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REVIEW PAPER

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IN THE FRAME OF GLOBALIZATION, SOME TRACKS FOR THE FUTURE OF CHEMICAL AND PROCESS ENGINEERING

In today's economy, chemical engineering must respond to the changing needs of the chemical process industry in order to meet market demands. The evolution of chemical engineering is necessary to remain competitive in global trade. The ability of chemical engineering to cope with managing complex systems met in scientific and technological problems is addressed in this paper. Chemical Engineering is vital for sustainability: to satisfy both the market requirements for specific end-use properties of products and the social and environmental constraints of industrial-scale processes. An integrated system approach of complex multidisciplinary, non-linear, non-equilibrium processes and phenomena occurring on different length and time scales is required. This will be obtained due to breakthroughs in molecular modelling, scientific instrumentation and related signal processing and powerful computational tools. The future of 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; (2) Design novel equipment based on scientific principles and new production methods: process intensification using multifunctional reactors and microengineering and microtechnology (3) Extend chemical engineering methodology to product design and engineering using the "triplet 3PE molecular Processes-Product-Process Engineering" approach; (4) Implement multiscale application of computational chemical engineering modelling and simulation to real-life situations from the molecular scale to the production scale.

Key words: Future of chemical engineering, Complex systems and chemical engineering, Multidisciplinary and multiscale approach of complex systems, The triplet "molecular Processes-Product-Process Engineering", Product design and engineering, End-use property, Soft solids, Complex fluids, Molecular modelling, Process intensification.

Chemical and related process industries are at the heart of a great number of scientific and technological challenges involving complex systems.

Chemical and related industries including process industries such as petroleum, pharmaceutical and health, agriculture and food, environment, textile, iron and steel, bituminous, building materials, glass, surfactants, cosmetics and perfume, and electronics are evolving considerably at the beginning of this new century due to unprecedented market demands and constraints stemming from public concern over environmental and safety issues.

To respond to these demands, the following challenges are faced by the chemical and process industries involving complex systems both at the process-scale and at the product-scale.

a) Processes are no longer selected on the basis of economic exploitation alone but rather, compensation resulting from the increased selectivity and savings

linked to the process itself are sought. Innovative processes for the production of commodity and intermediate products such as sulfuric acid, ammonia, calcium carbonate, ethylene, methanol, where patents usually do not concern the products but the processes, need to be researched. Economic constraints will no longer be defined as: sale price minus capital cost plus operating costs plus raw material and energy costs. The problem becomes more complex as other factors such as safety, health, environmental aspects, including non-polluting technologies, reduction of raw material and energy losses and product/by-product recyclability are considered. The industry will have to process with large plants supplying bulk products in large volumes. For such high volume bulk chemicals, the customer will buy a process that is non polluting and perfectly safe;

b) Progression from traditional intermediate chemistry to new specialities, active material chemistry and related industries involves the chemistry/biology interface of agriculture, food and health industries. Similarly, it involves the upgrading and conversion of petroleum feedstocks and intermediates, conversion of coal-derived chemicals or synthesis gas into fuels, hydrocarbons or oxygenates. This progression is driven by the new market objectives, where sales and competitiveness are dominated by the end-use properties of a product as well as its quality. The quality

Plenary lecture at SEEChe 1, Beograd, September 25-28, 2005

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Paper received and accepted: February 8, 2006

of a product is a function of its properties: size, shape, colour, esthetics, chemical and biological stability, degradability, therapeutic activity, solubility, mechanical, rheological, electrical, thermal, optical, magnetic characteristics for solids and solid particles, touch, handling, cohesion, friability, rugosity, taste, succulence, and sensory properties etc. Control of the end-use property, expertise in the design of the process, continual adjustments to meet changing demands, and speed in reacting to market conditions are the dominant elements. Indeed for these new specialities and active materials the client buys the product that is the most efficient and the first on the market. He will have to pay high prices and expect a large benefit from these short life-time and high-margin products.

It is important to note that today 60% of all products sold by chemical companies are crystalline, polymeric or amorphous solids. These complex materials must have a clearly defined physical shape in order to meet the designed and the desired quality standards. This also applies to paste-like and emulsified products. New developments require increasingly specialized materials, active compounds and special effect chemicals. These chemicals are much more complex in terms of molecular structure than traditional, industrial chemicals.

ORGANIZING SCALES AND COMPLEXITY LEVELS IN PROCESS ENGINEERING

In the previous frame, today chemical process engineering is concerned with understanding and developing systematic procedures for the design and optimal operation of chemical, pharmaceutical, food, cosmetics and process systems, ranging from nano and microsystems to industrial-scale continuous and batch processes. Figure 1 illustrates the concept of the chemical supply chain (Grossmann and Westerberg, 2000).

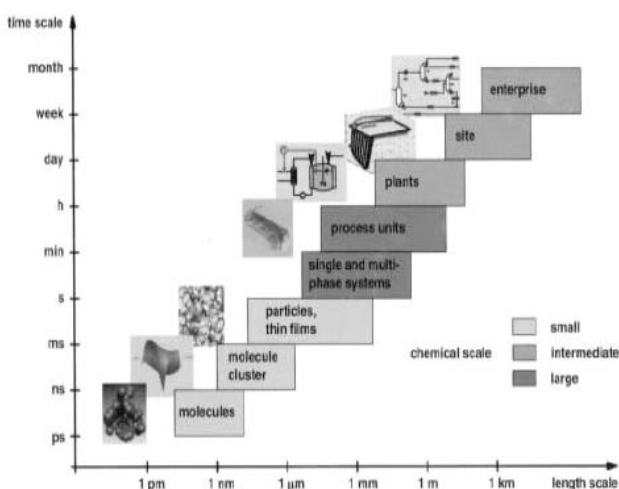


Figure 1. Chemical supply chain (Grossmann and Westerberg, 2000)

This chain starts 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 macroscopic 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. This site is part of the commercial enterprise driven by market considerations and product quality, once again in the framework of sustainability.

In this supply chain, it should be emphasized that product quality is determined at the micro and nano level and that a product with a desired property must be investigated for both structure and function. An understanding of the structure/property relationship at the molecular (e.g. surface physics and chemistry) and microscopic level is required.

The key to success is to obtain the desired end-use properties of a product, and thus control product quality, by controlling complexity in the microstructure formation. This will help make the leap from the nano level to the process level. Moreover most chemical processes are non-linear and non-equilibrium, belonging to so-called complex systems for which multi-scale structure is the common nature (Gallagher and Appenzeller, 1999). So an integrated system approach for a multidisciplinary and multiscale modelling of complex, simultaneous, and often coupled momentum, heat and mass transfer processes is required:

- Different time scales (10^{-15} to 10^8 s) from femto 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^{-8} to 10^6 m) are used in industrial practice and are shown in Figure 2 (Charpentier, 2002). Nanoscale measurements are used for molecular kinetic processes; microscale is used for bubbles, droplets, particles, and eddies; mesoscale is used for unit operations dealing with reactors,

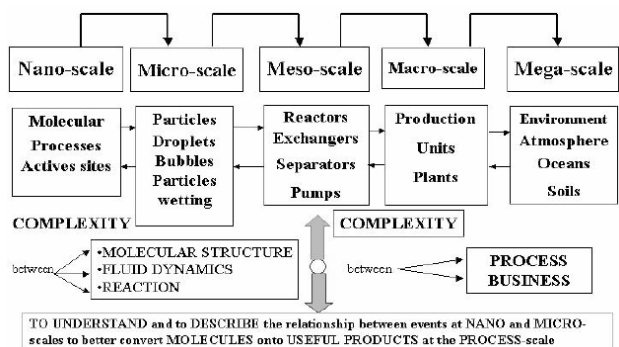


Figure 2. Scales and complexity levels in process engineering (Charpentier, 2002)

exchangers, and columns; macroscale is used for production units such as plants, and petrochemical complexes; and megascale is used for measurements involving the environment, atmosphere, oceans and soils. e.g., thousands of kilometers for the dispersion of emissions into the atmosphere.

Organizing scales and complexity levels in process engineering is necessary in order to understand and describe the events at the nano and microscales and to better convert molecules into useful products at the process scale. It is this approach involving a quantitative design and optimization of chemical systems based on detailed mechanisms that is required by chemical engineering today.

And any progress in the analysis of multiscale structures in chemical engineering, not to say any breakthrough in understanding complex systems, is bound to contribute to the formation of a new knowledge base for the process industry. This requires a complex system and multiscale methodology as shown by Li and Kwank (2004) with a special issue in Chemical Engineering Science.

Two illustrations of this multiscale and multidisciplinary approach of complexity are given.

Transport phenomena in catalysed olefin polymerisation

Polyolefins (essentially polyethylene in its different forms and polypropylene) are by far and away the most widely consumed polymers in the world in terms of tonnage. On the one hand there are different processes for their production, including a high pressure free radical process to make low density, highly branched structures and therefore amorphous products. On the other hand one can also consider processes where the molecules of ethylene and/or propylene (and/or other comonomers) are assembled at active sites to make products with different molecular structures, and thus properties.

If we consider this latter type of process, it can be viewed from a number of different length scales, as shown in Figure 3 (McKenna and Soares, 2001 – adapted from Ray, 1986). In this type of process, a catalyst particle is injected into a continuous medium in which the monomer is dispersed either in a gas stream (ethylene – C2, or propylene – C3), in an inert diluent (C2 and C3), or in liquid monomer (C3). The reaction

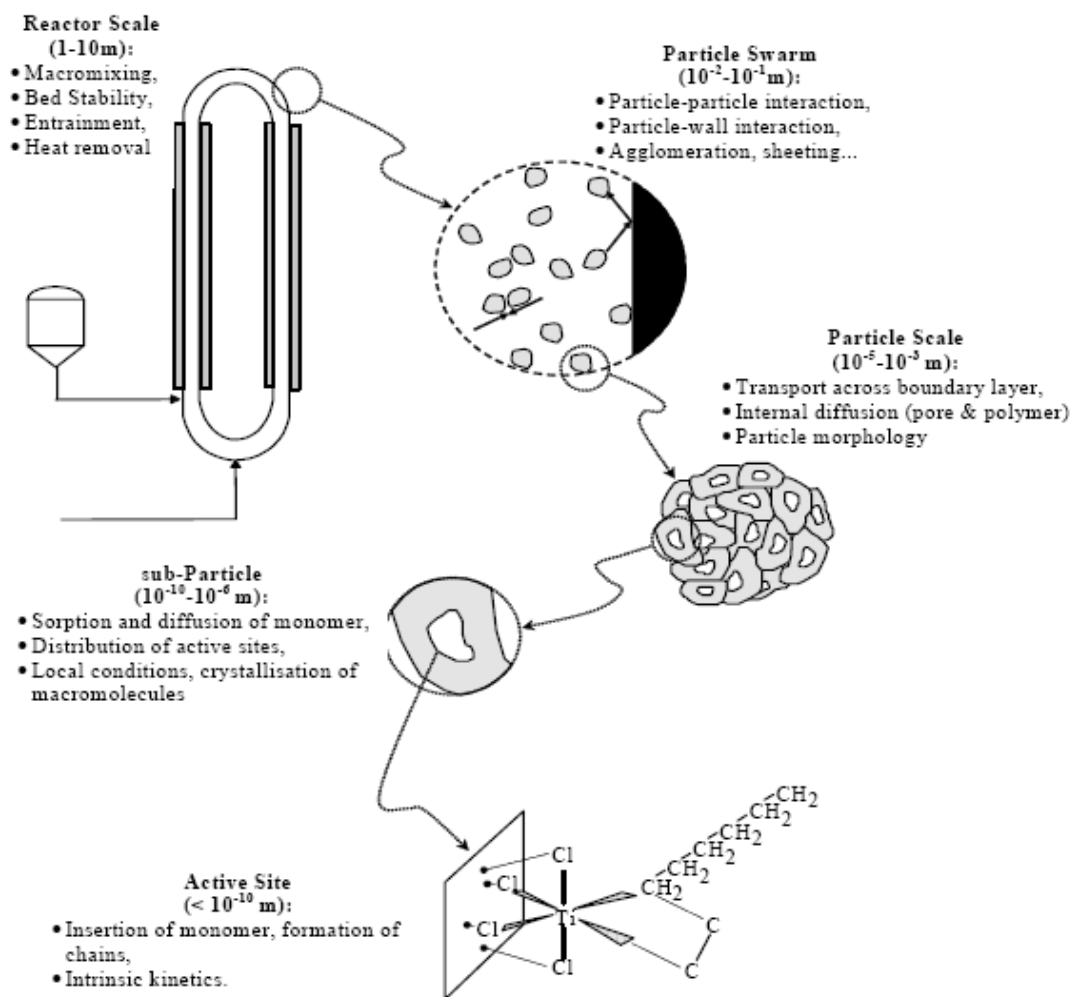


Figure 3. Different length scales to be considered from a process point of view in the polymerisation of olefins on supported catalysts

takes place on active sites deposited inside the solid support of the catalyst particles (typically MgCl_2 or silica). The particle retains its original shape because of the entanglement of the polymer formed inside it, but this fragmentation allows the reaction to continue because it keeps the length scale for diffusion through the polymer relatively short. Reactions are typically fast, with rates on the order of 1 to 60 kg of polymer per gram of catalyst per hour (kg/g/h). The transformation of particle morphology is very rapid, especially in the early stages, and, with heats of polymerisation on the order of 100 kJ/mol, enormous amounts of heat must be evacuated from the particles.

On the surface, the process might appear simple: one injects a porous catalyst particle into the reactor, and polymer is formed in its pores. This causes the particles of catalyst to grow. After a few seconds of growth the original support matrix is fragmented, and a sort of phase inversion occurs, with the polymer phase becoming the continuous matrix, with fragments of the support material carrying the active sites dispersed within it. However, the complexity of the process, and the need to consider different length scales become apparent if we look more closely at what is happening in the reactor.

Let us begin to look at the process at the scale of the active sites. An active site is essentially a metal ion (titanium for Ziegler–Natta catalysts, chromium or vanadium for Phillips catalysts, or other metals for metallocenes) that coordinates incoming monomer molecules and adds them to a growing polymer chain. Several phenomena are occurring at this length scale, including the insertion event, chain transfer, active site activation or deactivation, as well as the growth of the chain, and eventually the partial crystallisation of the latter.

