The Future of Chemical Engineering in the Global Market Context: Market Demands versus Technology Offers

KUI 21/2003
Received April 25, 2003
Accepted June 3, 2003

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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 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. A multidisciplinary, multiscale approach to chemical engineering is evolving 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 process control; (2) Novel design equipment based on scientific principles and new production methods: process intensification; (3) Extended chemical engineering methodology to product design and product focussed processing using the 3P Engineering "molecular Processes-Product-Process" approach; (4) Implemented multiscale application of computational chemical engineering modelling and simulation to real-life situations from the molecular scale to the production scale.

Keywords: *Future of chemical engineering, sustainability and chemical engineering, multidisciplinary and multiscale approach, product-oriented processing, the triplet "molecular Processes-Product-Process Engineering", end-use property, soft solids, complex fluids, molecular modelling, process intensification.*

Introduction

In the new consumer-based global economy, new needs and challenges arise. The key to survival for chemical engineering is the ability to cope with societal and economical problems encountered by the chemical process industry.[1,2] This report highlights some of the challenges faced by chemists and the awaiting chemical process industry in terms of market demand and sustainability. The new multi-disciplinary and multiscale approach to chemical engineering and the necessary tools to ensure the success of this integrated approach will also be presented. We propose that future research in chemical engineering is heading in four directions: tailoring materials with controlled structures, process intensification, product oriented engineering, and multiscale simulation and modelling from the molecular scale to the product scale.

Chemical and related industries are at the heart of a great number of scientific and technological challenges to be taken up by chemical engineering

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.

Chemical knowledge is also growing rapidly, and the rate of discovery is increasing every day, shown in Figure 1. Over fourteen million different molecular compounds have been synthesized and about one hundred thousand can be found on the market. Only a small fraction of them are found in nature. Most of them are and will be deliberately conceived, designed, synthesized and manufactured to meet a human need, to test an idea or to satisfy our quest of knowledge. The development of combinatory chemical synthesis is a current example.

Chemistry already plays an essential role in our attempt to feed the world's population, to tap new sources of energy, to clothe and house humankind, to improve health and eliminate sickness, to provide substitutes for rare raw materials, to design necessary materials for new information and communication technologies, and to monitor and protect our environment.

Thus, the challenges faced by chemical and related industries and the specific business of chemists is to imagine re-

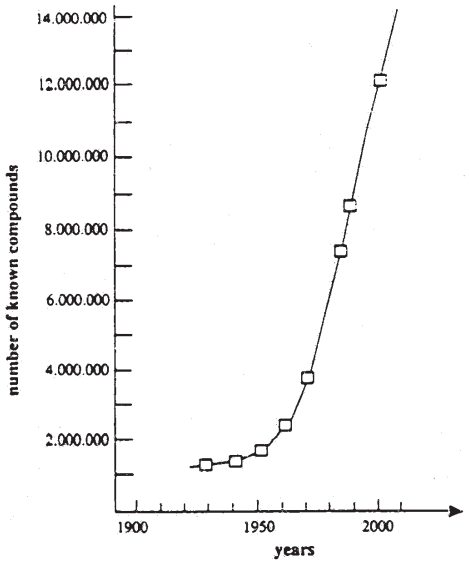

Fig. 1 – *Chemical knowledge is growing rapidly*
Slika 1 – *Znanje iz kemije naglo raste*

actions that will convert the chemical substances we find around us into substances or products that meet the consumer's needs. Modern chemistry has evolved to meet these new needs, such that the new keywords associated with it are: **life sciences**, **information and communication sciences**, **and instrumentation in the 21th century**.

What do we expect from chemical and process engineering?

There are two demands associated with the previous challenges to assure competitiveness, employement and sustainability in the process industry:

What products and processes will be competitive in the new global economy, where the keywords are globalization, technology, partnership and innovation (innovation means discovery + development)? The speed of product innovation is accelerating. For example, in the fast moving consumer goods business, to which the majority of the food businesses belong, product development time has decreased from 10 years in 1970, to an estimated 2–3 years in the year 2000.[3] This means that it is increasingly difficult to be the first on the market with an innovative product. Thus, speeding up the product/process development cycle is of paramount importance.

