ m) encountered in industrial practise with approaches on the Angstroms (for the electronic structure, H-bond, ion, ion pair, network), on the nanoscale (for molecular processes, aggregate, self-assembly, active sites), on the microscale (for bubbles, droplets, surface and particle wetting, and



**Figure 3:** The industrial practice time and length scales covered in the multiscale approach.

eddies), on the mesoscale for unit operation (reactors, exchangers, separation columns and equipment); 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).

For example, in oil refining industry, the range of length scales from the refining chemical reactor main dimensions to the thickness of the liquid diffusion layer on the catalyst is about  $10^6$  orders of magnitude.

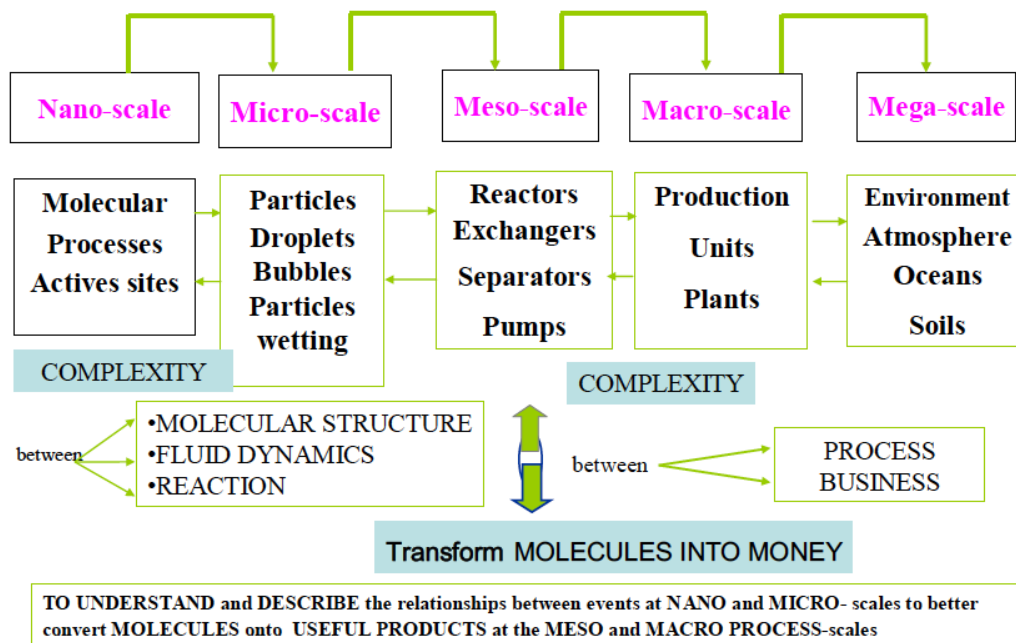
### 3.2. Organizing Scales and Complexity of the Chemical Supply Chain

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

This approach has been defined as “the triplet 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 of the chemical supply chain, 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 of the different length scales described in Figure 4 [15].

To illustrate, this multiscale approach is also encountered in biotechnology and bioprocess engineering to better understand and control biological tools such as enzymes and micro organisms biology’s catalysts and to manufacture structured products (drug-delivery systems and new therapies) [9, 65]. In such cases, it is necessary to organize the levels in terms of complexity, from the gene with known properties and structure, up to the product-process couple, through modelling of coupled mechanisms and process that occur at different scales, *i.e.*, the nanoscale (molecular and genomic processes, cellular phenomena and metabolic transformations), the microscale





**Figure 4:** Organizing levels of complexity underlie today view of chemical engineering: how to transform molecules into money at the production scales.

(respectively, enzymes in integrated enzymatic systems, biocatalyst environment, and active aggregates), the mesoscale for unit operations (bioreactors, fermenters, exchangers, separators, etc.) and the macroscale and megascale (respectively, for units and plants, and for the interaction with the biosphere).

More generally, the associated idea of multiscale modeling approach is the computation of some desired information on a fine scale to pass a coarser scale or vice versa, *i.e.* emphasizing the communication of information between scales. It is evident that efficient process development must rely on different simulation tools on different scales, one simulation on a given scale giving insights into the other in a two-way coupling approach.

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 micro scales characteristics are seen as vital to “designer” products. Combined with the meso and macroscale which are typical issues seen as vital to “designer” process at the equipment and plant levels, the emphasis on multiscale approach and representation will continue to grow for sustainable process innovation [13, 16].

So, it should be emphasized that, in addition to the basic and irreplaceable notions of unit operations and to the transport phenomena (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 conceptual integrated multidisciplinary and multiscale approach may be today considered as the 3<sup>rd</sup> paradigm of chemical engineering [17, 18]. When the fine analytical scientific instrumentation and the powerful numerical simulations are utilized at their utmost, this approach involves and led to a very thorough and detailed understanding of underlying mechanisms in all chemical engineering systems and processes, far beyond what it is possible to obtain with the paradigms of unit operations and transport phenomena only. Indeed, complementarily, this paradigm aims at the fully mechanism-based in-depth understanding of the entire domain related to chemical processes and production, which encompasses all forms of complexity of engineering interest (complex systems, non-linearity, multiple scales, green chemistry and sustainable production, sustainability, etc.) under the all-round support of modern analytic scientific instrumentation and computer science and techniques. Actually, this multiscale modelling paradigm is beneficial for multiscale process innovation and has considerable advantages for the development and success of a

modern chemical and process engineering in terms of concept and paradigms both for process intensification and for product design and engineering, especially in case of market driven approach for targeted products [5, 19, 20].

And it has to be underlined that the 3PE integrated approach is now receiving more and more attention thanks to the considerable developments, (i) in fine analytical scientific instrumentation and non-invasive monitoring techniques and related micro- and nano technologies in connection with signal and image processing, (ii) in the powerful computational tools and capabilities (clusters, supercomputers, cloud computers, central process unit, graphic processing units, numerical codes parallelization, many integrated core processors, etc.), and (iii) in the development and application of descriptive models of steady state and dynamic behaviour of the objects and events at the scale of interest: molecules, structure of the catalyst, sites and local fluid dynamics, surface state and local fluid dynamics, solid particles, catalyst particle, process unit, process plant, supply chain, and beyond including all control and operational support systems, if we take the applications in the oil and gas industries: Altogether, this involves molecular modelling (both theory and computer simulation), computer fluid dynamics and mixing, event-driven simulation tools and dynamic process system modelling.