One might think that this is lowest length scale that can be defined in such a process. However, in a review on the application of computational material science Kremer (2003) begins at this scale, and looks at even smaller dimensions! He defines the pertinent length scales starting at around 10^{-7} – 10^{-6} metres, and then differentiates between types of events at length scales that decrease by 10 Å all the way to sub-atomic phenomena. In this context, it is important to consider such well-defined length scales since different types of phenomena will dominate at a given level. For instance, at what Kremer (2003) refers to as the mesoscopic scale (10–50 Å), entropy-related phenomena will dominate, where as at the nanoscopic scale (1 Å) energy-related phenomena dominate. We will not consider such fine divisions of scales here, but this digression was meant to illustrate that even concepts such as length scales must be defined within a certain context. However it is interesting to keep in mind the idea that length scales can be associated with different types of phenomena,

and therefore different modelling approaches might be needed at different length scales.

The reactors for this type of process are typically on the order of tens of cubic metres in volume. Tubular loop reactors, such as the one picture in Figure 3, will have diameters of the order of tens of centimetres. Fluidised bed reactors (FBR) for gas phase polymerisations will have dimensions of height and diameter of the order of metres, as will stirred tank reactors for slurry processes. At these length scales, attention is usually focused on maintaining bed stability, and ensuring that the temperature and concentrations in the continuous phase are as homogenous as possible. Heat must be exchanged with the outside environment (and therefore the reactor is the interface between the process and the external environment). Heat is generated, and matter is converted to products or energy on the catalyst/polymer particles. These particles will also grow at a rate that depends on local conditions in the reactor, as well as on factors related to particle shape and the intrinsic kinetics of the catalyst system in use. Particle growth will most certainly influence fluidisation and bed stability... Thus, in order to understand what happens at the scale of the reactor, one must understand how particles interact at the level of a few particles, how the individual particles evolve in the reactor, and thus how the chains are produced. But perhaps more importantly, it is necessary to understand the interaction between all of these events!

Let us consider the lowest level of morphology in Figure 3: that of the active site and the chain growing off of it. At this level the rate of polymerisation will depend on the intrinsic chemistry of the active site itself (for certain types of catalyst, there can be many different types of active site chemistry), the local temperature, the concentration of monomer, hydrogen, and eventually catalyst poisons. As monomer arrives at the active site, it is inserted into the growing chain. This releases heat, as well as causing the chain to grow and to make it move away from the active site. As the chain moves away, and eventually detaches from the active site either due to a termination reaction, or a chain transfer event, it will either form crystals, or coil up upon itself to form an amorphous zone. At this level, modelling efforts can be focused on the material properties, and the relative rates of the different reactions (insertion, transfer, termination) that occur at the sites, and it is unlikely that one can really treat the phenomenon as taking place in a continuum. More and more, computational chemistry and/or molecular modelling can be used here.

At the next highest length scale defined in Figure 3, we need to consider the substructures inside the particles. The interaction between this level and the previous one is clear since monomer must be transported through these structures to the active sites. Monomer transport can occur at two levels: either through the polymer layer that covers the active sites

(via diffusion), or through the pore space of the particle (or via diffusion and eventually convection). Obviously the second route will be faster, but at one point diffusion must occur through the polymer. The rate at which this process takes place can determine the rate of reaction, and the thicker the polymer layer, the slower local mass transfer will be. In addition, the properties of this polymer layer will be important since monomer and hydrogen cannot be absorbed by crystalline polymer, nor can they diffuse through it. Therefore the degree of crystallinity of the polymer layer covering the active sites can reduce the rate of reaction. At this level, modelling will focus on sorption and diffusion, as well as on modelling the morphology of the polymer layer. The rate of reaction, the quantity of monomer sorbed in the polymer layer, the diffusion coefficients and the degree of crystallinity of the polymer layers will depend on a number of factors, not the least of which is the temperature inside the growing particle – which in turn of course depends to a certain degree on the rate of reaction as this type of polymerisation is an exothermic process.

The events happening at the level of the single particle are also extremely complicated, and are the key to smooth process operation. When a fresh particle is injected into the reactor, it consists of a porous, solid support, with the active sites being deposited in the pores of the support. Thus, the shape of the support, its degree of porosity, the pore size distribution and the catalyst loading will all play important roles in the observed rate of polymerisation of the particle. The pore volume and shape will obviously influence the rate at which monomer can diffuse to the active sites, as will the size of the particle (length of the pores). The concentration of active sites within the pores will have an influence on the rate of polymerisation, and subsequently on the rate of generation of energy and the local temperature (this can of course lead to runaway situations). During polymerization, the size of the polymer particle increases and mass transfer rates to the particle will increase. This is because the flux of monomer into the particle is proportional to the surface of exchange i.e. R^2 , R being the radius of the growing particle, whereas the rate of monomer consumption is proportional to the mass of catalysts in the particle. Mass transfer therefore becomes less and less difficult as the particle grows, and the polymerization rate, if controlled by diffusion into the particle, is expected to increase with polymerization time.

The size and structure of the subparticles, the thickness of the polymer domains through which monomer is transferred will also be determined to a large extent at the level of the single particle. In addition to the initial structure of the particle, its morphology will be determined by a very complex series of events that occur throughout the reaction, but especially in the early stages (Pater et al., 1998; Pater 2000; Grof et al., 2003; Kittilsen et al., 2001, 2003). As the initial polymer chains are formed inside the virgin catalyst particle, the support

ruptures into many fragments (often called micrograins, microparticles, or primary particles). The catalyst particle does not lose its overall integrity because the individual fragments are held together by the polymer already formed in the particle. The generation of pressure inside the particle will depend on what happens at the active site and in the subparticles. However the interaction of the different substructures will have a sort of feedback effect since the distribution of pressures inside the particle itself will determine to a large extent the overall morphology of these objects, and thus the rate of polymerisation in the particle itself.

Modelling at the level of the single particle can be approached in different ways depending upon the accuracy of the information that one needs (McKenna and Soares, 2001). It can be treated either as a pseudohomogeneous medium, or as an assembly of substructures (e.g. Kittilsen and Svendsen, 2003). Models will include moving boundary transport equations for energy and matter, but also should include models that incorporate the mechanical properties of the polymer phase to explore particle growth.

One step higher in morphology, particle temperature will also be determined by its interaction with its immediate environment, especially with particles of different size (see e.g. McKenna et al., 1999). Thus the modelling of heat transfer at the level of the particle cloud is an essential point in the development of a full scale model of this type of polymerisation process. This type of modelling is best done with computational fluid dynamics. An example of this is shown in Figure 4 (Charpentier and Mc Kenna, 2004). This Figure shows how the particle interaction leads to a moderation of the

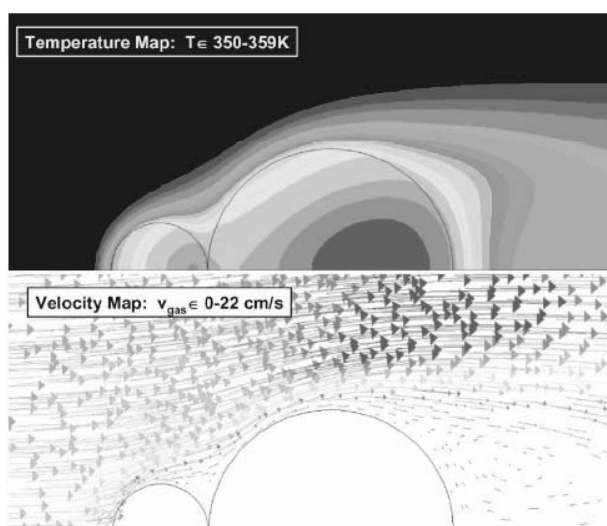


Figure 4. CFD image of the interaction between neighbouring particles in a gas stream. The top graph shows the temperature contour in the small and large particles (red is the hottest), whereas the bottom graph shows the velocity profile in the gas phase. Conditions: $d_p = 60 \mu\text{m}$ for small particles, $150 \mu\text{m}$ for large particles, nominal polymerisation rate = 20,000 g/g/h for both particles, and free stream gas velocity = 20 cm/s.

temperature. The example shown here is for a fresh catalyst particle with a diameter of 40 μm injected into a reactor at 350 K. After 5 seconds, this small particle has grown to a diameter of almost 60 μm and has come into contact with a larger one with the same intrinsic activity, but that has been in the reactor long enough to grow to a diameter of 150 μm from the same original particle size. Both particles are polymerising at a nominal rate of 20.000 g/g/h, but the volumetric heat flux of the small particle is obviously much higher since both particles contain the same amount of catalyst. If the small particle were left alone in a stagnant gas stream, it would overheat and melt down would occur. This is also the outcome predicted using standard chemical engineering correlations based on an estimate of the Nusselt number (see McKenna et al., 1999). However, as can be seen from Figure 4, the highest temperature in the small particle is just under 360 K, approximately 20 degrees below the melting point of linear low density polyethylene. In addition, the hot spot is shifted to the right, closer to the large particle. The hot spot in the large particle is also shifted toward the low velocity zone behind the trailing edge of the particle. McKenna et al. also showed that these steady state profiles are reached very quickly (less than 0.025 seconds), which clearly means that particle-particle interaction is important in defining heat transfer. Extending this conclusion to the other scales, it should be easy to imagine that the particle size distribution can influence heat transfer on this scale, and therefore the rate of particle grow and the evolution of particle morphology can both influence how heat transfer occurs in the reactor.

Finally, the full scale reactor model must incorporate all of the issues discussed above, and will, to a certain extent be described by a cascade of models for each of the process length scales considered.

Transport phenomena in biochemical engineering

This multiscale approach is now encountered in biotechnology and bioprocess engineering, to better understand and control biological tools such as enzymes and microorganisms and to manufacture products. In such cases, it is necessary to organize the levels of increasing complexity from the gene with known properties and structure, up to the product-process couple, by modelling coupled mechanisms and processes at different length-scales as shown in Figure 5 (Charpentier 2002). The nanoscale is used for molecular and genomic processes and metabolic transformations; pico and micro scales are used for enzyme and integrated enzymatic systems, and for the biocatalyst and active aggregates; mesoscale is used for bioreactors, exchangers, separators; and macro and megascales are used respectively for production units such as plants, and interactions with the biosphere.

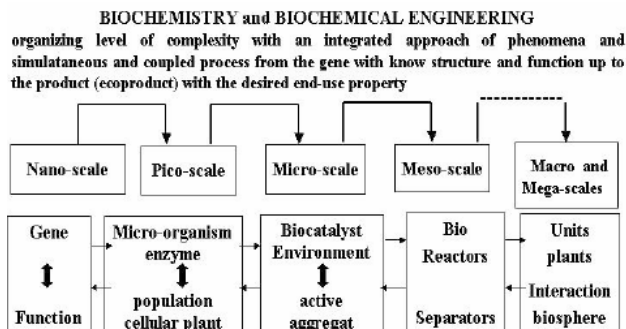


Figure 5. Organizing levels of complexity underline new view of biochemical engineering (Charpentier 2002)

Thus, organizing levels of complexity at different length-scales, associated with an integrated approach to phenomena, and simultaneous and coupled processes are at the heart of the new view of biochemical engineering. This capability offers the opportunity to apply genetic-level controls to make better biocatalysts, novel products, or develop new drugs and new therapies and biomimetic devices. Understanding an enzyme at the molecular level means that it may be tailored to produce a particular end-product (Engasser, 1998). Also 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 (Chakraborty, 2003).

In food process engineering today, there is significant scope for such approaches in linking scale to model process physics, process (bio) chemistry and process microbiology from the molecular and cellular scale to the full process plant scale (Bruin, 1997).

These examples are at the heart of the new view of chemical and process engineering: 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 a continuous process.

This can be defined by "**le Génie du Triplé Processus-Produit-Procédé (G3P)**" or "**the triplet 3PE – molecular Processes – Product-Process Engineering**": an integrated system approach of complex pluridisciplinary non-linear and non-equilibrium processes and phenomena occurring on different length and time scales.

In addition to the basic notions of unit operations, coupled transfers and the traditional tools of chemical reaction engineering, as well as the fundamentals of chemical and process engineering (separation engineering, chemical reaction engineering, catalysis, transport phenomena, process control), this integrated multidisciplinary and multiscale approach of complex systems involving non-linear and non-equilibrium

processes is beneficial and has considerable advantages for the development and the success of this engineering science in terms of concept and paradigms.

Now, chemical and process engineering involve a strong multidisciplinary collaboration with physicists, chemists, biologists, mathematicians and instrumentation specialists. This leads to the theoretical development and design of products with complex structures like emulsions, paste-like products, plastics, ceramics and soft solids. Developing new concepts within the framework of what could be called "physicochemical (bio) engineering" justifies the qualification of process engineering as an extension of chemical engineering and takes on its full meaning (Charpentier and Trambouze, 1998; Bacchin et al, 1999). **In such a context, biology is included as a foundation science of process engineering, along with physics and chemistry in order to involve chemical engineers to basic concepts of genetics, biochemistry and molecular cell biology** which will serve well the needs of the new chemical, pharmaceutical (such as chiral compounds) and biotechnology industries.

Improving both the design and evaluation of complex systems for the production of real products requires further research into strategies, methodologies and tools. These are oriented toward the acquisition of basic data in thermodynamics, kinetics, rheology and transport, and toward the conception of new integrated operations incorporating coupling and uncoupling of elementary processes (transfer, reaction, separation) or combining several functions in one piece of equipment.

This is clearing the way for smaller, cheaper installations, requiring improved knowledge of process modelling, automation and control. However, this requires mathematical models and scientific instrumentation which provide useful basic data that can be treated using powerful computational tools. For example, the treatment of generalized local information increasingly requires the help of computational fluid dynamics (CFD) and computational fluid mixing (CFM). This has been the case for a long time in combustion, automotive, and aeronautic applications, especially for the knowledge, control, stability of flows and the characterization and improvement of transfer phenomena.