The response to the evolution of market demands involves a double challenge: developing countries have low labour costs and less constraining local production regulations. Industrialized countries, on the other hand, have rapid development in consumer demand, and more regulatory constraints stemming from public and media concerns over environmental and safety issues.

To respond to these demands, the following challenges will be faced by the chemical engineering industry:

1) Processes will no longer be selected on a basis of economic exploitation alone but, rather, the compensation resulting from the increased selectivity and savings linked to the process itself will be 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 will become 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. Indeed, the customer will buy a process that is non polluting, is defect-free, and perfectly safe.

2) 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 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 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 will be the dominant elements. Indeed for these new specialities and active materials the client will buy the product that is the most efficient and the first on the market, thus strengthening the existing competition between the developed country producers.

In the framework of sustainability, these are examples of current problems and challenges faced by chemical and process engineering specialists in the chemical industry. What are the implications for chemical engineering?

The chemical and process engineering approach in 2003

The previous demands were satisfied by transforming material and energy to create new industrial processes with nearly zero pollution, zero defects and complete safety. The current chemical engineering approach accounts for new or emerging technologies such as biotechnology, microelectronics and microoptoelectronics, biomedical, nanotechnologies, and new polymer, ceramic and composite materials and simultaneously remains competitive in traditional technologies that involve solving the age-old problems of renewable energies, synthetic fuels, raw material and energy savings.

Fortunately chemical engineering is evolving to satisfy these numerous demands as the problem is not totally new to chemical and process engineering specialists. The objective of chemical process engineering, is the synthesis, design, scale-up or scale-down, operation, control and optimization of industrial processes, changing the state, microstructure and chemical composition of materials through physico (bio) chemical separations (distillation, absorption, extraction, drying, filtration, agitation, precipitation, fluidization, emulsification, crystallization, agglomeration, etc) as well as through chemical, catalytic, biochemical, electrochemical, photochemical and agro chemical reactions. Chemical engineering involves all of the scientific and technical knowledge necessary for physical, chemical and biological transformations of raw materials and energy into the targeted products required by the customer. Thus, it covers areas involving a wide variety of technologies, with increasing emphasis on the end-use properties.

It is important to note that today, 60 % of all products sold by chemical companies are crystalline, polymeric or amorphous solids. These 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.

The purpose of basic research in chemical and process engineering is still the development of concepts, methods and techniques to better understand, conceive and design processes to change raw materials and energy into useful products. However, due to the complexity of the phenomena involved in industrial processes, chemical process engineers and researchers are turning more often to other industries such as defense, automotive, aeronautical and medical to help them develop new concepts and methods.

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 2 illustrates the concept of the chemical supply chain.[4]

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 microstructure formation. This will help make the leap from the nano level to the process level. An integrated system approach for a multidisciplinary and multiscale modelling of complex, simultaneous, and often coupled momentum, heat and mass transfer processes is required (figure 3):

– Different time scales (10^{-15} to10^{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} to10^{6} m) are used in industrial practice and are shown in Figure 4. 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, exchangers, and columns; macroscale is used for produc-

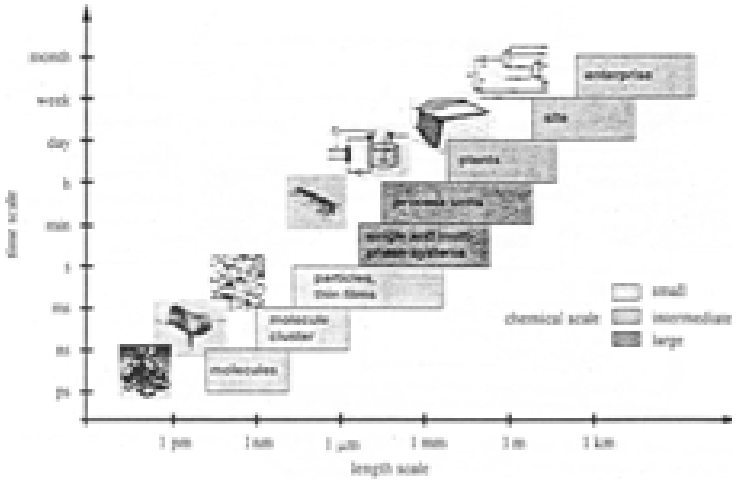

Fig. 2 – *Chemical supply chain*[4]
Slika 2 – *Ukupnost znanja u proizvodnji kemijskih proizvoda*[4]