We shall emphasize on these models and simulation tools in the next chapter.

#### 4. MODELS AND SIMULATION TOOLS FOR THE INTEGRATED “THE TRIPLET MOLECULAR PROCESSES-PRODUCT-PROCESS ENGINEERING (3PE)” APPROACH

The 3PE molecular Processes-Product-Process Engineering integrated modelling approach of complexity concerns the multiscale modelling to scale from the nanostructures and microstructures of the product end-use properties up to the scale of the equipment manufacturing this product. For example in petroleum industry, the integrated 3PE approach of the complexity concerns the modelling to scale from the atomic/molecular levels where the chemical reaction occurs on the catalyst surface up to the level of the catalytic unit in an oil and gas refining site.

Thus, the task of chemical engineering has been and always will be to design and implement the complete manufacturing systems up to the macro- and mega scales of the production units and environment. Complete systems involve both individual processes and plants for producing required products, as well as the integration of the individual processes into an overall production site, in terms of materials, energy, and logistics also taking into account the requirements of both customers and the larger society. Of course it would be unrealistic to expect that, in the near future, one single simulation tool will be able to address all subsystem levels simultaneously, e.g., to simulate simultaneously the many complex physical-bio-chemical, hydrodynamics, and momentum, mass and heat transfer phenomena occurring at the different time and length scales encountered in the units and the

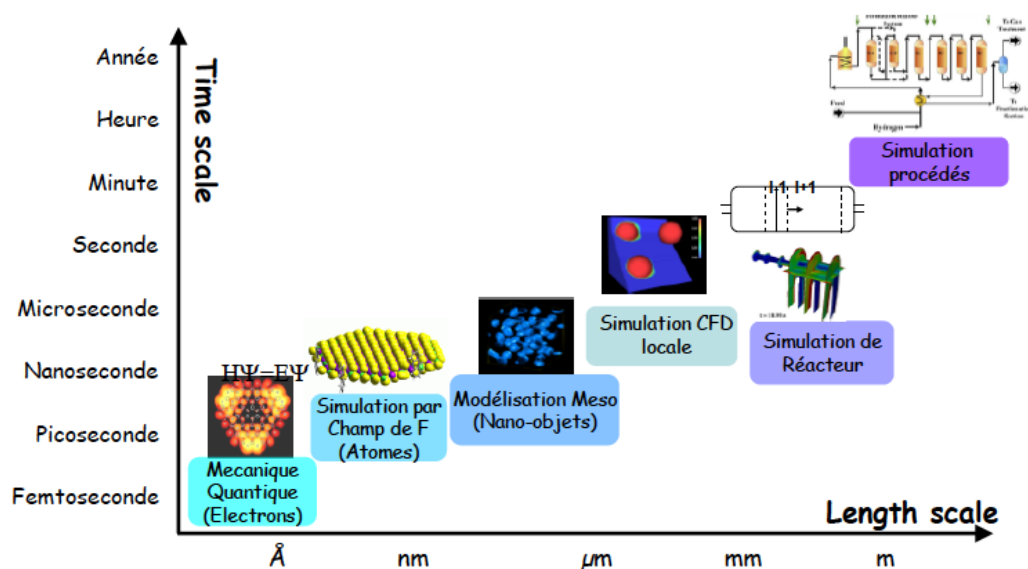


Figure 5: The scales of modeling and simulation in chemical engineering.



production site (Figure 5, [18]), (*i.e.*, to design a refinery from the Schrödinger equations!). As a result, a full CFD simulation of a process is today impossible, and may still remain impossible to some years to come, whatever the progress of CPU or GPU computing may be. Simplification is thus required, either by decoupling phenomena, or by considering a multiscale strategy combining different simulations on different scales, and often by making both. So, for process innovation, it continues to be the task of the chemical engineering to analyze subsystems at the scale level in the Figure 3 that is adequate to represent the individual problem's complexity. Then the models, based on this knowledge must reduce the complexity of the lower-level findings in such a way that the results can be integrated efficiently into the description of the problem solving at the higher levels presented in the Figures 3 and 4.

To illustrate the Figure 6 [13, 18] shows a schematic vision of the different step by step simulations of the events at different length scales in a catalytic multiscale fluidized-bed process: from the molecular scale up to the factory level including the flowsheet.

So, more generally it is clear that starting from the atomic and molecular scales, methods and simulation tools are required for the functional integration of the individual process steps and the integration of the individual production processes into the overall production complex or site (step by step integration).

This integrated multiscale approach necessitates the following models and computer simulations that enable to design individual step, structure the entire process, and place the individual process in the overall context of production.

#### 4.1. Models Used in the Multiscale Approaches

Models can be presented with decreasing time and length scales and can be distinguished into continuum models, mesoscale models, molecular dynamics and quantum mechanics models and they can be interconnected in a multiscale frame with macroscopic models.

##### 4.1.1. Continuum Models

Continuum models like fluid mechanics neglect the discrete nature of atoms, molecules, or particle and rely on macroscopic material properties. That way it is possible to simulate length scales significantly higher than molecular up to the size of reactors and provide important information on temperature, velocity, or particle concentration fields and residence times of a reactor as a result and as input at the smaller time and length scales. Continuum models also describe detailed reaction kinetics of precursors to identify rate-limiting reaction steps and develop more rigorous particle formation rates as input for population balance models (PBM) or to identify the most abundant nanocluster sizes (*i.e.* in operations such as