Due to recent rapid advances in software programs (e.g. CFDLIB, FLUENT, PHOENICS, FLOW 3 D, FIDAP, FLOW MAP, etc.), CFD is becoming more important every day for scaling up new equipment or for multifunctional unit operations. CFD is used for simulation of flow phenomena and processing generalized local information: for understanding the impact of complex flow geometries on mixing and reaction phenomena at the microeddy scale; for the numerical simulation of the complex hydrodynamics of multiphase catalytic gas-liquid-solid reactors; or for modelling sieve tray hydraulics; or for analyzing local

hydrodynamics parameters of both liquid and gas phase in the riser of external loop airlift reactor; or for simulating flow in complex geometries such as reactor internals (industrial distributor devices). Calculations can be carried out for any geometric complexity and for single and two-phase flow, provided that physical models are available. Nevertheless, the use of this tool becomes possible only when the calculation time is acceptable, i.e. less than a few days. CFD is thus a good link between laboratory experiments, conducted with common fluids like air, water, organics and hydrocarbons, etc., and industrial operations involving complex fluids, and severe temperature and pressure conditions. An important advantage of CFD techniques is that geometry and scale effects are automatically accounted for. Imaging complements CFD and CFM, especially for validation purposes complementarily to experimental data obtained with sophisticated techniques such as laser Doppler velocimetry (LDV) and particle image velocimetry (PIV), computer automated radioactive particle tracking (CARPT), or positron emission tomography (PET) and positron emission particle tracking (PEPT) for opaque systems.

TODAY'S TOOLS FOR THE SUCCESS OF CHEMICAL AND PROCESS ENGINEERING FOR MODELLING COMPLEX SYSTEMS AT DIFFERENT SCALES

It is possible to understand and describe events on the nano and microscale in order to convert molecules into useful products on the process and unit scales thanks to significant simultaneous breakthroughs in 3 areas: molecular modelling (both theory and computer simulations), scientific instrumentation and non-invasive measurement techniques, and powerful computational tools and capabilities for information collection and processing (Charpentier, 2003).

At the nanoscale, molecular modelling assists in maintaining better control of surface states of catalysts and activators, obtaining increased selectivity and facilitating asymmetrical syntheses such as chiral technologies, or explaining the relationship between structure and activity at the molecular scale in order to control crystallization, coating and agglomeration kinetics.

At the microscale, computational chemistry is very useful for understanding complex media such as non-newtonian liquids, molten salts, supercritical fluids, multiphase dispersions, suspensions and more generally, all systems the properties of which are controlled by rheology and interfacial phenomena such as emulsions, colloids, gels, froths, foams, hydrosoluble polymers and particulate media such as powders, aerosols, charged and viscous liquids. Computational chemistry also helps us understand fractal structures of porous media and their influence on mass and heat transfer and on chemical and biological reactions. Also non-invasive measurement techniques (such as spectroscopic or monochromatic ellipsometry, i.e.,

diffusing wave spectroscopy, NMR, Computer Automated Radioactive Particle Tracking, tomographic techniques, etc) coupled with 2D or 3D image reconstruction techniques are very helpful to obtain hydrodynamics data at the time and space microscale. Among available tomography techniques, electrical tomography (either resistance and capacitance) seems the most promising technique for the dynamic flow imaging purpose, i.e., to visualize gas hold up in gas-liquid systems such as stirred tanks (Mann et al., 1997), or in bubble columns (Fransolet et al., 2001; 2005) and flow pattern inside packed beds (Bolton et al., 2004), or to visualize the transient phenomena and hydrodynamic characteristics in bubble columns, and in two and three phase fluidized beds (Du et al., 2004; Warsito et al., 2005), or even both to visualize solid distribution in solid-liquid stirred tank and to monitor phase dispersion and separation for liquid-liquid processes relevant to the pharmaceutical industry (Ricard et al., 2005). Electrical tomography is also used for the quantification of mixing with chemical reaction in batch stirred vessel reactions (Wabo et al., 2004). Nuclear Magnetic Resonance coupled with Magnetic Resonance Imaging presents a non-invasive means to obtain specific information about structural heterogeneity of materials and porous media (Stapf, 2005). Also for multiphase flow in catalytic porous media, this sophisticated technique leads to simultaneous measurement of the parameters characterizing hydrodynamics, mass transfer and chemical conversion (Gladden, 2003, Koptug, 2003). This technique leads also to the time and space dependent droplet separation kinetics in granular bed filters (Nguyen et al., 2005).

At the meso and macroscales, computer fluid dynamics is required for the design of new operating modes for existing equipment such as reversed flow, cyclic processes, unsteady operations, extreme conditions like high temperature and pressure technologies, and supercritical media. CFD is also required for the design of new equipment or unit operations. It is especially useful when rendering process step multifunctional with higher yields in coupling chemical reactions with separation or heat transfer. It provides a considerable economic benefit. More generally, CFD is of great assistance concerning the design of new equipment based on new principles of coupling or uncoupling elementary operations (transfer, reaction, separation).

At the production unit and multiproduct plant scale, dynamic simulation and computer tools for simulation of entire processes are more and more required and are applied to analyze the operating conditions of each piece of production unit equipment. They are used to predict both the material flows, states and residence times within individual pieces of equipment in order to simulate the whole process in terms of time and energy costs. New performances (product quality and final cost) resulting from any change due to a blocking step or a bottleneck in the

supply chain will be predicted in a few seconds. Many different scenarios may be tested within a short time, allowing the rapid identification of an optimal solution. For instance, the simulation of an entire production year (steady state flow sheet simulation) may take only 10 minutes on a desktop. It is clear that such computer simulations enable the design of individual steps, the structure of the whole process at the mega-scale and place the individual process in the overall context of production.

CHEMICAL AND PROCESS ENGINEERING: QUO VADIS?

The previous considerations on the necessary integrated approach of chemical engineering for managing complex systems led to propose four main parallel objectives for engineers and scientists.

Total multiscale control of the process to increase selectivity and productivity

This necessitates the "intensification" of operations and the use of precise nano and micro technology design. This is the case of molecular information engineering, where instead of using porous support for heterogeneous catalyst, synthetic materials with targeted properties are now conceived and designed. The development of an effective catalyst (a complex system) in both composition and functionality is central to a successful catalytic process. The ability to better control its microstructure and chemistry allows for systematic manipulation of the catalyst's activity, selectivity, and stability.

Nanotailoring of materials with controlled structure

Through the control of pore opening and crystallite size and/or proper manipulation of stoichiometry and component dispersion, there now exists the ability to engineer novel structures at the molecular and supramolecular levels via nanostructure synthesis (Figure 6, Ying 2000). This leads to the creation of nanoporous and nanocrystalline materials. Both these materials possess an ultrahigh surface-to-volume ratio, which offers a greatly increased number of active sites for carrying out catalytic reactions.

Nanocrystalline processing includes tailoring size-dependent electronic properties, homogeneous multicomponent systems, defect chemistry, and excellent phase dispersion. Nanocrystalline catalysts

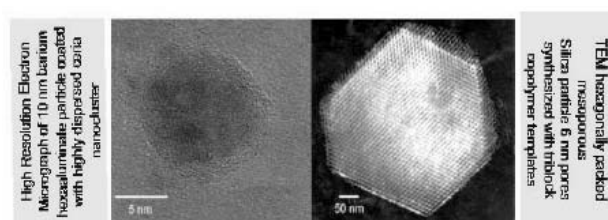


Figure 6. Nanotailoring of materials with controlled structure

have greatly improved catalytic activity over conventional systems and multifunctionalities necessary for complex applications. For example, the catalytic activity of structure-sensitive reactions such as photocatalysis over titania, used for the decomposition of chemical wastes such as chloroform and trichloroethylene, depends not only on the number of active sites, but also on the crystal structure, interatomic spacing and the crystallite size of the catalytic material. By varying the crystal size and phase through molecular engineering, it is possible to manipulate and optimize the catalyst design. Titania crystals of controlled size (4–100 nm) and phase were systematically synthesized by sol-gel hydrolysis-precipitation, followed by hydrothermal treatment (Ying, 2000). Specifically, 10 nm anatase crystallites, due to their greater redox potential, present the best photonic efficiency for the photodecomposition of chloroform and trichloroethylene.

High volume fraction of surface/interfacial atoms in nanocrystalline materials presents a great opportunity to control the surface chemistry and defect concentration. The design of such materials, with flexible control of stoichiometry and electronic properties that are important for redox catalysis can be exploited in a variety of catalytic processes. For example, the elaboration of a cerium oxide catalyst, involving a high intrinsic oxygen mobility, which is synthesized with a high surface area and a reservoir of oxygen vacancies through modified magnetron sputtering of cerium in argon, followed by controlled post-oxidation. The resulting 6 nm CeO_{2-x} nanocrystals are excellent catalysts for SO_2 pollutant treatment, as they enable 100% selective conversion of SO_2 to S at 460°C compared to 580°C needed by ultrafine stoichiometric CeO_2 powder (Ying, 2000).

The implications of tailored nanostructures for high-temperature catalysis are also of a great interest for many industrial processes such as steam reforming, catalytic combustion and the selective oxidation of hydrocarbons. The catalytic combustion of methane or natural gas makes it possible to generate power with reduced emissions of greenhouse gases compared to the burning of coal or higher hydrocarbons. This requires a catalyst that can sustain activity and mechanical integrity at flame temperatures as high as 1300°C . The catalyst must also be active at low temperatures for start-up and transient periods. Noble metal catalysts exhibit excellent light-off behaviour at 400°C , but suffer from deactivation by $700\text{--}800^\circ\text{C}$. To achieve high-temperature stability, one system considered is barium hexaaluminate (BHA) which is stopped in particle growth and sintering once it is crystallized. A discrete BHA nanoparticle preserving a surface area higher than $100\text{ m}^2/\text{g}$ at 1300°C was achieved using a reverse microemulsion mediated sol-gel synthesis. This technique allows molecular-level

chemical homogeneity to be achieved, so that the desired spinel-like crystalline phase is induced at relatively low temperatures. This minimizes subsequent particle growth at the high flame temperature of catalytic combustion. Nanostructured materials with great thermal stability are now used to support transition metal and rare earth oxides, to create highly dispersed nanocomposite systems, i.e. CeO_2 nanoclusters coated on stable BHA nanoparticles (Figure 6) retain a crystal size of 20 nm even at 1100°C and allow methane light-off by 400°C (Zazur and Ying, 2000). Such nanocomposites display a low-temperature activity that is comparable to noble metal systems; they are less expensive and present superior thermal and hydrothermal stability.

Moreover, vapour phase and wet-chemical synthetic approaches have led to unprecedented control of material structures at the atomic and molecular levels, and have brought about ensembles of such features in the shape of nanocrystalline systems involving crystallite-size tuning. Now, complex nanocomposite systems can be built to fulfill various roles required for the reaction mechanism and conditions. Nanocomposite processing and tailoring also lends itself readily to intelligent combinatorial approaches in material design and rapid catalyst screening (Engstrom and Weinberg, 2000).

Also, through supramolecular templating, nanoporous systems can now be derived with well-defined pore size and structure, as well as compositional flexibility in the form of particles and thin films. Nanoporous structures hold many possibilities in materials applications, with further development in molecular engineering, in areas such as the surface functionalization of inorganic structures and the extension of supramolecular templating to organic systems. A self-assembly of nanostructured building blocks (e.g. nanocrystals) and combining porosities on different length scales will lead to interesting hierarchical structures. Systems with multiple levels of intricacies and design parameters offer the possibility to simultaneously engineer molecular, microscopic and macroscopic material characteristics, which, in response to societal demands, may lead to the construction of such advanced systems as biomimicking medical implants or electronic/photonic devices.

In general, nanoscale characteristics can be achieved using either "bottom-up" or "top-down" techniques. In "top-down" techniques, a larger scale structure is created and nanoscale characteristics are obtained by etching or by microelectronic fabrication. In "bottom-up" synthesis, the materials are assembled at the molecular level by aerosol reactor synthesis or self-propagating high-temperature combustion synthesis (SHS). There are numerous advantages to generating materials using the flexible and powerful combustion technique. SHS can be used to generate

materials with controlled micro- and macrostructures, such as foams, whiskers, composites, near-net shapes and functional grade materials (Varma et al, 1998), and for high-value-per gram materials such as bio-implant materials, high-temperature super conductors and nanostructured materials (Pampuch, 1999). The gas-phase combustion synthesis (GPSC) of powders is another combustion technique used to create nanocrystalline materials such as tin oxide particles. Advantages of GPSC techniques include the ability to control the composition and microstructure of the particle, continuous processing, high purity products, readily scalable technology and integration of synthesis and assembly steps (Kimm et al. 2001).

In the field of homogeneous catalysis, a supramolecular fine chemistry has been recently established. It extends the principle of self-organization of the enzyme (catalyst) molecule to non biological systems, using supramolecular compounds as catalysts for the shape selection of molecules. Such catalysts are formed in situ by self-organization, i.e, chemical bionics (Kreysa 2001).

In general, where the tailoring of materials with controlled structure is concerned, the previous approaches imply that chemical engineers should and will go down to the nanoscale to control events at the molecular level. At this level, new functions such as self-organization, regulation, replication and communication have been observed and can be created by manipulating supramolecular building blocks. The latest advances in nanotechnology have generated materials and devices with new physical, chemical and biochemical characteristics for a wide variety of applications.

With their broad training in chemistry, physical chemistry, processing, systems engineering, and product design, chemical engineers and researchers are in a unique position and play a pivotal role in this technological revolution concerning the management of complex systems.

Increase selectivity and productivity by supplying the process with a local "informed" flux of energy or materials

At a higher microscale level, detailed local temperature and composition control through staged feed and heat supply or removal would result in higher selectivity and productivity than the conventional approach, which imposes boundary conditions and lets a system operate under spontaneous reaction and transfer processes. Finding some means to convey energy at the site by supplying the process with a local "informed" flux of energy, where it may be utilized in an intelligent way is therefore a challenge. Such a focused energy input may be achieved by using ultrasonic transducers, laser beams or electrochemical probes, but a more fundamental approach is required to progress in

this direction. Some kind of feedback between the process and the energy source is needed to convey the exact amount of energy, at the precise location where it must be utilized to promote transfer or reaction. Driving the elementary processes within the unit is a challenge, but combining microelectronics and elementary processes, like tuning the selectivity by controlling catalytic reactions at the surface of electronic chips, is a direction that should be explored.