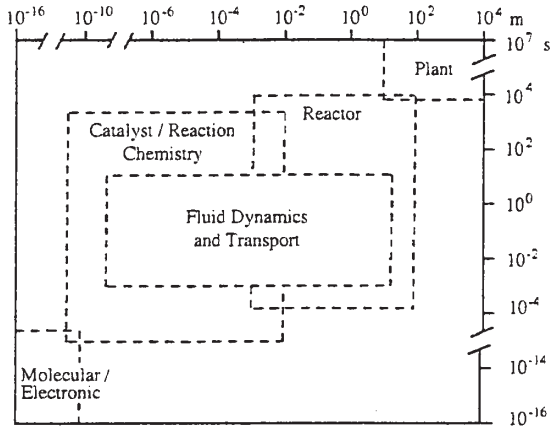

Fig. 3 – *The length and time scales covered by the multiscale approach*[5]

Slika 3 – *Prostorno i vremensko mjerilo obuhvaćeno u multirazinskom pristupu*[5]

tion units such as plants, and petrochemical complexes; and megascale is used for measurements involving the environment, atmosphere, oceans, 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 that is required by chemical engineering today.

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

Transport phenomena in polyolefin polymerization

This example is borrowed from polymerization engineering, and illustrates the fact that even for processes that have been used on an industrial scale for a long time, it may be necessary to re-examine the fundamental mechanisms involved at the microscopic level. This is presently the case for the polymerization of olefins using both highly active Ziegler-Natta type catalysts as well as more recently supported metallocene catalysts, which offer the possibility of producing tailor-made polymers in rather mild, and therefore, less expensive, process conditions.

Many attempts have been made to design properly, optimize, and control reactors by modelling the kinetics of polymerization; the evolution of the particle morphology formed by the catalyst and the polymer; the heat and mass transfer around the growing particles. Figure 5, puts the problem into perspective by illustrating the different length scales and the transfer phenomena involved in cases of, both gas-phase fluidized-bed reactors (FBR) (left side) and liquid phase slurry or liquid pool reactors (SBR) (right side).

Let us consider gas-phase processes, which in theory, are particularly interesting because they use no solvents and, because the final product is easily separated from the reaction medium. If the models available in the literature are used in conjunction with the traditional transfer equations and transfer coefficients correlations, they predict that experimentally observed polymerization kinetics are theoretically impossible: they would lead to temperature gradients so high during gas phase polymerization, that the center of the polymer particles would melt. If this happened, the pores of the growing particles would fill with molten polymer and the resulting increase in mass transfer resistance would then completely extinguish the reaction. This does not mean that significant temperature gradients at particle levels do not exist. It means that the fundamental descriptions currently available for such situations are inadequate. Since the reaction is very fast, very high levels of activity and typical rates in the order of 30 to 60 kg of polymers/g of catalyst/hour are obtained, and melt-downs are encountered in industry. The models simply do not explain why or how.

If we consider the length scales shown in Figure 5, it is easy to see that events taking place on the nano-scale (kinetics, Figure 4), the microscale (internal mass and energy transport), and the mesoscale (particle-particle, particle-wall interactions) have a significant impact on macroscale (global reactor behaviour) and even megascale (reactor run away, use of energy) events. It is, therefore, absolutely criti-