Step by step multiscale approach

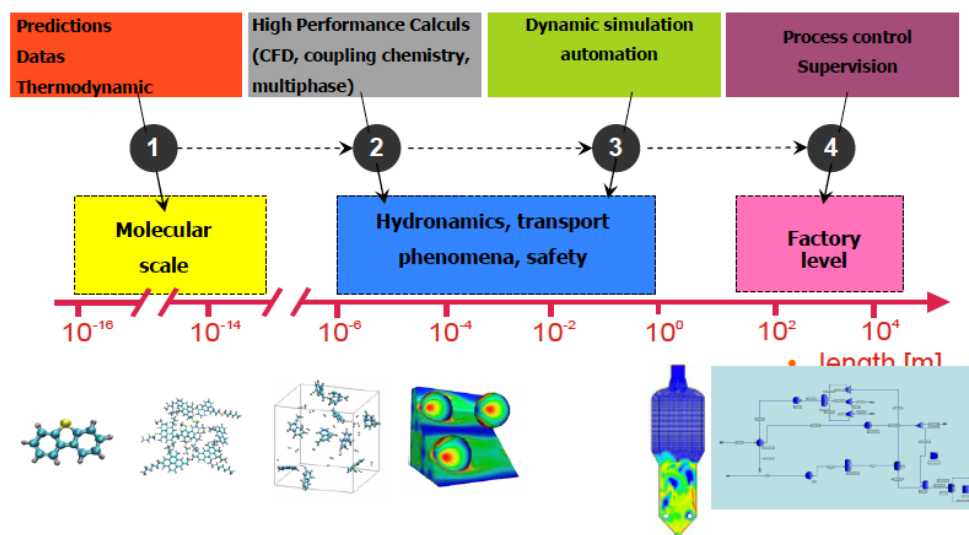


Figure 6: Schematic different length-scales simulation of a catalytic fluidized-bed process.

crystallization, sintering or gas-phase nanoparticle synthesis).

Reactors and units models based on computational fluid dynamics (CFD) simulate laminar or turbulent flow, temperature, and particle concentration fields by accounting for the reactor and internals geometry, particle dynamics and chemistry. Turbulent flows require, with increasing accuracy and computational demand, either additional models like the Reynolds-averaged Navier-Stokes (RANS) model (standard and realizable  $k-\epsilon$  model and the Reynolds shear stress model), the large eddy simulation (LES), or resolution of all turbulence scales as in direct numerical simulations (DNS). Direct numerical simulation is a powerful tool which has become more useful with the proliferation of high-performance computing [21]. DNS is unique in predicting physicochemical process consistent with the basic equations describing the phenomena of interest by resolving all length and time scales, *i.e.*, to model catalyst particle flows with heat transfer encountered in oil and gas industry (namely, fluidisation, sedimentation or transport) [22-24].

However, industrially relevant problems often require too big range of scales to be resolved by DNS. Thus, an increasing popular approach to reduce the computational costs is LES [25-28], which requires significantly less grid points than DNS. Large-scale features and interactions are resolved explicitly but the small-scale fluctuations and interactions are modelled by a subgrid-scale model to reduce the required resolution and compute-time. However, modeling these small-scale fluctuations, especially in turbulent, reacting, multiphase flows, is still a significant challenge and the high computational costs have often limited the application of LES and DNS to local phenomena revealing, *i.e.* the nanoparticle concentration gradients inside of turbulence eddies in multiphase reactors or complex turbulent flows in structured packings.

Still, at local scale in multiphase reactors, another type of CFD multiphase flow simulations, based upon the Finite Volume Method (FVM), deals with the Volume Of Fluid (VOF) approach [29]. The VOF method consists in an Eulerian description of each phase on a fixed grid, the interface between the two phases being calculated using the transport equation of the local volume fraction of one phase. The Navier-Stokes equations are solved according to a standard one-fluid formulation. The purpose of the one-fluid formulation is to describe the physical parameters for

both phases using only one equation valid in the entire computational domain. Combined with appropriate turbulent modelization, this method has been used to simulate the gas/liquid flow at liquid film scale, *i.e.*, wetting phenomena, effective interfacial area and liquid hold-up within structured packings [30-32], to simulate a single rising bubble with surface compression [33] or to simulate dispersed gas/liquid flows in bubble columns at high phase fractions [34].

Moreover, concerning the petroleum industries, in offshore exploitation conditions, a reactive gas absorption unit is on a floating vessel such as Floating Liquefied Natural Gas Vessel (FLNG) or a Floating Production Storage and Offloading (FPSO) vessel. The absorption column undergoes wave oscillation motions and significant accelerations and rolling conditions that might affect transfer efficiency and fluid distribution. It is interesting to underline that the use of VOF approach has been particularly interesting for the evaluation and design of high-performance and compact distribution technologies that are less sensitive to motion, and thus, reducing the floating absorption unit investment cost [35].

A review presenting the CFD methodologies applied to process development in the oil and gas industry with a focus on refining technologies is presented in [36]. It is shown how CFD can be used at all steps of the development of a new process, with a focus on refining techniques (distillation, trickle-bed reactors, FCC, new technologies such as distributor and new packings) and on new detailed design rules for the reactors or columns equipped with the latter, and the evaluation of the corresponding gain). Complementarily and also important for petrochemical industries, a comprehensive review of CFD methodologies to study the global and local fluid dynamics in bubble columns is presented in [37].

#### **4.1.2. Mesoscale Models**

Mesoscale models represent (gas, liquid, solid) agglomerate particles as geometric bodies (*e.g.*, spheres) and use rate models to describe their motion, size change, and overlap during surface growth, sintering, coagulation, crystallization or more generally any particle fragmentation. Mesoscale methods are also developed to model materials of the structure with length scale of hundred of nanometers, close to that of CFD. For example, such models provide important information about the evolution of the fractal dimensions and the agglomerate sintering rates which

can be used as input for the continuum particle population balance simulations while the primary particle coordination numbers define the setup of molecular dynamics simulation.

The particle population modelling (PBM) is a powerful modelling framework that allows predicting the dynamics of distributed properties of a population of individuals at the mesoscale (e.g., evolution of the particle size and morphology distribution) [38-41]. Though this modelling requires rates such as those describing coagulation, sintering, granulation and particle formation from mesoscale, and molecular dynamics or quantum mechanics simulations, particle population models are also ready to be coupled with fluid dynamics models to include the effect of spatial heterogeneities, *i.e.* in fluid-bed granulation processes [42].