The necessity to increase information transfer in the reverse direction, from process to man

It is highly desirable to develop a variety of intelligent sensors, visualization techniques, image analysis and on-line probes giving instantaneous and local information about the state of the process. This opens the way to a new "smart chemical and process engineering" and requires close computer control, relevant models, and arrays of local sensors and actuators. Field-programmable analog arrays coupled with microreactor technology promise to change the way plants are built, as well as the methods by which their processes are designed and controlled. Rapid progress is noticeable in this area, although sensors for opaque materials and particulate solids in bulk systems are still scarce.

Design of novel equipment based on scientific principles, new operating modes and new methods of production: Process intensification

The progress of basic research in chemical engineering has led to a better understanding of elementary phenomena and it is now possible to imagine new operating modes of equipment or design novel equipment based on scientific principles.

Process intensification refers to complex technologies that replace large, expensive, energy-intensive equipment or process with ones that are smaller, less costly, more efficient, or that combine multiple operations into a single apparatus or into fewer devices.

Process intensification using multifunctional reactors

Such is the case with the "multifunctional" equipment that couples or uncouples elementary processes (transfer – reaction – separation) to increase productivity and/or selectivity with respect to the desired product and to facilitate the separation of undesired by-products. In recent years, extractive reaction processes involving single units that combine reaction and separation operations have received considerable attention as they offer major advantages over conventional processes due to the interaction of reaction, mass and energy transfer. Thermodynamic limitations, such as azeotropes, may be overcome and the yield of reactions increased. The reduction in the number of equipment units leads to reduced investment

costs and significant energy recovery or savings. Furthermore, improved product selectivity leads to a reduction in raw material consumption and hence, operating costs. Globally, process intensification through the use of multifunctional reactors permits significant reductions in both investment and plant operating costs. Cost reductions between 10 and 20% are obtained by optimizing the process. In an era of limited profit margins, it allows chemical producers more leverage for competing in the global market place.

Reactive separation processes involving unit operation hybridation

A great number of reactive separation processes involving unit operation hybridation exist.

The concept of reactive or catalytic distillation has been successfully commercialized, both in petroleum processing, where packed bed catalytic distillation columns are used, and in the manufacture of chemicals where reactive distillation is often employed (Malone and Doherty, 2000; Taylor and Krishna, 2000; Guo et Lee, 2004) Catalytic distillation combines reaction and distillation in one vessel, using structured catalysts as the enabling element (Gorak and Hofman, 2001). The combination results in a constant-pressure boiling system, ensuring precise temperature control in the catalyst zone. The heat of reaction directly vaporizes the reaction products for efficient energy utilization. By distilling the products from the reactants in the reactor, catalytic distillation breaks the reaction equilibrium barrier. It eliminates the need for additional fractionation and reaction stages, while increasing conversion and improving product quality. Both investment and operating costs are far lower than with conventional reaction followed by distillation (Xu et al. 2002).

The use of reactive distillation in the production of fuel ethers such as tertiary-*amyl*-methylether (TAME) or methyl-*tertiary*-butyle ether (MTBE) or methyl acetate, clearly demonstrates some of the benefits. Similar advantages have been realized for the production of high purity isobutene, for aromatic alkylation; for the reduction of benzene in gasoline and in reformat fractions; for the production of isopropyl alcohol by hydration of propylene; for the selective production of ethyleneglycol, which involves a great number of competitive reactions; and for the selective desulfurization of fluid catalytic cracker gasoline fractions; as well as for various selective hydrogenations. Extraction distillation is also used for the production of anhydrous ethanol. The next generation of commercial processes using catalytic distillation technology will be in the manufacture of oxygenates and fuel additives (Dudukovic, 1999) or in the synthesis of a range of fatty acid esters used in the manufacturing of cosmetics, detergents and surfactants (Omota et al. 2003), or in the recovering of lactic acid from fermentation broth (Choi and Hong, 1999).

Liquid maldistribution (large-scale and small-scale maldistribution) in packed column distillation columns is probably one of the most described effects influencing the efficiency of the column (Zuiderweg, 1999). A general trend is the emerging of multifunctional packings and their application in combined systems like catalytic distillation (Spiegel and Meier, 2003), or multiphase catalytic processes (Kapteijn and Moulijn, 2003).

Monolith is an example of structured catalyst or reactor, the borders vanish for this catalyst application either as catalyst or as a functional reactor internal. The use of these structured reactors allow to decouple the chemistry, transport phenomena, and hydrodynamics and hence to tailor the reactor/catalyst independently to satisfy optimal operation conditions. Monoliths can be used both for co- and counter current operation in gas-liquid reactions (Heibel et al., 2003). They can combine the advantages of the slurry and trickle-bed reactor and eliminate the disadvantages such as discontinuous operation, stirring energy input and catalyst attrition or ineffective catalyst use, liquid maldistribution and local hot-spots that may develop and cause runaways. They can be contacted in virtually any desired way, opening up new processing routes, (Roy Sharbal et al., 2004; Boger et al., 2004). Catalytic conversion can be combined, heat integration is possible, and lead to process intensification. In the laboratory monolithic structures provide a tool for scaling down catalyst testing units, with a wink to microreactor technology and combinatorial catalysis. It is expected that monoliths will be increasingly applied to chemical and biochemical conversion processes, from bulk and fine chemical production processes and in clean-up processes. Indeed the motivation of the use of monoliths (or capillary channels in other configurations), and proof of the concept has been established with great certainty, leading often to very accurate predictions of the performance (Kreutzer et al., 2005; Baurer et al., 2005).

Moreover one of the major aims of the researches on novel (micro-) structured reactor beds and catalytic support is process intensification, or herein, among others, a marked reduction of the size of the current reactor units is pursued. This involves monolith reactors, bead-string reactors, ceramic foam packings, composite structured packing reactors, three-levels of porosity reactors, etc. For example, Desmet et al. (2003) have presented a global optimization analysis of a general class of perforated monolithic bed reactors for the case of an isothermal first-order reaction and for laminar flow conditions. The resulting design rules indicate how a given amount of catalyst material should best be perforated or distributed in space as a function of the available inlet pressure. It is shown that, in applying, the more advanced reactor designs involving beds with ultra-small flow-through pores, proposed in

the past years, the productivity gain of these advanced concepts can even amount up to a factor of 100.

An alternative reaction–separation unit is the chromatographic reactor. It uses differences in the adsorptivity of the different components involved rather than differences in their volatility. It is especially interesting as an alternative to reactive distillation when the species involved exhibit small volatility differences, are non–volatile or are sensitive to temperature, as in the case of small fine chemical or pharmaceutical applications. There are several classes of reactions to which reactive chromatography is applied. The widest class of reactions is given by esterification reactions catalyzed by acidic ion–exchange resins or by immobilized enzymes, as the polarity difference between the two products (ester and water) makes their separation easy on many different adsorbents. Other applications include trans–esterifications, alkylation, etherification, (de)hydrogenations and reactions involving sugars. Reactive chromatography has also been used for methane oxidation. In all these applications, special care has to be devoted towards the choice of the solid phase for sorption selectivity, sorption capacity and catalytic activity. Typical adsorbents used are activated carbon, zeolites, alumina, ion–exchange resins and immobilized enzymes (Lode et al., 2001).

Concerning the coupling of reaction and crystallization, there exist myriads of basic chemicals, pharmaceuticals, agricultural products, ceramic powders and pigments produced by reactive crystallization based processes: processes that combine crystallization with extraction to solution mine–salts. These separation processes are synthesized by bypassing the thermodynamic barriers imposed on the system by the chemical reactions, and the solubilities of the components in the mixture. By combining crystallizers with other unit operations, the stream compositions can be driven to regions within composition space where selective crystallization can occur. Berry and Ng (1997a) have shown how to selectively crystallize desired solid products after a reaction step and how to use compound formation to affect the separation of a mixture. They have also presented a systematic method to synthesize flow sheets to separate binary mixtures by crystallizer–extractor hybrids. The use of decanters, countercurrent extraction, and fractional countercurrent extraction is discussed for several phase behaviours including complex systems with multiple reactions.

The complementary nature of crystallization and distillation is also explored. Hybrids provide a route to bypass thermodynamic barriers in composition space that neither the distillation, which is blocked by azeotropes and hindered by tangent–pinches in vapour–liquid composition space, nor the selective crystallization, which is prevented by eutectics and hampered by solid solutions and temperature–

insensitive solubility surfaces, can overcome when used separately (Berry and Ng, 1997b). Extractive and adductive crystallization are solvent–based techniques that require distillation columns. They are applied to high melting, close–boiling systems. Extractive crystallization uses a solvent to change the relative solubility of the solutes to affect separations. The distillation column is used to create solvent swings and to recycle the solvent. Commercial examples include solvent dewaxing, solvent deoiling and separation of sterols. Another advantage of such crystallization–distillation hybrid separation processes is that they do not require the addition of solvents, which may increase the process flows, create waste streams, propagate throughout a chemical plant and require costly separation and recycle equipment.

Membrane technologies respond efficiently to the requirement of so–called process intensification because they allow improvements in manufacturing and processing, substantially decreasing the equipment–size/production–capacity ratio, energy consumption, and/or waste production and resulting in cheaper, sustainable technical solutions (Howell, 2002). The paper by Drioli and Romano (2001) documents the state–of–the–art and includes progress and perspectives on integrated membrane operations for sustainable industrial growth. The first studies on membrane reactors used membranes for distributing the feed of one of the reactants to a packed bed of catalyst. They were used in order to improve selectivity in partial oxidation reactions. Other methods like the immobilization of biocatalysts on polymeric membranes have attempted selective product removal from the reaction site in order to increase the conversion of product–inhibited or thermodynamically unfavorable reactions. With such membrane bioreactors, provided that membranes of suitable molecular weight cut off are used, the chemical reaction and physical separation of biocatalysts (and/or substrates) from the products can take place in the same unit. Substrate partition at the membrane/fluid interface can be used to improve the selectivity of the catalytic reaction toward the derived products with minimal side reactions. Bioreactors based on hollow–fiber design are used to produce monoclonal antibodies for diagnostic tests, to mimic biological processes or to produce pure enantiomers, when a membrane separation is combined with an enantiospecific reaction. As for general membrane reactors, the result is a more compact system with higher conversion. This technology can respond to the increasing demand for food additives, feeds, flavors, fragrances, pharmaceuticals, and agrochemicals. Phase–transfer catalysis can also be performed in membrane reactor configurations by immobilizing the appropriate catalysts in the microporous structure of the hydrophobic membrane. Catalytic membrane reactors are also proposed for selective product removal to

remove equilibrium limitations, i.e., catalytic permselective or non-permselective membrane reactors, packed bed (catalytic) permselective membrane reactors, fluidized bed (catalytic) permselective membrane reactors. So the reaction step can be improved through the integration of a separation step, as for example in membrane reactors for dehydrogenation reactions where hydrogen is withdrawn from the reaction mixture using permselective Pd-membranes thereby shifting the reaction equilibrium to the desired products. Alternatively, also the separation step can be improved due to the integration of a reaction step, as for instance in membrane reactors for the catalytic partial oxidation of methane using permselective dense perovskite membranes for the air separation, where the high consumption rate of oxygen at the permeate side helps increasing the chemical potential difference of oxygen across the membrane and hence the oxygen fluxes (van Sint Annoland et al. 2003). The development of such membrane reactors for high-temperature applications only became realistic in the last few years, with the development of high-temperature-resistant membranes (palladium membranes) mainly for dehydrogenation reactions, where the role of the membrane is simply hydrogen removal.

We should add that a new field of chemical and process engineering is now wide open with the coupling of supercritical fluids and membrane concepts to the design of very attractive and powerful processes, to improve the transfer, reaction and handling of highly viscous liquids. This major interest of all the processes thus created, is to safeguard the environment and the products. This is particularly essential when the processes are of a biological nature (Sarrade et al., 2002; Knez et al., 2003).

For more general applications, material scientists must solve the problem of providing inorganic membranes of perfect integrity, that have mechanical and thermal stability and that will allow large fluxes of desired species. Secondly, chemical engineers must resolve the heat transfer problem that now threatens successful scale-up. It might seem reasonable to expect membrane reactors, which combine oxygen transfer membranes with selective catalytic layers for the partial oxidation of hydrocarbons. However, a continuous research effort in the dynamics of these processes and in the study of advanced control systems applied to integrated multi-membrane operations is now necessary.

A formal classification of multifunctional reactors.

Multifunctional reactors are not new to the chemical and process industry as they have been used for absorption or extraction with chemical reaction. Only recently have reactors incorporating several "functions" in one reactor been formally classified as being

multifunctional. The great benefits obtained in integrating the progress of knowledge at different time and length scales have been acknowledged by the process industries. This was illustrated by the first international symposium on multifunctional reactors (Moulijn and Stankiewicz, 1999) with a presentation of research and development in the main domains of reaction and heat exchange, reaction and membrane separation, reaction and sorption, reaction and power generation, reactions and distillation, reaction and catalyst regeneration and the use of non-traditional structured packing. This was also illustrated by the second symposium on multifunctional reactors (Agar, 2002) which shows that although two areas – reactive distillation and membrane reactors – still dominate the subject, several others, such as chromatographic reactors, are catching up rapidly and exotic newcomers, involving the electrochemical processes in fuel cells for example, are emerging. Moreover this was recently illustrated by the 3rd International Symposium on multifunctional reactors held in Bath 2003 (Kerhsenbaum, 2004) with contributions on reactive distillation, adsorptive reactors, membrane reactors, autothermal reaction systems, and structured reactor configurations. And finally a Working Party of the European Federation of Chemical Engineering was created on that topic in 2005 regrouping a great number of academic and industrial partners.

In summary to achieve optimal performance with multifunctional reactors, it is important to lead a scientific approach to understand where the integration of functionalities occurs, as explained by Dautzenberg and Mukherjee (2001) (Figure 7) and illustrated in a survey by Krishna (2002).