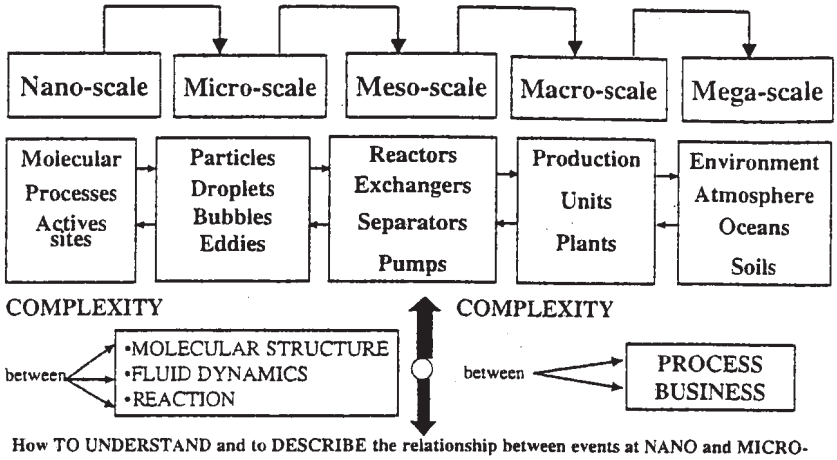

Fig. 4 – *Scales and complexity levels by process engineering*

Slika 4 – *Razine i složenost kemijskog procesnog inženjerstva*

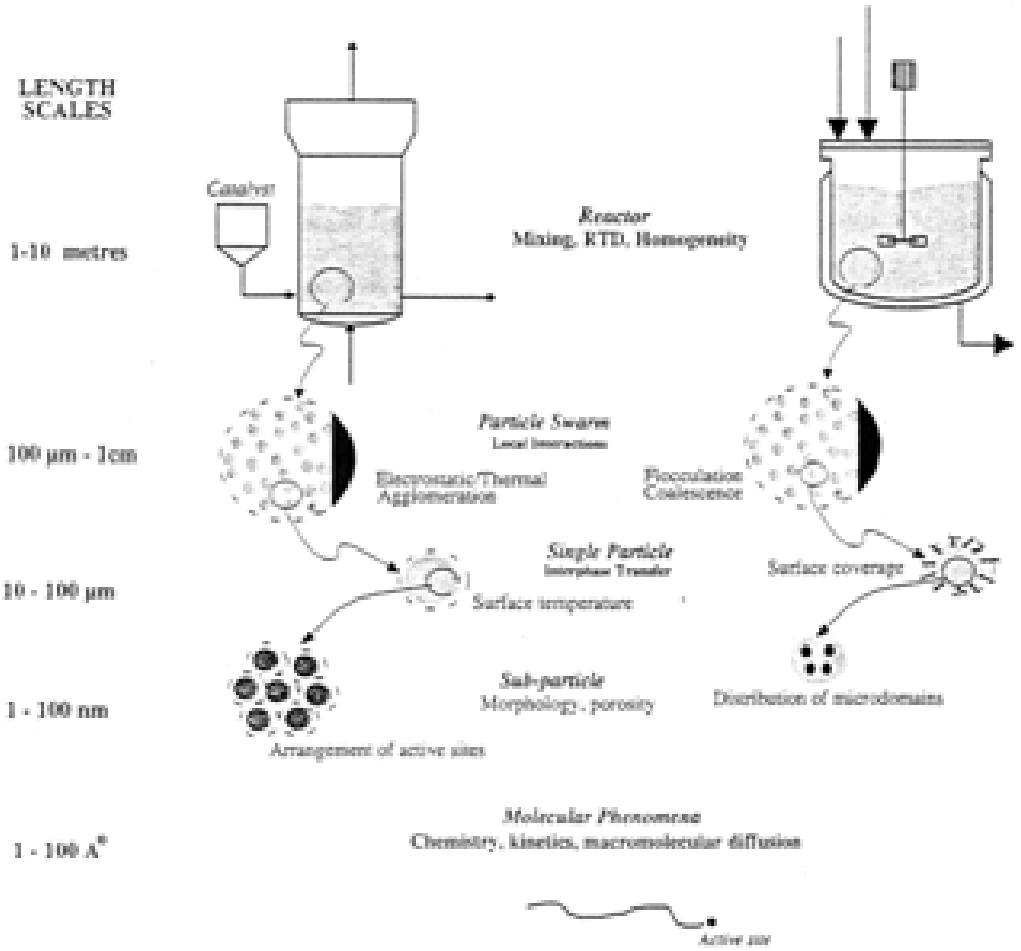

Fig. 5 – *Problems to be solved and related length scales in the heterogeneously catalysed polymerization of olefins*[6]
Slika 5 – *Problemi koje treba riješiti i odgovarajuće prostorno mjerilo pri heterogeno kataliziranoj polimerizaciji olefina*[6]

cal that the process engineer has a fundamental understanding of events at all complexity levels.