There exist also other fundamental mesoscale models taking into account the relevant details of fluid-particle interactions. Lattice-Boltzmann model and the particle-particle interactions such as the discrete particle model (DPM) or Euler-Euler based models are used to develop closure laws to feed previous continuum models which can be used to compute the flow structures on a much larger industrial scale, *i.e.*, the formation and evolution of heterogeneous structures that strongly affect the performance of the process. To cite but a few among many applications in oil and gas industries, the Lattice Boltzmann approach has been used to investigate on the drag force in bubble swarms [44], to describe multiphase flow and phase-change heat transfer [43,88], to describe and elucidate the nature of in-line interactions and coalescence between bubbles rising in line in viscoelastic non-Newtonian fluids [47], to describe the dynamic behaviour of multiphase flows in a 1-D Fischer-Tropsch reactor [45], to describe a wide variety of problems including relative permeability and viscous fingering as well as membrane transport in fuel cells [46], or to provide new insight for understanding the microscale flow of shale gas in variable cross section nano-channels such as those encountered in shale gas reservoirs [89].

Besides, it is interesting to mention a comparative assessment of Lattice Boltzmann and Volume of Fluid approaches for generic multiphase multiscale problems (*i.e.*, two immiscible liquids like oil and water undergoing a mixing process) in terms of the accuracy of these techniques and their computational efficiency [48]. The LBM solver is based upon an in-house code

(written in FORTRAN 90) which uses the pseudopotential technique for multiphase flows. The VOF method was implemented using two Finite Volume Methods solvers, the OpenFOAM 2.3.0 (an open source framework in C++) and FLUENT 15.7 (a wide used commercial package). Among several results a comparison is presented for two cases of chlorobenzene droplets falling in water, with results compared to experiments. It appears that LBM clearly outperform VOF when comparing spurious velocity profiles and computational time (LBM is much faster than VOF). And VOF is generally more versatile in simulating droplets of various Reynolds numbers, in different shape regimes, which could not be done with the in-house LBM formulation.

#### **4.1.3. Molecular Dynamics and Quantum Mechanics Models**

Molecular dynamics (MD) models and various Monte-Carlo (MC) techniques such as kinetic MC or lattice MC account for the discrete nature of atoms, which is neglected in continuum and mesoscale models, thus limiting MD to shorter length and time scales. They have been used to investigate reaction pathways, transition states, evaporation, sintering rates and mechanisms to full coalescence or mechanisms of laser ablation. For example in operation such as gas-phase nanoparticle synthesis, the MD simulations provide detailed insights into sintering rates and mechanisms as function of particle size, composition, and crystal phase and with this, the major part of the product particle performance (end-use property) [49]. They are also used to drive the mesoscale models or describe the evolution of the surface area concentration in particle population balance models.

Quantum mechanics (QM) simulations are applied to develop simple force fields for molecular dynamics models or to determine thermochemical properties and reaction mechanisms which are required for the simulation of reacting flows using continuum fluid mechanics. More precisely, quantum mechanics is used to calculate the electronic structure of materials and quantum mechanics models describe molecules and matter very accurately. But they are often limited to very small systems of 1 to ca several 100 atoms due to the high computational costs. Among the various QM methods, Density Functional Theory (DFT) has become very popular since the development of improved functionals, which cannot be derived analytically, describing the exchange and correlation interactions to solve the electron-electron many body problem. DFT requires a relatively low computational

effort compared with other methods. The derivation of the functionals by fitting is the main reason why DFT leads to good results in many cases. A disadvantage is that local approximations do not allow accounting for van der Waals forces properly. However, DFT elucidates reaction rates and mechanisms, crystal structures or nanocluster structures and their dynamic behavior, or models chemical and physical processes at surfaces, or DFT investigates thermochemical properties of molecules to develop, e.g., gas-phase reaction system. And finally QM calculations are the most accurate simulations of matter, and methods like DFT in combination with new high-performance computing tools extends its range of application to particle/cluster sizes relevant for nanomaterials science [49]. Also to improve certain catalysts with a knowledge of details on how the chemical reaction occurs at the atomic/molecular level on the catalyst surface, it is important to mention that the empirical reactive force field ReaxFF, trained on the basis full quantum mechanical DFT calculations, has been proven as an effective approach to transfer information from the microscopic to mesoscopic space and time scales, hence overcoming limitations in computational capacities [50]. And as ReaxFF can manage the description of bond formation and breaking, but at much lower computational costs than DFT, larger systems (ca  $10^6$  atoms) can be simulated with trajectories at the nanosecond timescale.

It has to be underlined the applications of molecular simulation in the oil and gas industry since at least two decades [51]. And today computational modelling using DFT and related nanoscale approaches is allowing a *priori* prediction of catalyst performance (rates and selectivity), reducing the number of empirical formulations that must be prepared and tested. Of course, the ultimate performance must be validated experimentally to be credible, often using multi-throughput laboratory reactors or high throughput screening microreactors, but predictive capability is saving time and cost in preparation and characterization of new catalysts formulation.

For petroleum industry it is also interesting to mention investigations on the use of both molecular dynamics and Montecarlo methods for the predictions of different thermophysical properties for 25 primary, secondary and tertiary amines which are employed in gas absorption processes [52]. The calculations are based on a force field for amines developed at IFP Energies Nouvelles that follows the Anisotropic United Atom approach (AUA) to predict the behaviour of different amines [53-54]. It is clearly shown the role and

power that molecular simulation can play when predicting thermodynamic and transport properties such as surface tensions, viscosity coefficients, excess properties and Henry constants of gases in an amine aqueous solution. These results are also of first importance in the frame of industry problem of post-combustion flue gas CO<sub>2</sub> capture at coal-fired power plants.

Summarizing, it can be said that at the nano-and microscopic scales computers have opened the way for process innovation in the reaction pathway synthesis or in the modeling of molecular and physical properties, e.g. estimation of bulk phase thermodynamic and transport properties. And there is no doubt that molecular modeling and the application of the principles of statistical molecular mechanics computational techniques (e.g., molecular dynamics and various Monte-Carlo techniques) and quantum mechanics have also today an increasingly important role in the problem-oriented approach concerned in process innovation. To illustrate, relationships between materials structural and physicochemical properties (i.e., electronic structure, electronic conductivity, effective molecule gas diffusion coefficient) at the nanoscale for a catalyst particle and mesoscale for a catalyst packing cell can be built on the basis of molecular simulations (i.e., Coarse Grained Molecular Dynamics such as Monte-Carlo or dissipative particle dynamics).