In general, the use of hybrid technologies encountered in a great number of multifunctional reactors is limited by the resulting problems with control and simulation. The interaction between simultaneous

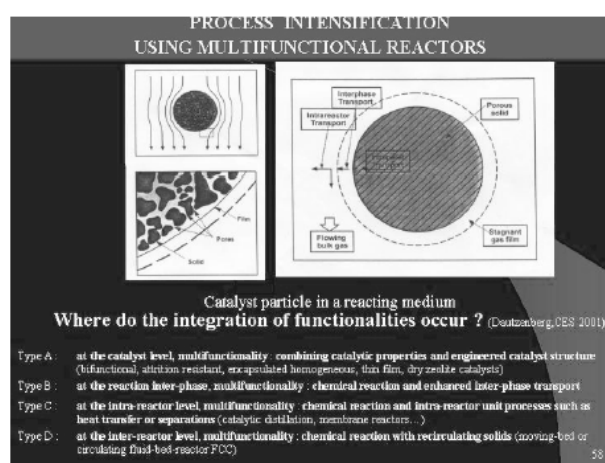


Figure 7. Process intensification using multifunctional reactors: where do the integration functionalities occur? (Dautzenberg and Mukherjee, 2001)

reaction and distillation introduces more complex behaviour, involving the existence of multiple steady states and output multiplicities corresponding to different conversions and product selectivity than those achieved in conventional reactors and ordinary distillation columns. This leads to interesting challenging problems in dynamic modeling, design, operation, and strong non-linear control. Indeed, the response of a reactive separator with marginal changes in design parameters, such as feed position, feed flow, number of stages, height, type of packing or plates, etc...may be drastic and unforeseen and, consequently, the simulation of this hybrid equipment should be based on reliable models with high accuracy. Their control requires sophisticated model predictive control, robust control and adaptative control, where mathematical predictive control may have to run 50–500 times faster than real time.

There is also an increasing awareness that the full potential of multifunctional reactors may only be realized if the reaction and the unit operation integrated are properly harmonized and too much integration can even exert a negative influence, requiring detailed modeling of the underlying processes and careful selection of the chemical and physical system properties and operation conditions (Stitt, 2002). It is suggested that many of the potential benefits can be achieved by a partial approach to multifunctionality and that further integration has a low increment value (Stitt, 2004).

Process intensification using new operating modes

The intensification of processes may be obtained by new modes of production that are also based on scientific principles. New operating modes have been studied in the laboratory and/or pilot stage: reversed flow for reaction–regeneration, unsteady operations, cyclic processes, extreme conditions, pultrusion, low-frequency vibrations to improve gas–liquid contacting in bubble columns, high temperature and high pressure technologies, and supercritical media are now seriously considered for practical applications. Reactors can be operated advantageously with moving thermal fronts that are created by periodic flow reversal. Low level contaminants or waste products such as volatile organic compounds can be efficiently removed in adiabatic fixed beds with periodic reversal by taking advantage of higher outlet temperatures generated in earlier cycles to accelerate exothermic reactions. Energy and cost savings are affected by this substitution of internal heat transfer for external exchange (Dautzenberg and Mukherjee, 2001).

Some attractive options for improved catalytic reactor performance via novel modes of operation are the periodic (symmetric) operation of packed beds with exothermic reaction, coupling of an exothermic and endothermic reaction in a periodically operated (asymmetric) packed-bed, and induced pulsing liquid

flow in trickle beds to improve liquid–solid contacting at low liquid mass velocities in the co-current downflow mode (Silveston and Hanika, 2004; Nigam and Larachi, 2005). Also such periodic operation with respect to liquid flow may help in providing process intensification for gas–limiting reactions or for petroleum applications where filtration and bed plugging are serious threats (Iliuta and Larachi, 2005). Moreover non–conventional research on magnetic–driven process intensification is worth noting for mini trickle bed reactors especially in non–petroleum applications such as in fine and pharmaceuticals chemical processes. It has been shown that a positive–gradient in homogeneous magnetic fields promote larger values of liquid holdup (and thus wetting efficiency in trickle flow regime) and two–phase pressure drop (Iliuta and Larachi, 2003). Also, when high conversions are required and the gaseous by–product of the reaction is known to inhibit the rate, as in hydrodesulfurization, or in selective hydrogenation, countercurrent flow operation of traditional trickle beds is now preferred (Julcour et al. 2001). Also, improving the product selectivities in a parallel–series reaction by feeding one reactant through the reactor by stage wise reactant dosing will be applied (Morbidei et al. 2001) and the use of ultrasonic and microwave technologies to enhance the rates and improve the selectivities of catalytic reactions should be underlined (Mikkola et al. 2002). It should also be emphasized that in recent years, among non–conventional bioreaction media, supercritical fluids and ionic liquids have recently appeared as interesting "green" alternatives to classical organic solvents to carry out enzymatic reactions for the preparation of valuable and active organic materials, opening the door for a clean chemical industry in the near future (Laudani, 2005).

Process intensification using microengineering and microtechnology

Current production modes will be increasingly challenged by decentralization, modularization and miniaturization. Microtechnologies developed, especially in Germany (i.e., IMM, Mains and Forschungszentrum, Karlsruhe) and in the USA (i.e., MIT and DuPont) lead to microreactors, micromixers, microseparators, micro–heat–exchangers and microanalyzers, making accurate control of reaction conditions possible with respect to mixing, quenching, and temperature profile. Microfabrication techniques and scale–up by replication have shown spectacular advances in the electronics industry, and, more recently, in microanalysis by biological and chemical applications. Microfabricated chemical systems are now expected to have a number of advantages for chemical kinetic studies, chemical synthesis, and more generally, for process development. Indeed the reduction in size and integration of multiple functions has the potential to produce structures with capabilities that exceed those of the conventional

macroscopic systems and to add new functionality, while potentially making possible mass production at low cost.

Miniaturization of chemical analytic devices in a micro-total-analysis-system (μ TAS) (Berg et al, 2000) represents a natural extension of microfabrication technology to biology and chemistry, with clear applications in combinatorial chemistry, high throughput screening, and portable analytical measurement devices. Also, the merging of μ TAS techniques with microreaction technology promises to yield a wide range of novel devices for reaction kinetic and micromechanism studies, as well as the on-line monitoring of production systems, as explained by Jensen (2001) in a publication on the state of the art on microreaction engineering.

Microreaction technology is expected to have a number of advantages for chemical production (Ehrfeld et al., 2000; Hessel et al., 2004, 2005). The high heat and mass transfer rates possible in microfluidic systems allow reactions to be performed under more aggressive conditions with higher yields than conventional reactors. Also, new reaction pathways considered too difficult for application in conventional microscopic equipment, such as the direct fluorination of aromatic compounds, could be pursued because if the microreactor fails, the small amount of chemicals released accidentally could easily be contained. The presence of integrated sensor and control units could allow the failed microreactor to be isolated and replaced, while other parallel units continued production. In addition, these inherent safety characteristics could allow a production scale system of multiple microreactors, enabling a distributed point-of-use synthesis of chemicals with storage and shipping limitations, such as highly reactive and toxic intermediates like cyanides, peroxides, and azides.

Microchemical systems for combinatory synthesis and the screening of small molecules and systems for nucleic acid synthesis and detection have already revolutionized drug discoveries in pharmaceutical companies (Borman, 2000). Similarly, the rapid screening of small molecules and systems for nucleic acid synthesis pathways could lead to an analogous productivity increases in chemical industry laboratories. Experimentation at the conventional bench-scale is limited by the high costs of reagents and safety concerns, which the small volumes and inherent safety characteristics of the microreactors could effectively eliminate (Hendershot, 2000 ; Jachuck, 2002). Moreover, scale-up to production by replication of the microreactor units used in the laboratory would eliminate costly redesign and pilot plant experiments, thereby shortening the development time from laboratory to commercial-scale production. This approach would be particularly advantageous for pharmaceutical and fine chemical industries where production amounts are often less than a few metric tons per year. Others more

recently have begun to apply microchannel technology to larger scale applications such as methane steam reforming, propylene oxide, hydrogen peroxide production, etc, some with industrial partnership, Degussa, FMC, UOP, etc, as referred by Tonkovich et al., 2005.

Small reactors are already used for testing process chemistries, like catalyst testing. Chemical detection is the rate-limiting step in most techniques since detailed product information must be obtained using sequential screening. However, with the continual advances in μ TAS and microfabrication techniques, these macroscopic test systems could be replaced by PC-card-sized microchemical systems consisting of integrated microfluidic, sensor, control, and reaction components requiring less space and utilities, and producing less waste. Moreover, the small dimensions imply laminar flow, making it feasible to fully characterize heat and mass transfer and extract chemical kinetic parameters from sensor data.

As an illustration de Bellefon et al. (2000) proposed a new concept for high throughput screening (HTS) experiments for rapid catalyst screening based on dynamic sequential operations with a combination of pulse injections and micromachined elements. The principle used for the test microreactor is a combination of pulse injections of the catalyst and the substrate, a static IMM micromixer with negligible volume and residence time less than 10^{-2} s mounted in a dynamic microactivity test, and a tubular stainless steel capillary reactor (Figure 8). The pulses mix perfectly in the micromixer and the liquids or the gas-liquid mixtures thereby emulsify and behave as a reacting segment, which then travels along the tubular microreactor. Collection and analysis at the outlet of the reactor provides the conversion and selective data. The catalyst library was then screened for 2 test reactions, a liquid-liquid isomerization of allylic alcohols and a gas-liquid asymmetric hydrogenation. The results of this technique lead to the selection of the best catalyst

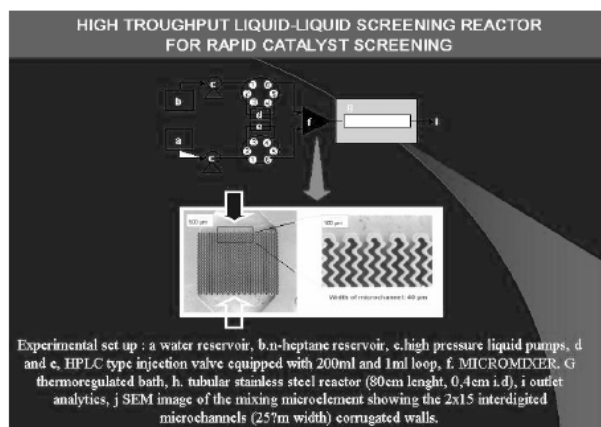


Figure 8. The IMM micromixer for high throughput screening (de Bellefon et al. 2000)

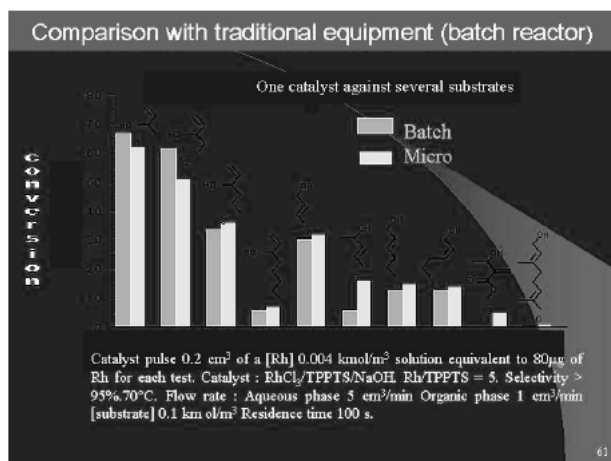


Figure 9. High throughput screening: comparison with traditional equipment (de Bellefon et al. 2000)

showing activity towards a large class of allylic alcohols and similar results obtained in a traditional well mixed batch reactor (40 cm³) proves the validity of the microreactor concept (Figure 9). Indeed using these microreactors for HTS of fluid–liquid molecular catalysis offer considerable advantages over traditional parallel batch operations by ensuring good heat and mass transport in a small volume, reducing sample amounts (to µg levels), a large range of operating conditions (temperature, pressure), fewer, simpler electro–mechanical moving parts and throughput testing frequencies of more than 500 per day.

Complementary data concerning part of a high throughput catalyst screening facility have been presented by Tesar et al (2004) which developed a microfluidic unit for sequencing fluid samples for composition analysis. The novel feature is that the key components are the use of an array of microfluidic valves having no moving parts and operating at very low sample flow Reynolds numbers, typically below 100.

Another illustration is the design of a prototype miniature bioreactor for high throughput automated bioprocessing. Indeed a major challenge for drug discovery now is to elucidate the relationship between proteins produced by each gene, and disease. In this respect, advances in proteomics and automated HTS based on the shaken microwell plate system have provided the technology platform for a significant increase in the number of potential drug candidates that are likely to come forward. A related challenge is the need to define the conditions from the translation of results, from the microwell systems to conventional laboratory scale. Recently Lamping et al. (2003) described a new miniature gas–liquid bioreactor designed to have the same diameter as that of a single well of a standard 24–well plate but being mechanically agitated and aerated with a microfabricated – bladed turbine impellor such that its operation mimicked the flow conditions in a conventional mechanically stirred

reactor. They used experimental and theoretical analysis to establish its performance as a fermenter. Microfabricated fibre optic probes were used for in–situ measurement of the process parameters including dissolved oxygen, pH, temperature, and cell density. The volumetric oxygen transfer data were obtained for air–water and *Escherichia–coli* fermentation for different operational conditions. The results were compared with data obtained from parallel experiments using a 20 l mechanically agitated fermenter with a working volume of 15 l and with predictions using Higbie's penetration model with the contact time obtained from the CFD simulations of the turbulent flow in the bioreactor. The predicted and measured volumetric mass transfer coefficients in the miniature bioreactor were in the range 100–400 h⁻¹, typical of those reported for large–scale fermentation which assessed its engineering performance as a fermenter.

The examples reported here represent a small fraction of the many designs for microreactors being pursued or envisioned by different research groups. Microengineered reactors have some unique characteristics that create the potential for high performance chemicals and information processing on complex systems. They can provide significant advantages in information generation for high throughput experimentation and process development, and reduce difficulties to obtain operating regimes. In terms of chemical manufacture, they allow distributed, mobile and intensified processing (Gavriilidis et al. 2002). However, when applying microengineered reactors, it should be suggested to conduct a fair comparison between microchannel reactors and their conventional counterparts. The new reactor type has to be tested against the best alternative reactor for the given application (kinetic measurements, catalyst screening, production, etc) (Walter et al., 2005). Moreover in developing microreaction technology for process intensification, it is essential to focus on systems where microfabrication can provide unique process advantages resulting from the small dimensions, i.e. not only the high transport rates, but the forces associated with a high surface area–to–volume ratio.

In summary for process intensification, Tsouris and Porcelli (2003) have shown that many new technologies are being developed in chemical industries motivated by improved chemistry, enhanced safety, improved processing energy and environment benefits, low inventories, capital cost reduction, enhanced corporate image, novel or enhanced products and value to customers. Stankiewicz (2000) has even schematically proposed a vision of how a future plant employing process intensification may look compared to a conventional plant (Figure 10 a). This has already been obtained in certain cases (Figure 10 b).