For example, a fundamental analysis of mass and heat transport equations, reveals that convection might play a very important role during polymerization, especially during the early stages of operation, which are critical for the development of particles, as illustrated in Figure 6. After the first few seconds at most, the hydraulic forces created by the formation of solid polymer inside the particle cause the original structure to rupture or fragment. The particle retains its original shape because of the entanglement and/or crystallization of the macromolecules formed in the porous structure of the originally porous support.

Particles grow rapidly from approximately 10 μm for fresh catalyst to approximately 1 mm for polymer particles. Thus, the values generally retained for the heat transfer coefficient around these growing particles must be increased by one order of magnitude to account for experimental observations. Furthermore, it seems necessary to revise the description of the basic mechanism for heat transfer in the gas phase around the particles, because the correlations used until recently are based on the assumption that heat transfer takes place only via convection.

Traditional chemical engineering correlations have been developed for particles diameters > 400 μm, whereas particles are actually in the order of 20 – 40 μm in diameter during the critical stages of low pressure olefin polymerization. Computational fluid dynamics software package have been used to study heat transfer from spherical particles of different sizes, under different heat transfer conditions. These studies show that the traditional heat transfer correlations for the case where particles do not interact, are not true for densely packed reactors, such as those commonly encountered in olefin polymerization.[6,7] The authors have also demonstrated that convection is not the only means of removing heat from small, highly active particles. Conductive heat transfer, between large and small particles present in the same reactor, appears to help alleviate previous problems of overheating, and explains why earlier models of heat transfer in olefin polymerization overpredicts the temperature rise during early polymerization.

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

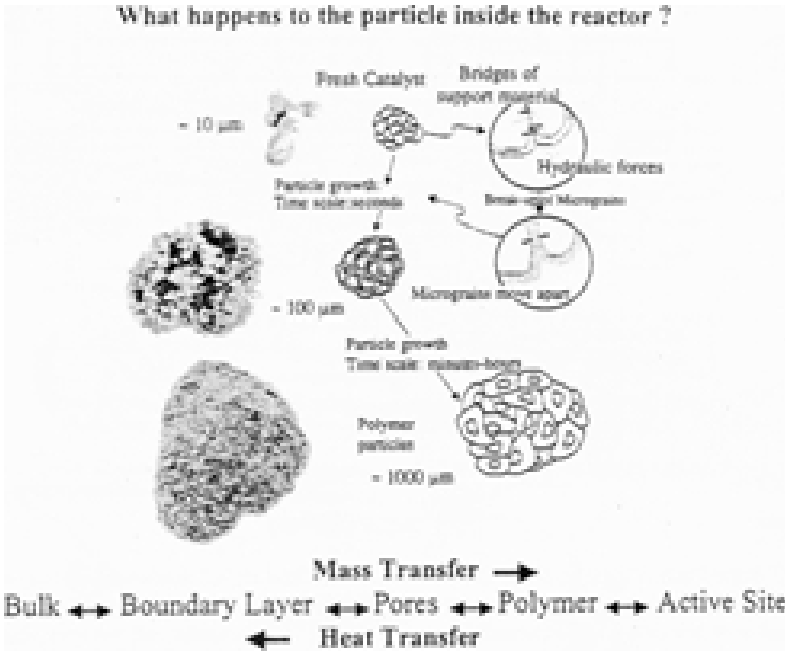

Fig. 6 – *Schematic transformation of a fresh catalyst particle into a polymer particle, and evolution of particle morphology and growth*[7]

Slika 6 – *Shematski prikaz transformacije čestice svježeg katalizatora u česticu polimera, razvoj morfologije čestice i rast*[7]

Figure 7. The nanoscale is used for molecular and genomic processes and metabolic transformations; pico and micro scales are used for enzyme and integrated enzymatic systems; mesoscale is used for the biocatalyst and active aggregates, and macro and megascales are used for bioreactors, units and plants involving interactions with the biosphere.

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 on biochemical engineering. Understanding an enzyme at the molecular level means that it may be tailored to produce a particular end-product.[8]

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[3].