To illustrate also, if we take the case of chemical product design where the molecular design problem is transformed into a computer-aided molecular design (CAMD) or a computer-aided mixture/blend design (CAM<sup>b</sup>D) problem [55], the solution of the molecular and mixture/blend design involves various multiscale approaches [56-58]. CAM<sup>b</sup>D is defined as follows: given a set of chemicals and a set of property constraints, determine the optimal mixture and/or blend consisting of a sub-set of chemicals [55]. CAM<sup>b</sup>D problems are usually formulated and solved as Mixed Integer Non Linear Programming (MINLP) or Mixed Integer Linear Programming (MILP). 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 CAM<sup>b</sup>D methods employ problem specific models based on property-molecular structural relationships of the end-use property.

Also let mention an integrated optimization-based CAM<sup>b</sup>D methodology proposed for cosmetics products formulation using integer programming which explicitly incorporates available heuristic rules (regarding ingredients functionality, and its recommended/allowed concentrations). These heuristic rules are converted into mathematical forms that are explicitly included in the optimal design problem, side by side with property models. Then a lab scale validation of the designed products, as obtained from the solution of the optimization algorithm, was carried out and showed excellent results concerning the rheological, textural and microstructural characteristics [123].

Main efforts on computer-aided product design have been recently directed to the design and analysis of a wide range of blended products, such as, polymer blends, formulated liquid products, solvent mixtures and lubricants, diesel surrogate, tailor-made jet fuel blend [77-81].

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 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 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, as already previously mentioned, 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 still often to combine the thermodynamics and physics of local structure-forming processes like network formation, phase separation, agglomeration, nucleation, crystallization, sintering, etc., with the multiphase computer fluid dynamics (CFD) models presented in § 4.1.1 and 4.1.2. Complementarily a list of today computer softwares which are predominantly used for

molecular mechanics calculations can be found with [https://en.m.wikipedia.org/wiki/Comparison\\_of\\_software\\_for\\_molecular\\_mechanics\\_modeling](https://en.m.wikipedia.org/wiki/Comparison_of_software_for_molecular_mechanics_modeling).

#### 4.1.4. Macroscale Models

Turning to the macroscopic scales of production units and multiproduct plants, dynamic process system modeling (PSM) as well as process synthesis methods 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, this requires analysis and optimization of the supply chains and the times taken by individual process stages and/or individual equipment (exchangers, reactors, pumps, storage tanks, etc.). 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 process 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 [59]. Actually, when such real-time simulation is finally achieved, this means that the operators can actually see the real process inside the control and monitored system, rather than some input and output parameters only. Moreover they may safely venture into abnormal or accident scenarii, so as to understand the reaction of the facility in these cases and develop proper measures to prevent and harness the situation.

So, the integration and opening of modeling and event-driven simulation environments, in response to the current demand for diverse and more complex models in chemical and 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 [60]. CAPE-OPEN is a set of standards that defines

interfaces to allow the compatibility and 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: see CAPE-OPEN Laboratories Network-CO-LaN Consortium, [www.colan.org](http://www.colan.org). The result of CAPE-OPEN has been vital for the improvement of openness in commercial process modelling software and for the development of open simulation platforms such as CHEOPS for polymer manufacturing (modelling and simulation) [61].

And in the future, for process innovation it is obvious that more effective CAPE will continue to be 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, particularly to evaluate the process sustainability [62, 63].

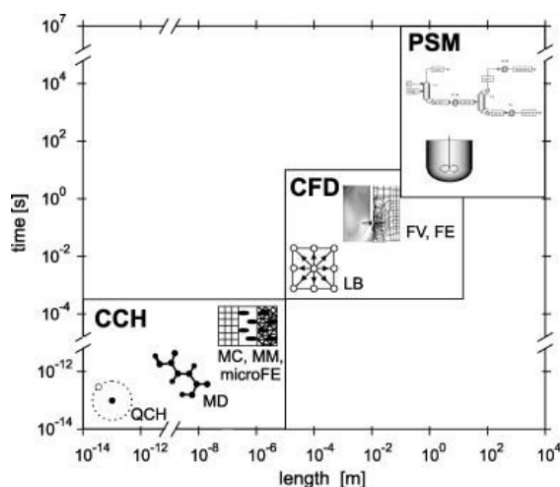
#### 4.2. Challenges and Opportunities for the Multiscale Modelling Approach with Integration of Simulation Codes

It is clear that challenges and opportunities yet exist for multiscale process engineering 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. Indeed, as explained previously, in all cases, integration of the product and process design problem is achieved only by solving simultaneously some aspects of the individual product and process design.

So, there still exist a need of a framework for employing the integrated 3PE multiscale approach - molecular processes-product-process- for product/process design and optimization with using computer-aided methods and tools to develop systematic model-based solution approaches that can be applied to a wide range of products and their corresponding processes in the supply chain design and optimization [64]. Such a framework could help to find a solution, especially in terms of getting the targetted product faster and cheaper to dynamic and competitive markets, *e.g.*, concerning a systematic multiscale method for studying the structure-performance relationship of drug-delivery system [65] or for designing and analysing mixture blended products such as solvent mixtures or fuel surrogates [77, 78].

Furthermore, it is interesting to note that for the integration of the modelling and simulation methods, the concept of multiscale modelling of product manufacturing can be interestingly presented based on integration of three modelling and simulation methods currently applied at previous different scales of length and time: they are respectively process system modelling (PSM), computational fluid dynamic (CFD) and computational chemistry (CCH) [66]. Figure 7



PSM – process system modeling, CFD – computational fluid dynamics, CCH – computational chemistry, FV – finite volume, FE – finite element, LB – lattice-Boltzmann approach, MC – Monte Carlo, MM – mesoscale, microFE – micro-finite element, MD – molecular dynamics, QCH – quantum chemistry.

**Figure 7:** Computational tools in multiscale modelling.



shows schematically the ranges of both length and time characteristics for individual means of numerical analysis in process engineering where it is indicated within each group the scales corresponding to different models presented in § 4.1. The software categories focus respectively on the efficacy of the production system, on the transport processes in individual equipment units, and on the molecular structure and thermodynamics of the molecular processes.