Figure 10a. One vision of how a future plant employing process intensification may look (right) versus a conventional plant (left) (Stankiewicz and Moulijn, 2000).



Figure 10b. One vision of a contemporary plant employing process intensification

But several important barriers must be overcome before process intensification is widely adapted such as the maturity and economic competitiveness of the new technologies compared to conventional technologies. The conservatism of plant owners, batch processors will not easily accept continuous processing solutions.

Anyway, it must be underlined that today's microreaction technology contributes substantially to the fields of chemistry, chemical engineering and energy generation, to name but a few. It is seen that this technology which on the reaction level already shows a broad variety of facets concerning different applications, has now reached the field of downstream processing to influence industrial pilot and also production processing. The availability of complete plants with microstructured reactors has led to commercial interest. The current impact of microreaction technology on chemical and process engineering is reflected in the fact that two consecutive issues of the Chemical Engineering and Technology Journal 2005, 28, N°3 and N°4, edited by V. Hessel have been dedicated to this topic, showing both

breathtaking scientific results and their process application. It is clear that there exists today a current trend which can be called from microreactor design to microreactor process design.

Manufacturing end-use properties: product design and engineering

This is the answer for today's ever-growing market place demand for sophisticated products that combine several functions and properties: cosmetics, detergents, surfactants, foams, lubricants, textiles, inks, paints, rubber, bituminous emulsions, plastic composites, pharmaceuticals, drugs, foods, agrochemicals, and more.

In practice, the end-use property of such products is often more important than its chemical composition for the consumer. As explained earlier, these functions and end-use properties have to be built and scaled up from nano or microscale liquid or solid structures inside the process equipment in order to meet consumer demands on the product mesoscale. In practice, these technologies mostly concern complex media and particulate solids. Indeed, complex media such as non-Newtonian liquids are often used, including gels, foams, hydrosoluble polymers, colloids, dispersions, microemulsions and suspensions for which rheology and interfacial phenomena play a major role. Similarly, they apply to the so called "soft solids": systems which have a detectable yield stress, such as ceramic pastes, foods, gels, solid foams, and drilling muds.

Moreover, product engineering concerns particulate solids encountered in 70% of the process industries. This involves the creation and the control of the particle size distribution in operations such as crystallization, precipitation, prilling, generation of aerosols and nanoparticles as well as the control of the particle morphology and the final shaping and presentation in operations such as agglomeration, calcination, compaction, and encapsulation. Both types of applications (complex media and particulate solids) require better understanding, as they control the end-use property and quality features, such as taste, feel, smell, color, handling properties, sinterability or biocompatibility of the product. Product engineering also concerns solids, which are considered vehicles of condensed matter in solventless processes. Non-passive or "intelligent solids" may be obtained by multiple layer coatings and are used to accomplish intelligent functions such as controlled reactivity or the programmed release of active components.

It is clear that the properties of these materials are determined primarily not by their overall composition, but rather by their nano and microstructure. Indeed the quality and properties of such emulsified or paste-like and solid products is determined at the micro- and nano-level. Therefore, to be able to design and control the product quality and make the leap from the

nano-level to the process level, chemical and process engineers involved with the complexity of structured material, face many challenges in fundamentals (structure-activity relationships on the molecular level, interfacial phenomena, adhesive forces, molecular modelling, equilibria, kinetics, and product characterization techniques); in product design (nucleation growth, internal structure, stabilization, additive); in process integration (simulation and design tools based on population balance); and in process control (sensors and dynamic models) (Wintermantel – 1999).

This explains why numerous process companies that manufacture structured materials (fluids, soft solids, and solids) collaborate with university partners in multidisciplinary research-development programs on the formation and handling of solid particles; on emulsification and homogenisation; on soft solids for the control of the end-use properties of the product; and more generally on the manufacturing of a product with the desired qualities. Indeed, the manufacturing cost, as well as the research and development expenses which constitute about 30–35% of product cost are equally important.

For illustration, we may cite the control of the quality of microemulsions for foodstuffs containing microorganisms that could spoil and the growth of which can be prevented by enclosing them in a water-in-oil emulsion of aqueous droplet size not significantly larger than 1 μm and of a narrow size distribution, which namely characterizes the product quality (Schubert, 1997). Such miniemulsions can only be generated in high-pressure homogenizers with a high-energy input and customized nozzle geometry. However the droplets generated must not coalesce during emulsification which makes it necessary to find emulsifier systems which also stabilize the droplets sufficiently fast. So, in modelling the emulsification process, the overall process must be divided into two substeps: the generation of droplets by mechanical energy and stabilization of the droplets before they re-coalesce. The resulting product quality is determined not only by how well the dispersed phase has been broken up into small droplets but also by how well the equipment, process conditions and emulsifier have been matched to one another (Schubert and Engel, 2004).

Complementary in topics such as microemulsions for the chemical, food and pharmaceutical industries (drug delivery systems), investigations on monodisperse emulsion formation with a micro-fabricated microchannel (MC) array, called a straightthrough microchannel, i.e. a silicon array of elongated through-holes for monodisperse emulsion droplets should be emphasized (Kobayashi et al. 2002). Such oblong straightthrough MC equipment allows the production of monodisperse oil in water emulsion droplets with an average diameter of 32.5 μm and a coefficient of variation of 1.5% verifying their excellent monodispersity (Figure 11). Such monodispersed droplets in emulsions have advantages for the control of their

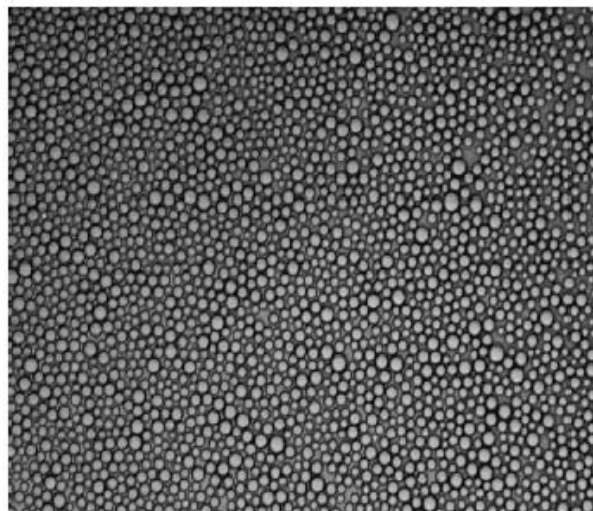


Figure 11. Monodispersed emulsion formed with a micro-fabricated microchannel array

physical and functional end-use properties, stability and application to other processings. The same microchannel technique was applied to obtain monodispersed microbubbles using surfactants and proteins as dispersing agents. The average bubble size ranged from 34 to 51 μm and a coefficient of variation below 10% (Yasuno et al., 2004).

For topical delivery especially on the skin, novel multiple lipidic systems account for the sustained release and optimized stabilization of active ingredients as well as drugs. Topical delivery for cosmetic products combines aspects of optimized skin release of actives and an optimized match to the sensorical features of a product. Prominent examples for the preparation of such kind are multiple emulsions of the water in oil in water type (W/O/W type), produced by the partial-phase sol-inversion technology (PPSIT), and solid lipid nanoparticles (SLN, lipopearls) and multicompartiment solid lipid nanoparticles (MSLN).

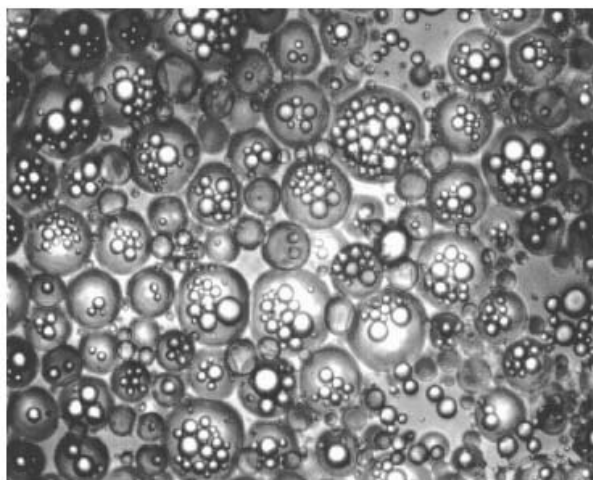


Figure 12. Multiple W/O/W emulsion manufactured by partial-phase solinversion technology (Gohla, 2002)

Multiple emulsions based on the PPSIT technology (Figure 12) combine the protecting and occluding effects of classical W/O emulsions and the easy application feature of classical O/W formulations. Besides, the W/O/W base as such already shows excellent skin caring properties, as exemplified by improving the skin's microrelief, short-, mid-, and long term moisture holding capacity (adaptogenic moisturization) and skin firmness improvement. Such multiple emulsions are manufactured by a novel one step manufacturing technology even facilitating industrial scaling up to large scale (up to 1 t batches).

The formulation of oxidation-instable ingredients such as Lipoic Acid and Retinol are preferentially stabilized in solid lipid nanoparticles (SLN) suspensions, which can either coat the instable materials as a solid shell or even can entrap additional solving oil compartments to be detected active (Figure 13). SLN particles can be manufactured based on proloxamer derivatives as well as non-ethoxylated lipids, such as Compritol or Dynasan. High pressure homogenization also reveals an ultra narrow particle size distribution in the nanometer range and an excellent stabilization of lipophilic ingredients such as Ubiquinone Q10 and Vitamin E and derivatives. Due to the solid character of this carrier, active ingredients can be protected against both oxidation and hydrolysis.

Retinol and sunfilters are e.g. successfully encapsulated and stabilized by SLN technology. Thus multiple lipidic formulation technologies (both new topical application technologies – W/O/W – type and SLN – type) are now in the focus of cosmetic as well as pharmaceutical product design and formulation technology with particular gain in knowledge about emulsifiers and microencapsulation technologies concerned with potential to stabilize fragile ingredients and to obtain typical sustained release properties.

Control of the shape and size of crystals in an industrial crystallization process can also be cited as an

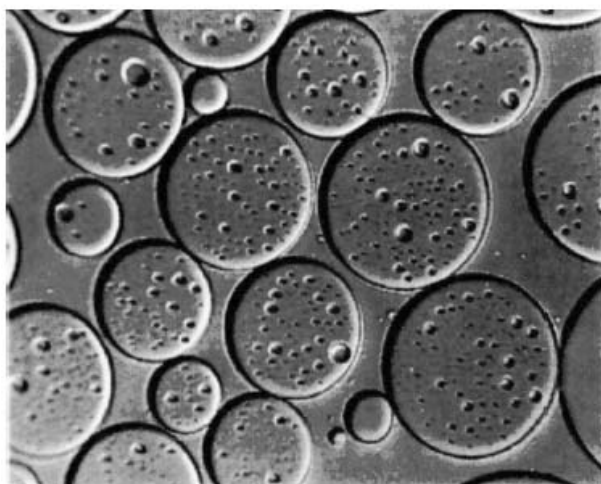


Figure 13. Solid-lipid-nanoparticles

example. Wintermantel (1999) has shown that much improved process control, in terms of both crystal purity and defined size distribution could result by detailed computer studies of the crystallization process, which could be markedly changed by the presence of small traces of foreign substances such as unwanted by-products in the feed solution. In order to understand the mechanisms causing these changes in crystal size and shape, and to utilise them in a controlled manner, we must explain the structure-activity relationships on a molecular level. With computer simulations, diagrams of the molecular structure of the most important crystal surfaces may be generated from x-ray crystal structure data. In the same computer simulation, contaminant molecules as well as molecules with an expected beneficial effect on the crystallization process can be placed on each crystal surface, and their adsorption energy could be calculated. The hypothesis is that the growth rate of the surface decreases with increasing adsorption energy, and by comparing relative adsorption energies, the expected modified crystal shape could be predicted. This was illustrated with the results of crystallization from a feed ammonium sulphate solution containing amaranth dye. It was shown that the amaranth molecule is adsorbed onto the 001 surface of ammonium sulphate crystals with the highest adsorption energy in comparison with the other crystal surfaces. According to the calculations, the somewhat block-shaped crystal produced in the pure system becomes a flat shaped crystal having a large 001 surface area, which was experimentally verified (Figure 14). Similar results were predicted and experimentally verified when aluminium-ions were added as an impurity (Rauls et al. 2000) (Figure 15).

So many quality features can only be designed in a targeted way if the molecular processes are understood at this level. And as shown by this example, the analysis, both by theoretical and by experimental means must be carried out at the molecular level to obtain results of real value. To understand the

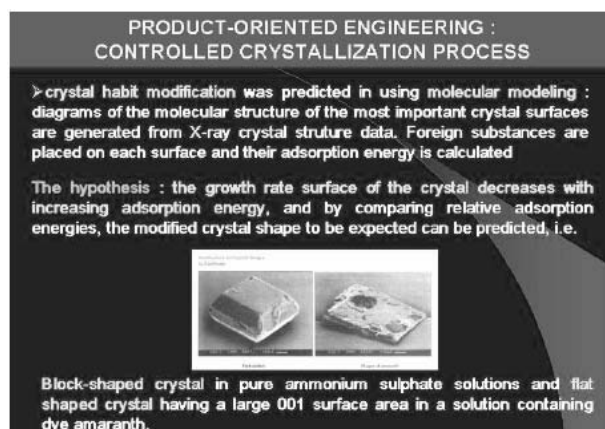


Figure 14. Product-oriented engineering: controlled crystallization process (Wintermantel, 1999)

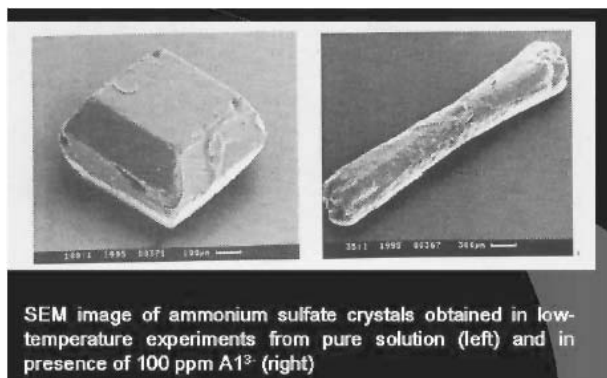


Figure 15. SEM image of ammonium sulfate crystals obtained in low temperature experiments from pure solution and in the presence of Al^{3+}

relationship between a certain set of product qualities and the physical product state, let us take for example two pain killing tablets that may have the same chemical composition, but different routes of production, which may lead to different crystallinity and porosity profiles and therefore to totally different dissolution and solubility properties, namely different bioavailabilities. The rate and extent of adsorption in the human body are often determined by the dissolution rates of different crystal faces (Villadsen, 1997). The coming years will see more and more investigations on that topic named polymorphism.