The important demand of the markets for the production of targeted products requires the integration of the numeric tools of the computational fluid dynamic CFD with tools of modelling and simulation of the computational chemistry CCH and also with the tools of the process system modelling PSM at scales which are higher than those of the computer fluid dynamic. Figure 7 shows that there exists a small gap in the integration of CCH and CFD and it seems that the Lattice-Boltzmann (LB) and Volume of Fluid (VOF) approaches are the best candidates to link CFD with CCH, e.g., for modelling colloidal dynamics with mesoscopic features [67], for the simulation of the expansion of polyurethane foams of industrial interest [68] or for the modelling of surface chemistry for the simulation of catalytic fluidized bed reactors [69]. In addition, another interesting potential option is the integration of the mesoscale modeling (MM) techniques, i.e., micro finite elements (microFE) with CFD approach, which could provide information on properties of pure components or complex materials [66].

Also along with progress in molecular modelling, new reports on numerical modelling in nanoscale are published and the two boundary modelling methods, i.e. PSM and CCH deliver and use different types of informations, namely, the CCH models are used for determining the missing thermodynamic data in process simulators (PSM) [70]. These informations are complementary to different extent with that required for use in CFD simulations or resulted from them. Moreover, there exists a general scheme of data exchange between the PSM and CFD software packages involving a middleware which participates in data exchange and management, as being a part of either a PSM package or a CFD package or an independent interface [66].

Anyway more generally, it is clear that solving large-scale, complex, multi-scale supply chain models still poses a technical challenge that must be addressed. Indeed, towards computer-aided multiscale modelling needs a methodology overarching the 3 CCH, CFD, PSM domains and a computer-based support of

conceptual modelling which could provide a generic set of tools (i.e., development of a Computer-aided Conceptual Modelling Tool which should be a prototypical tool for conceptual modelling [71]). For example, in case of gas solid fluidization, focusing on the mesoscale hydrodynamics phenomena, a multiscale computing paradigm termed the energy minimization multiscale (EMMS) modelling has been proposed as a variational multiscale methodology to model the circulating fluidized bed riser, i.e., to predict hydrodynamic structures as a function of scale [72, 73]. Actually the computational intensity is high, which needs more efficient approaches and algorithms. But the targeted goal is “Virtual Process Engineering (VPE)” for *a priori* development and design of new processes from first principles [72]. Similarly, in case of product design and engineering, “Virtual Product-Process Design Laboratory (virtual PPD-lab) Excel based software is proposed as an overarching tool for chemical product and process design and for managing the complexity in the verification of formulated products [74-76].

Finally, if the multiscale computational chemical engineering approach will led towards thorough ultimate mechanism-based in-depth understanding of chemical processes and precise application [82], it is also clear that this theoretical analysis and modelling approach still require reducing the voluminous amount of digital figures obtained from numerical simulations into concise formulation for facile application. This need is further emphasized with the opportunity due to the dawn of the Big Data movement (i.e., involvement of big data obtained by artificial intelligence and machine learning), which will provide in the future the supply chain designers even more detailed data that can help to bridge the spatial and temporal scales of the supply chain [83, 84].

Summarizing, the Figure 7 shows the challenges still encountered with the multiscale modelling approach applying integration of simulation codes: there is a need of a methodology which should be grounded on a unified hierarchical framework of multiscale systems theories to achieve a high degree of generality. And it seems that an efficient candidate for successful linking the three package systems (CCH, CFD and PSM) stays yet today the CAPE-OPEN standard. Indeed, as explained above, CAPE-OPEN defines rules and common interfaces for integration and interoperability of process modeling software components. Information transfer between a process simulator and individual modules can be carried out

through software tools for interfacing packages applied in different operating systems.

It can be added that the widening span of the scales of the supply chain and the increasing diversity of processing methods offer the great opportunity of a call for a joint effort with the multiscale process intensification (PI) methodology, which aims at better utilization of physical resources and an associated reduction in numbers and sizes of multiphase process equipment. [85-87, 90].

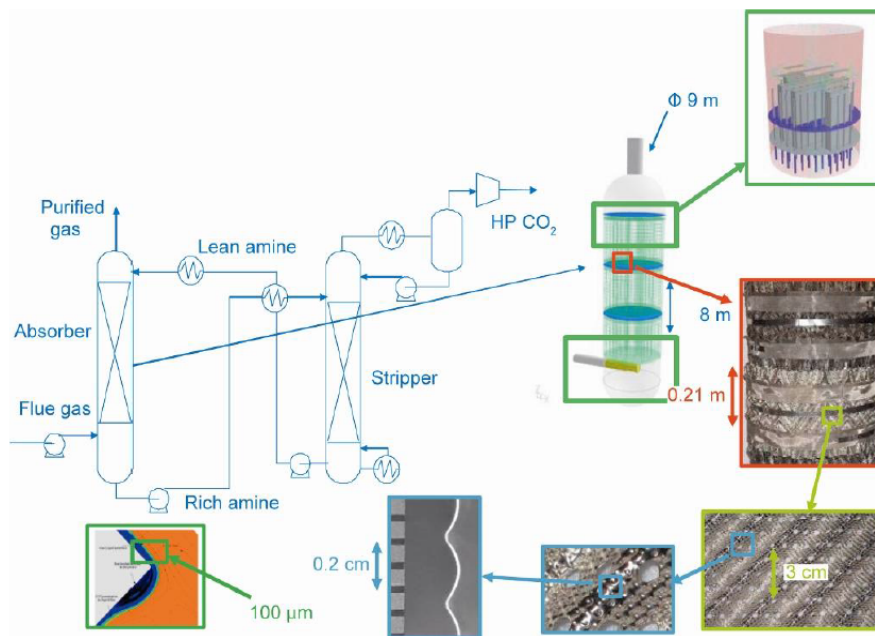
## 5. CONCLUSION: WHAT KIND OF MODERN “GREEN” CHEMICAL ENGINEERING FOR PROCESS AND TECHNOLOGIES INNOVATION AIMING THE DESIGN OF “THE FACTORY OF THE FUTURE”?

The increased ability to monitor phenomena on the molecular and nanoscale has brought a fascination with molecular and nanoscale research, especially applied for reaction pathway synthesis or chemical product design. Undoubtedly many important discoveries await us at these scales. But the previously mentioned pressing challenges requiring process innovation for product type and market segments relative to different types of industries, especially oil, gas and energies industries require further development and implementation of rational methodologies for the transfer of molecular and nanoscale research and discoveries to production scales and commercial practice.

This is done by focusing simultaneously on process development and scale-up, and on developing technologies, 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 (sustainable) processes, including process intensification for example. Clearly, process innovation for the factory of the future requires the methodology of the 3<sup>rd</sup> paradigm of chemical engineering, *i.e.*, the integrated multiscale approaches leading to both sustainable products and processes, which necessitate a good understanding and comprehension of the interplay between the phenomena concerned on different scales.

In oil and gas industries, as previously described and explained, significant progress has been made in recent years on a variety of levels, both experimentally and computationally, with the description of catalysts, adsorbents, solvents, complex feedstocks and multiphase flows, and process system control. Individually, these efforts have already had an impact on process design and modeling, and process performance.

To illustrate, the Figure 8 presents an efficient process development strategy approach based on differential simulation tools used at different length



**Figure 8:** The different scales of the different simulations of a gas treatment process or a post-combustion CO<sub>2</sub> capture process.

scales, one simulation at a given scale giving insights for the other in a two-way coupling approach [18, 28].

To reduce significantly the costs of a gas treatment process or a CO<sub>2</sub> capture process, several types of simulations can be used. First of all, a quick techno-economical study performed with appropriated simulation tool can be used at process global scale to show how capex and associated column designs are important. Second, process simulations (based on thermodynamics, kinetics and mass transfer) can be used to identify the most important drivers that control the design of the absorption columns. Last, computational fluid dynamics (CFD) simulations can be performed to determine flow characteristics in the packed columns. CFD is used with several approaches, from small scale to large scale through mesoscale. For example CFD can be used at small scale for gas/liquid volume of fluid (VOF) simulations, and at column scale for studying entrance effects. The combination of all these simulations, performed in two-way coupling methodology, has allowed for determining optimum designs and appropriate choices of packing and fluid distribution technologies for a gas treatment process or a post-combustion CO<sub>2</sub> capture process [28, 32].

Thus, as shown in this illustration, it is clear that multiscale approaches are now emerging in force offering significant opportunities for process innovation. But, more generally, it has to be precised that the integrated multiscale approach still today requires detailed knowledge, description, experiments, modeling and simulation at the different scales of the chemical supply chain e.g. in case of petroleum industries: molecules, feed molecular species, structure of the catalyst, sites and local fluid dynamics, surface state and local fluid dynamics, catalyst particle, process unit, process plant, and beyond including all control and operational support systems. This approach also still requires as a first step of investigations the comprehension of the interplay between the phenomena concerned only for a small number of scales among all the scales concerned by the integrated 3PE approach, *i.e.* the scales between molecular species and catalyst sites and particle, or the scales between catalyst pellets and contacting fluids, or the different scales encountered for fluid-particle and particle-particle interactions in multiphase reactors or contactors, and so on.

Coming back to process innovation for the design of the factory of the future which is confronted with the constraints of globalization of the markets, acceleration

of partnerships and innovation, and to offer a contribution to the fight against environmental destruction and not always sustainable behaviour of the today world production, it has to be underlined that the chemical, petroleum and related industries militate for this evolution of chemical engineering *in favour of a modern process engineering voluntarily concerned by sustainability* (the green process engineering) that will face new challenges and stakes bearing on complex systems at the molecular scale, at the product scale and at the process scale, as previously described.

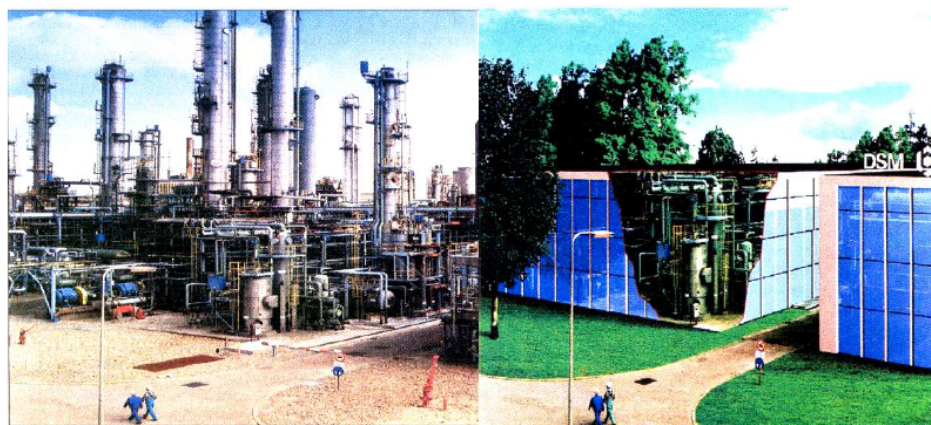
We have seen also that these last constraints require an integrated system modelling approach of complex multidisciplinary, non-linear, non equilibrium processes and transport phenomena occurring on the different time and length scales of the chemical supply chain. This modelling approach is also expected to play a central role in addressing scale-up, risk, and safety issues.

Thus, it is clear that this modern scientific multiscale approach of chemical engineering « *the green approach of process engineering* » that combines both market pull and technology push is totally involved in the design of the eco-efficient Factory of the Future whose objectives are strongly oriented on process intensification and on the couple green products/green processes “*to produce much more and better in using much less*”, and to sustainably produce molecules and products responding to environmental and economic challenges at process scale, aiming to economic growth. Such today and future trends 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 [3, 85].

In that framework and approach, the Figure 9 presents a schematic vision of the eco-efficient factory of the future, compared with a conventional plant [91]. The eco-efficient factory of future involves process intensification, operating with multiscale multifunctional equipment such as catalytic distillation columns, dividing wall columns as well as membrane technology allowing simultaneously reaction and separation processes [90, 92-94], or through the use of micro technology, such as microchannel (less than about one millimetre scale) mixers, heat exchangers and continuous flow microstructured reactors [95-97, 116].