Recent models recognize the significance of complex interfacial phenomena in crystal shape modeling, and lead the way for future developments, such as new simulation and/or group contribution methods for interfacial free energy production. Thus, an important and challenging area for chemical engineering research is to link interfacial models, capable of capturing the solvent or other process conditions to process models, leading to the end-product quality specifically required in the specialty and fine chemical, as well as in the pharmaceutical and life science industries. This explains why for practical purposes, idealized process models are proposed to describe the interactions of the flow pattern in agitated vessels with precipitation processes taking place on different scales, ranging from the macroscopic scale (macromixing) to the microscopic scale (micromixing). Coupled with the population balance, such mixing models may be used to model the influence of meso and microscale vessel hydrodynamics on continuous and semi batch crystal precipitation characteristics, quality nucleation rates and particle size distribution (Zauner and Jones, 2002, Marchisio et al. 2003, Kulikov et al., 2005).

Another good illustration of this multilevel research effort in crystallization has been proposed in the area of electrical engineering: microelectronics. It concerns correlations between the operating conditions and microstructure of Low Pressure Chemical Vapor Deposit (LPCVD) silicon based films prepared from silane SiH_4

**How to design theoretically
the best industrial equipment and procedures (at mesoscale)
(tubular reactor, length 2 metres, diameter 0,2 metre)
to obtain the desired material
structure and properties of use (at nanoscale)**

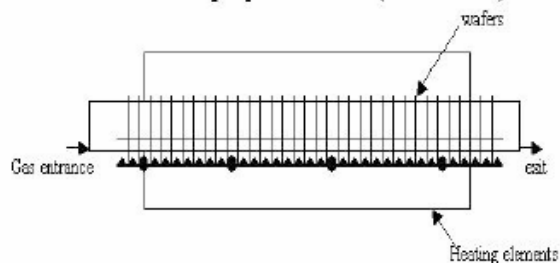


Figure 16. Schematic diagram of a horizontal hot wall microelectronic reactor

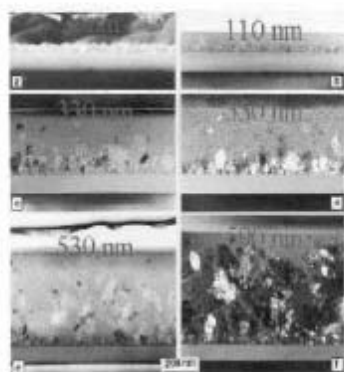
(Dollet, Caussat, Couderc, & de Mauduit, 2000). A multidisciplinary working group of French and Spanish laboratories involving Motorola Semiconductors SA has been created to progress in this new and very ambitious research domain relative to LPCVD reactor modelling: mechanisms existing at the substrate surface, and finally nucleation and crystal growth phenomena.

The main aim of the study was the development of a rigorous simulation model for the interpretation of the layer growth experimental data by taking into account both the mass transfer resistance at the boundary layer and the solid layer growth kinetic expression. It has been possible to treat, first, the kinetic questions such as to find sets of conditions producing the desired thickness with the desired degree of uniformity. In a second step, one could solve the questions of material structure (amorphous, partially or totally crystallized silicon) end-use properties. The thin CVD layers were produced in a so-called hot wall tubular reactor (2 m length, 20 cm in diameter) schematically presented in Figure 16. Numerous characterization techniques have been used to study the layer microstructural evolutions as a function of their elaboration conditions.

The local state of the reactor was simulated by a CVD2 model including the gaseous flow hydrodynamic parameters, the mass transfer parameters and chemical reaction parameters both in the heterogeneous phase (gas-solid interface) and in the homogeneous phase (solid phase). The mechanism existing at the surface substrate and nucleation and crystal growth phenomena together with the dynamic characteristics of the microstructure formation were modelled using a simple geometric and statistic approach based on concepts of the mechanics of continuous media (instead of using molecular dynamic models requiring too much computer power).

The final model that necessitates the local conditions of elaborations at the substrate surface and nucleation and crystal growth laws is able to calculate

Influence of deposit thickness or duration



Silicon films from pure silane
 T = 600°C - P = 0.2 Torr

Figure 17. Influence of the substrate surface on the microstructure of LPCVD films (Caussat et al., 1999)

the thickness, the fraction of crystallized silicon and the space distribution of silicon crystallites in the deposit layer films from operating conditions such as gas-phase components, temperature, pressure and initial substrate nature or surface state.

Figure 17 shows transmission electronic microscopy micrographies of silicon films from pure silane for a deposit duration of 29 and 85 nm thickness at 570°C and 0.2 Torr on different substrates: silica SiO₂, nitride Si₃N₄, amorphous and polycrystalline silicon substrate. Only the silica substrate exhibits a partial crystallization. Concerning the crystal state and growth, the Figure shows the influence of deposit duration of silicon films from pure silane on a silica substrate. For thin films (short duration) silicon is practically amorphous, for intermediary films, silicon is partially crystallized and for long duration, silicon becomes again totally crystallized. A comparison between these experimental data and the simulation results of the model has shown a good approximation for the crystallized fraction x_c and the space distribution of the crystallites (Dollet et al., 2000, Figure 18). The results also emphasize the dynamic characteristics of the film microstructure. Similar results were obtained for a complex SIPOS SiO_x deposit elaborated from silane and nitrogen protoxide and in situ boron silicon deposits from silane and boron trichloride (Caussat et al., 2001). It is interesting to note that the quality of the simulation results so obtained demonstrates the validity of the approach proposed and suggests that the way is now opened to develop complete product engineering or engineering of materials elaborations, able to predict the kinetic and structural characteristics of LPCVD films by numerical simulation.

MICROSTRUCTURE OF SILICONE LPCVD FILMS FROM SILANE AT DIFFERENT TEMPERATURES

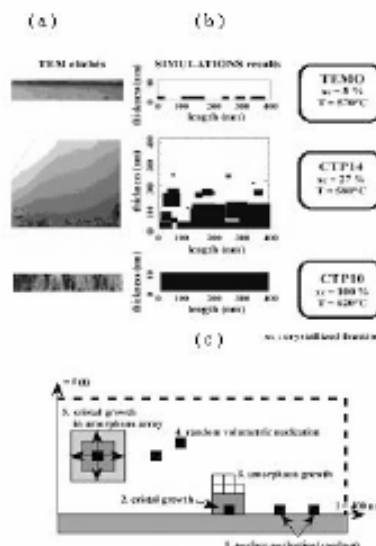


Figure 18. Microstructure of silicon LPCVD films at different temperatures: (a) TEM images, (b) simulation results, (c) schematic structure of the film deposit thickness (Dollet et al., 2000)

More generally, and not only focused on microelectronics, it will be possible to envisage a complementary but more global approach to control the material microstructure for thin film growth and nano-structured coatings processing applications, in using multiscale distributed systems. Indeed in addition to achieving spatially uniform deposition of thin films in chemical vapor deposition processes, one would like to control film properties such as composition and microstructure that characterize film quality. While deposition uniformity control can be accomplished on the basis of continuum type distributed models, precise control of the film properties requires multiscale distributed systems that predict how the film state is affected by changes in controllable processes parameters. Multiscale distributed systems constitute coupled molecular models, such as Monte Carlo and molecular dynamics simulation, that capture the evolution of microstructure formation and growth (including nucleation, impurities, cluster-cluster coalescence and adsorbate-adsorbate interactions) and continuum distributed models, based on conservation equations of momentum, energy and species, that describe spatio temporal process behaviour in macroscopic length and time scales.

While multiscale modeling provides a computationally attractive alternative with respect to direct modeling of the entire deposition process using a molecular model, it still leads to dynamic models that cannot be solved fast enough for real-time estimation and control purposes. Thus future research should focus on the study of the dynamics of multiscale

distributed models, the development of order reduction techniques for constructing low-order models that describe film properties directly from microscopic (Monte Carlo and molecular dynamics) film simulations (Raimondeau and Vlachos, 2000), and the integration of multiscale models, advanced sensing capabilities for online thin film microstructures/composition monitoring, and control theory to develop control systems that can be implemented in real time (Christofides, 2001).

In general, with respect to the manufacture of chemical-based consumer products, complementary industrial examples oriented on product-centered processing have been proposed by Wibowo and Ng (2002), including the production of dry toner, detergent, shampoo, and cosmetic lotion. In addition, examples on the formulation and manufacturing process development of pharmaceutical tablets and of a solution dedicated to roll web coating on smooth surfaces have been given by Favre et al. (2002) specifically to illustrate the potential of chemical product engineering. Also based on a multiscale approach which considers plant, equipment and particle scale issues, a systematic product-centered process synthesis and development procedure for tablets and capsules was formulated by Fung and Ng (2003).

Finally, we must underline that much progress has been made in the last few years in product oriented engineering and in process control using the scientific methods of chemical engineering. Thermodynamic equilibrium states are examined, transport processes and kinetics are analyzed separately and are linked by means of models with or without the help of molecular simulation and by means of computer tools for simulation, modeling and extrapolation at different scales for the whole supply chain up to the laboratory-scale (BASF, Unilever, Degussa, Astra Zeneca, Nestlé).

Since the processing of structured products usually alter their properties, process design cannot be decoupled from product design for these products. This highlights the need for concurrent product and process design (Hill, 2004).

But how can operations be scaled up from laboratory to plant? Will the same product be obtained and will its properties be preserved? What is the role of equipment design in determining product properties? Indeed, as mentioned many times in this paper, the control of end-use properties is a key issue for which general scale-up rules are still lacking. The development of this new "systemic" physical chemistry and biology where qualitative explanations will be translated with the help of fine modeling into formal laws for process development requires close cooperation between chemical engineering specialists and their systemic approach, with specialists in physical chemistry, biology, mechanics and mathematics. These questions have also justified the launch of a new

multidisciplinary section of the European Federation of Chemical Engineers entitled "Product Design and Engineering", involving both academic and industrial partners. The overview by Voncken et al. (2004) of the presentations at the 1st European Symposium on Product Engineering emphasizing the many facets of the product technology must also be underlined.

Summarizing the modeling required leads to the 4th main objective for the future development of chemical and process engineering.

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 involving control and safety

In the previous sections we have emphasized the necessary multidisciplinary and multiscale integrated approach of complexity applied to the 3P molecular Processes-Product-Process to scale from the nano and microstructures of the end-use properties of the product to the mesoscale of the equipment manufacturing the product. However, the task of chemical and process engineering has been and always will be to also design and implement the complete manufacturing systems up to the macro and megascales of the production site and the environment. Complete systems involve both individual processes and plants for producing products with specifically defined product properties as well as the integration of the individual processes into an overall production site in terms of materials, energy and logistics, 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 tackle all subsystem scale levels simultaneously. It continues to be the task of chemical engineering to analyze subsystems at the scale level that is adequate to represent the individual problem complexity. However, 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 higher levels (see Figure 2). Moving up from the subsystem level, methods and 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. This necessitates computer simulations that enable us to design individual steps, structure the whole process and place the individual process in the overall context of production, thus optimizing the supply chains from the nanoscale to the macroscale.

Computers have opened the way for chemical and process engineering in the modelling of molecular and physical properties on the microscopic scale. For molecular modelling, the application of the principles of

statistical molecular mechanic computational techniques (Monte-Carlo and molecular dynamics) and quantum mechanics constitute an area for the problem-oriented approach of chemical and process engineering. Indeed, molecular modelling starts with a consideration of microscopic structure and molecular interactions in a material system and derives thermodynamic, transport, rheological, mechanical, electrical, electronic or other properties through rigorous deductive reasoning based on the principles of quantum and statistical mechanics. Compared to more phenomenological approaches like correlations of the group contribution type, it offers the advantages of greater generality and reliability. Molecular modeling work can be classified broadly into theory and computer simulation. Theories provide closed-form descriptions of relationships between molecular constitution and macroscopic properties; typically, mathematical approximations have to be introduced in order to reach such tractable descriptions. Simulations, on the other hand, are numerical solutions of quantum and statistical mechanics formulations, which may be free of the simplifying approximations invoked in theories.

There is no doubt that molecular modelling is now playing an increasingly important role in future chemical and process engineering research and practice (Chen and Mathias, 2002 ; de Pablo and Escobedo, 2002; Frenkel and Smit, 2002; Papadopoulos and Linke, 2005). Recent advances in the fundamental molecular sciences, in computer hardware and in numerical algorithms and the development of new methods for simulation of complex fluids and materials have greatly accelerated its development. There are still many challenges to be met, stemming from the very large number of degrees of freedom needed for the molecular-level description of real-life systems (i.e. interatomic interactions), as a result, the computational requirements become excessive. The quantitative prediction of properties from chemical constitutions calls for hierarchies of theoretical and simulation methods that can be developed through systematic coarse-graining of the microscopic representation invoked in the modeling calculations. And connecting design with reality and its complexity, the consensus seems to be that simulation is useful un initial screening, but that experimental data are still essential for final design (Harvey and Laesecke, 2002).

Through the interplay of molecular theory, simulation, and experimental measurements a better quantitative understanding of structure-property relations evolves, which, when coupled with macroscopic chemical engineering science, can form the basis for new materials and process design.

Turning to the macroscopic scale, dynamic process modeling and process synthesis are being also increasingly developed. Indeed one must remember the targeted products in question are generally not

mass-produced products but ones which are produced in small batches and just in time for delivery to the customer whose needs are constantly changing and evolving.

To be competitive under these conditions, it is particularly important to analyse and optimize the supply chains shown in Figure 1, for which we are interested in the time that individual process steps take. These also have to be simulated and evaluated in terms of costs. In chemical and related process industries, the location of a particular component in the supply chain at a given time is not well defined. In the process industry a batch can be found in a stirred tank, a filter, a dryer, a pump, a mill and a storage container simultaneously. New event-driven simulation tools help solve these problems by simulating both material flows and states within the individual pieces of equipment. This dynamic simulation may enable us 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. The event-drive simulation also shows which alternative plant and storage strategies provide the greatest cost benefit (Wintermantel, 1999).

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 taking a more important place: see the Computer Aided Process Engineering European Brite Euram program CAPE-OPEN "Next generation computer aided process engineering open simulation environment," which involves a great number of simulator sellers, European clients and university researchers in computing and simulation. The aim is to promote the adoption of a standard of communication between simulation systems at any time and length-scale level (thermodynamic unit operations, numerical utilities for dynamic, static, batch simulations, fluid dynamics, process synthesis, energetics integration, process control) in order to simulate processes and allow the customers to integrate the information from any simulator onto another one.

In the future, more effective CAPE is required to be competitive in the process industry. The Global CAPE-OPEN (GCO) project is expanding and developing interface specification standards to ensure the interoperability of CAPE software components. A standardization body (CAPE-OPEN Laboratories Network, CO-LaN) has been established to maintain and disseminate the software standards in the CAPE domain that have been developed in the international projects CAPE-OPEN and Global CAPE-OPEN (Pons M. 2004) (Figures 19, 20, 21). The CO-LaN ensures that software tools used by the process industries reaches a level of interoperability that will sustain growth and competitiveness. Pons et al. (2001) have described the goals and means of the CO-LaN, especially its work

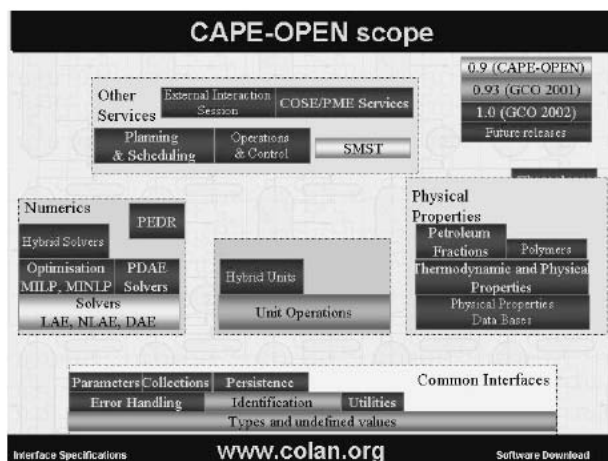


Figure 19. CAPE-OPEN scope (Pons, 2004)

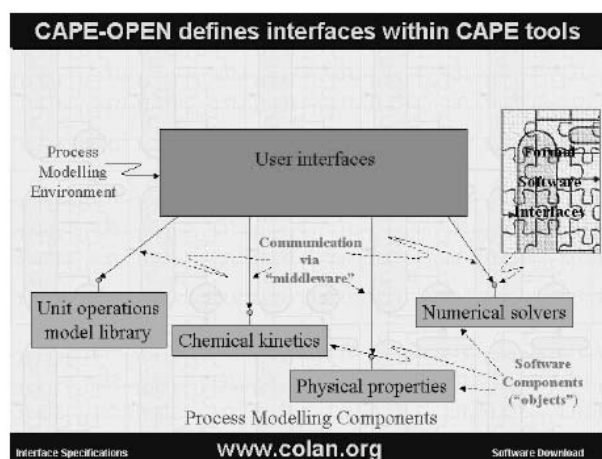


Figure 20. CAPE-OPEN defines interfaces within CAPE tools (Pons, 2004)

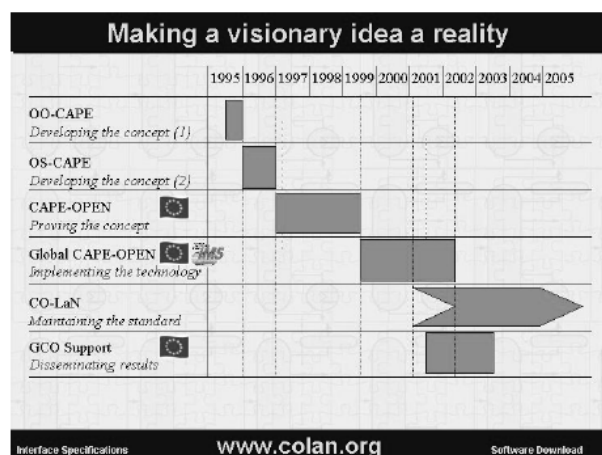


Figure 21. CAPE: Making a visionary idea a reality (Pons, 2004)

process related to testing procedures applied to software components, in order to assess their compliance with the published CAPE-OPEN interface specifications. A paper by Gani (2002) highlights for a class of chemical products, the design process, their

design with respect to the important issues, the need for appropriate tools and finally, lists some of the challenges and opportunities for the process systems engineering PSE/CAPE community.

Modeling should not be confused with numerical simulation. Especially for university and industry researchers, modeling must be an activity that requires knowledge of scientific facts, experience, skills, and judgment (Villiermaux, 1996). Attention should be focused on the systemic analytical models based on the multi-scale integrated approach previously referred that considers the global behaviour of complex systems as a whole, instead of looking at more details. Novel principles of the analytical models in chemical and process engineering should be sought at the highest level of integration.

For this purpose, the "equation-free" approach of Kevrekidis et al. (2004) should be underlined. They have developed and validated a mathematically inspired, computational enabling technology that allows the modeler to perform macroscopic tasks acting on the microscopic models directly, i.e. to look to the computer to explore the macroscopic behaviour, based on microscopic description. The main idea is to consider the microscopic simulator as a (computational) experiment that one can initialize and run at will. The results of such appropriately designed initialized, and executed brief computational experiments, allow us to estimate the same information that a macroscopic model would let us evaluate from explicit formulae. The final objective is to develop a computational approach for studying the simple collective, coarse-grained behaviour of any complex, multiscale system when we know in principle how to model such systems at a very fine scale (e.g., through molecular dynamics). And if enough control authority exists to initialize laboratory experiments "at will" this computational enabling technology can lead to experimental protocols for the equation-free exploration of complex system dynamics.

Finally, concerning modeling, what is needed is less anatomy and more physiology. This approach is required for a good understanding of the behaviour of the interactions in the process to be controlled. And it should be reminded that automation in world-scale plants provides high work force productivity, while in high margin multi-purpose plants it provides the capability to reach quality specifications and required throughputs quickly when restarting the process.

CONCLUSIONS: Chemical and Process Engineering: a multidisciplinary technology for managing complex systems in the context of society and market demands versus technology offers

Chemical and related industries are confronted with a great number of challenges in the framework of trade globalization and competition. These challenges have been presented and concern society and market

demands versus technology developments (Charpentier, 2000, 2003, Bertrand et al., 2004). First, it is necessary to research innovative processes for the production of commodity and intermediate products with non-polluting, perfectly safe industrial processes, and defect-free products. This affects "process driven" industries such as paper, iron and steel, glass, and commodity chemicals. Second, we need to progress from traditional intermediate chemistry to new specialties and active material chemistry, dominated by the synthesis of the end-use property of the product required by the customer. This affects "process enabled" industries, where both the product and process technologies not only evolve rapidly, but also must also be well synchronized, as the product and process capabilities are mutually dependent. Moreover, when used, the product should be safe and not significantly impact the environment.

To satisfy these consumer needs and market trends, the development of chemical and process engineering requires an integrated multidisciplinary and multiscale approach from the molecular scale up to the scale of the entire production site. We have defined it as the triplet "molecular Processes – Product – Process" Engineering or 3P Engineering (Charpentier, 2002). This approach is necessary for the understanding and modeling of complex, simultaneous and often coupled transport phenomena and processes taking place on the different scales of the chemical supply chain. This has been illustrated with examples involving polyolefin polymerization and biochemical process engineering. It has been emphasized that this integrated approach is possible today, thanks to considerable progress in the use of molecular modeling, scientific instrumentation and powerful computational tools and capabilities, as illustrated with the determination of physical and chemical parameters necessary for the modelling at different time and length scales (Boyer et al. 2002, Wild et al. 2003). This approach calls for a high degree of integration of process system engineering with other basic sciences, and for close collaboration among engineers and scientists of different backgrounds.

Therefore, for the future of chemical engineering, it is proposed to undertake simultaneous research in four directions: (1) Total multiscale control of the process to increase selectivity and productivity, a good illustration is the nanostructural tailoring of required materials with controlled structure, (2) Process intensification by design of novel equipment based on scientific principles and new production operating methods (Figures 10a and 10b). Examples concern multifunctional reactors, and the use of micro technology for high-throughput rapid catalyst screening experiments, (3) to synthesize structured products, combining several functions and properties required by the customer, with special emphasis on complex fluids and solids technology. Examples dealt with the quality of microemulsions for

Table 1.

TRENDS IN EUROPEAN CHEMICAL ENGINEERING					
	1999 Montpellier ECCE2	2001 Nürnberg ECCE3	2002 Praha CHISA	2003 Granada ECCE4	2005 Glasgow WCCE7 ECCE5
1. Increase Productivity and Selectivity through multiscale control of the process Molecular information engineering Nanotailoring of porous and crystalline Materials supplying local « informed » flux of energy or materials	33 %	15 %	22 %	24 %	25 %
2. Process Intensification Multifunctional reactors New operating modes Microengineering μ technology	25 %	39 %	30 %	22 %	18 %
3. Formulation Product design and engineering. Emphasis Complex Fluids Emulsion Solids technology	22 %	25 %	14 %	18 %	21 %
4. Multiscale and multidisciplinary Computational Chem Eng Modelisation and simulation. Optimization-Control-Safety	20 %	21 %	34 %	36 %	36 %

foodstuff and cosmetic and pharmaceutical products and the control of the shape, size and structure of crystals in crystallization processes encountered in chemical and microelectronics industries, (4) to implement multiscale and multidisciplinary computational modeling and simulation to real-life situations.

Table 1 shows the distribution of the contents of the lectures presented during the recent European congress on chemical engineering. The increasing part of academic and industrial investigations in modelisation, simulation, optimization, control and safety is seen, but it should be emphasized that modelisation and simulation should be oriented towards the understanding of the physics, chemistry and biology of interactions rather than the refinement of numerical codes the sophistication of which is not at all concerned with real life problems met in plants and in industrial practice (make models as simple as possible, but not simpler, Einstein citation).

It seems clear that the future of chemical and process engineering is heading in these four directions and requires the integrated approach presented as the 3P Engineering. Moreover, chemical and process engineering will also be increasingly involved and concerned with the application of Life Cycle Assessment to the 3PE Engineering approach, i.e. the application of LCA not only to product design and its use, but also to the plant and the equipment together with the associated services (Burgess and Brennan, 2001). Thus, this multidisciplinary and multiscale integrated approach for managing complex systems will be of great help, in responding to the increasing environmental, societal and economic requirements and to the transition towards sustainability, (environmental protection, security, societal demands, and business including better conversion and selectivity of raw materials and energy for consumer desired product quality), regardless of the industries where chemical engineers work.

We should add that a greater number of both scientific and technical articles on the four main objectives will be required in order to return the discipline closer to practices in industry and to reinforce its interdisciplinary ties. Indeed one must never forget that engineers and scientists in chemical engineering are complex interdisciplinary problem solvers, which means that interdisciplinarity will be more and more related to chemical engineering, just as solfeggio (sol-fa-music) is related to music. Music may be composed ignoring solfeggio, but no great composer has ever ignored solfeggio!

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IZVOD

BUDUĆI RAZVOJ HEMIJSKOG I PROCESNOG INŽENJERSTVA U SVETLU PROCESA GLOBALIZACIJE

(Pregledni rad)

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U svetlu današnje ekonomije, hemijsko inženjerstvo mora da odgovori na promenjene zahteve hemijske industrije u cilju zadovoljenja potreba za određenim materijalima na tržištu. Stoga je neophodna evolucija hemijskog inženjerstva kako bi se očuvala konkurentnost hemijske industrije na svetskom tržištu. U ovom radu se posebno potencira sposobnost hemijskog inženjerstva da se bavi i upravlja kompleksnim sistemima koji se susreću kod osnovnih i primenjenih tehnoloških istraživanja. Hemijsko inženjerstvo je posebno angažovano na problemima rešavanja i definisanja održivog razvoja, kako sa zadatkom da se zadovolje zahtevi tržišta u pogledu razvoja proizvoda sa željenim i zahtevanim karakteristikama ali i u pogledu osnovnih socioloških i ograničenja u odnosu na životnu sredinu. Neophodan je stoga integrisani pristup multidisciplinarnim, nelinearnim i neravnotežnim procesima i fenomenima koji se javljaju u različitim razmerama i vremenskim skalama. To se može ostvariti daljim probojem na polju molekuskog modelovanja, razvoja instrumentalnih tehnika, načina odgovarajuće obrade prikupljenih informacija i moćne kompjuterske tehnike. Budućnost hemijskog inženjerstva se može sumirati kroz četiri zadatka: (1) Povećanje produktivnosti i selektivnosti primenom intenzifikacije i inteligentnih operacija sa značajno povećanim odnosom prema kontroli procesa; (2) Razvoj novih naučno zasnovanih uređaja koji će zadovoljiti nove metode kao na pr.: proces intenzifikacije korišćenjem višefunkcionalnih reaktora i inženjerstva odnosno tehnologije na mikro nivou (3) Proširenje primene metodologije hemijskog inženjerstva u cilju razvoja novih proizvoda i tehnologije na osnovu principa "trostrukog P" kao 3P: Proces na molekuskom nivou–Proizvod–Procesno inženjerstvo" (4) Implementacija kompjuterizovanog hemijsko–inženjerskog modelovanja i simulacija realnih situacija u životu analiziranjem procesa od molekuskog nivoa do industrijskih razmera.

Ključne reči: Budućnost hemijskog inženjerstva, Kompleksni sistemi i hemijsko inženjerstvo, Multidisciplinarnost kompleksnih sistema, Razmera kompleksnih sistema, 3P sistem, Proces na molekuskom nivou–Proizvod– Procesno inženjerstvo, Razvoj proizvoda, Krajnje osobine proizvoda, Meka čvrsta faza, Kompleksni fluidi, Modelovanje na molekuskom nivou, Intenzifikacija procesa.