The most important features achievable using microreacting systems are the improve heat and mass transfer. This turns also into improved safety and in

One vision of how a future plant employing Process Intensification  
may look (right) vs. a conventional plant (left).  
(Rendering courtesy of DSM)



OPERATING with NON POLLUTING and VERY EFFICIENT PROCESSES involving  
PROCESS INTENSIFICATION for the production of products with required end-use properties

SAVINGS ABOUT 30% (RAW MATERIALS + ENERGY + OPERATING COSTS)

**Figure 9:** One vision of the factory of the future.

most cases into higher selectivity and productivity. The scale-up strategy of these microreactors involves the parallel numbering up, the consecutive or the scale-out by selective dimension enlarging [96-100]. The continuous operating condition rates may vary from several litres per hour for pharmaceutical and cosmetic applications, specialty chemicals, polymers, nanomaterials synthesis and energy applications such as microcombustors, up to several tens of m<sup>3</sup>/hour for chemical and petroleum applications such as, polymer or oxygenate production and vapour catalytic reforming [101-103].

It is interesting to precise that such operating conditions with multiscale multifunctional equipment and/or microstructured equipment and reactors may lead to about 30% cost savings (raw materials, energy and operating costs) [85].

Besides, it appears clearly that the use of multiple parallel microreactors technology has increased productivity in catalyst testing and process development in chemical and petroleum industries [87, 104]. Moreover, the term of flow chemistry has appeared to describe chemistry performed in continuous flow in microreactor, in contrast to the conventional batch chemistry. Actually, the high rates of heat and mass transfer, minimum axial dispersion, high interfacial area and the mixing time faster than 1 s allow micro/milli channel reactors to run high exothermic, toxic or even explosive reactions safely,

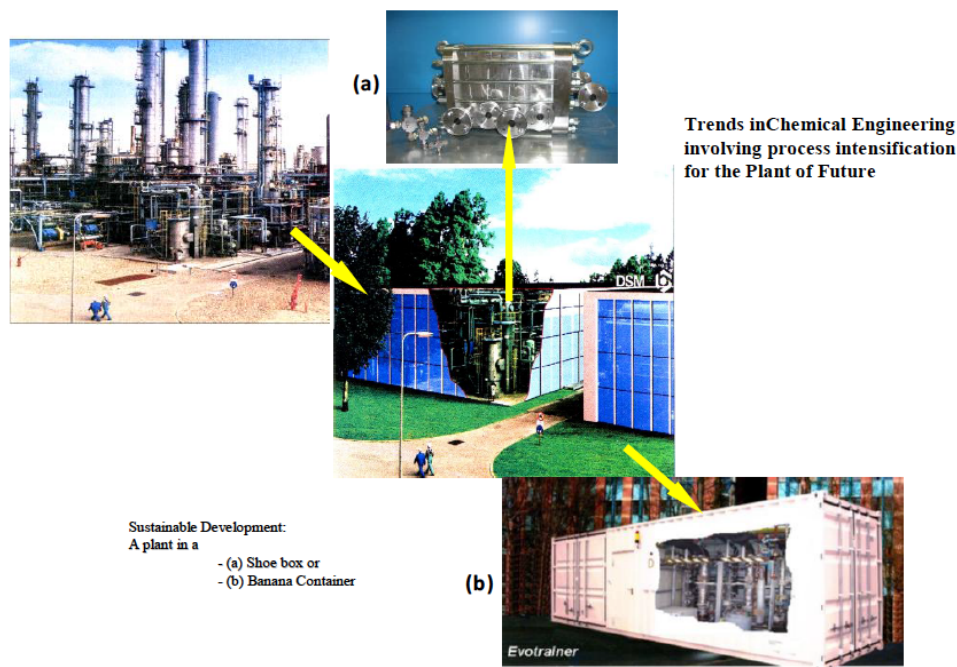
permitting greener routes for processing. And much broader operating conditions may be explored, thus opening the way to reaction unrealizable otherwise.

This has led to the concept of Novel Process Windows giving the chemist more opportunities for synthesizing and processing complex molecules [95, 105-107].

Complementarily, driven by the advantages of continuous processing, efforts have been 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 with downstream purification and formulations in the same container [108]. This has led to the concept of platforms and modular plants or container format approach to achieve faster product development and address the growing trend of individual and customized products [109-112]. The concept of modular plants is today the focus of several industry and academic intense research efforts to achieve faster product development, so aiming also to the design of the factory of the future [113-115].

These evolutions may finally led to the representation of the Figure 10 that represents schematically one evolution of the production due to the process intensification encountered in the factory of the future. It is seen that with operating with microreactor technology and modular plants, it has





**Figure 10:** Examples of the utilisation of the technologies of process intensification: schematic vision of a plant in a shoe box (a) or in a banana container (b).

appeared the notion of a plant in a shoe box for the production of several tons/hr of polymers (Figure 10a) and the notion of a plant in a banana container for flexible productions up to several hundreds of tons/year for specialties products (Figure 10b), which are production rates encountered in conventional plants [103].

Continued development of compact manufacturing units, such as the systems schematically described in Figure 10a and 10b, promises localized, on-demand production of a wide range of products, including pharmaceuticals, flavours and specialty polymers. Moreover, the emerging engineering potential approach of additive manufacturing (AM) will continue to accelerate the design and fabrication of specialized reaction microequipment, e.g. the potential of 3D printing of devices to achieve process equipment for micromixing and droplet formation for liquid extraction [117], to achieve on demand configuration of microreactors for chemical synthesis and analysis [118, 119] or to improve traditional chemical manufacturing processes, such as the well-known steam methane reforming (SMR) process [120], or to design and fabricate reactors and structured catalysts [122].

In the framework of the (r) evolution in the manufacturing environment coined as Industry 4.0 involving new model of production, the factory of the future in the chemical, petroleum and gas and energy

production industries require the previous new innovative process and technologies. The future technology developments will invariably come from combining the designs of new chemical reactor and selective separation technologies with new catalysts or unconventional reaction conditions, and challenging with the development of both more complex and simpler predictive mathematical models and simulation codes.

In that sense, the present papers has emphasized the today multiscale approach of process engineering in the chemical supply chain and has shown the models and simulation tools that may be used with this integrated approach for process innovation. Also various aspects of innovative small- and medium-scale production concepts in lab-, pilot plant- as well as production scale have been considered aiming to the design of the factory of the future. It has to be added that in a very next future, these results will have to be completed by the concept of the laboratory of the future because our future environment will comprise not only the factory of the future or the laboratory of the future, but a strong connection even a shared vision between them [121]. Just mention that the laboratory of the future may be a unit composed of several expert laboratories, with different geographic locations, mobilized on the basis of the specific research requirements (chemical reactions, separation methods, purification, modelling, etc.).

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