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" or "3P Engineering- molecular Processes-Product-Process Engineering": an integrated system approach of complex 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 is beneficial, and has considerable advan-

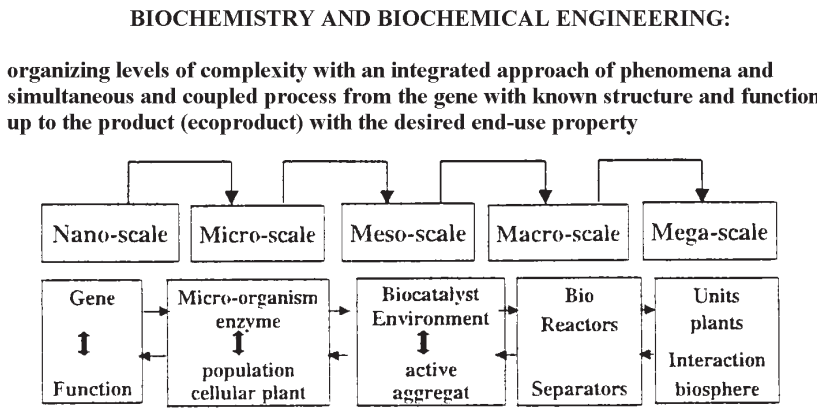

Fig. 7 – *Organizing levels of complexity underlie new view of biochemical engineering*

Slika 7 – *Razine organizacijske složenosti koje ukazuju na novi pogled na biokemijsko inženjerstvo*

tages for the development and the success of this engineering science in terms of concept and paradigms.

In the future, chemical and process engineers will involve a strong multidisciplinary collaboration with physicists, chemists, biologists, mathematicians and instrumentation specialists . This will lead 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.[9,10]

Improving both the design and evaluation of complex systems for the production of real products requires further research into strategies, methodologies and tools. These should be 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). 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 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 few days. CFD is thus a good link between laboratory experiments, conducted with common fluids like air, water, organics and hydro-carbons, etc., and industrial operations involving complex fluids, and severe temperature and pressure conditions.

Today's tools for the success of chemical and process engineering

It will be 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 three areas: molecular modelling (both theory and computer simulations), scientific instrumentation and non-invasive measurement techniques, and powerful computational tools and capabilities.

Modelling at different scales

– **At the nanoscale**, **molecular modelling** assists in maintaing 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 whose properties 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

– 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** are required still more and more, and are applied to analyse the operating conditions of each piece of production of 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 year production takes only 10 minutes on a computer. 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.

But the previous modelling, simulation, transcription, translation and interpretation at different scales also require the recent breakthroughs in information collection and processing.

Breakthroughs in scientific instrumentation and non-invasive measurement techniques

The development of sophisticated instrumentation and non invasive measurement techniques leads to noteworthy progress in matter-radiation interaction knowledge. In this context, increased cooperation with physicists and physical-chemists is essential as they possess considerable expertise in the application of fine, precise and instantaneous methods, which are not yet widely exploited in process engineering.

Nuclear magnetic resonance (NMR) is a good example. Used in medicine, NMR allows the characterization and the monitoring of chemical and physical phenomena that occur over a wide range of length and time scales and thus provides information on structure and structure dynamics (speed of particle agglomeration, rate of bubbles or drop coalescence, speed of nucleation in crystallization, rate of coagulation of colloids, etc) at the molecular or Angström scale.[11] Magnetic resonance imaging (MRI) is a non-invasive means to obtain specific information about structural heterogeneity of materials and porous media as well as concentration, temperature and velocity profiles in such media.[12] Thus, with the help of performing 3D image analysis techniques such as laser scanning microscopy, one accesses to local momentum, heat and mass transfer.

Tomographic techniques, optical, acoustical and impedance (both resistance and capacitance) are useful local non-intrusive techniques for flow characterization and on-line control of molecular processes. Capacitance tomography allows for the microscopic scale determination of instantaneous local velocities, mean lengths and shape coefficients of drops and bubbles, and the local fraction of each phase in multiphase flow in porous media. The computed gamma-ray tomographic technique is very promising for the measurement of porosity and gas-liquid flow distribution in trickle bed reactors of large diameter. Computer-assisted X-ray transmission tomography for liquid imaging in trickle flow columns, is also promising.

We should also highlight a Positron Emission Particle Tracking technique that uses a radioactive tracer particle to obtain the trajectories of solid or fluid elements in real time, either inside rotating blenders or inside agitated vessels containing non-Newtonian fluids. Spectroscopic and monochromatic ellipsometry is used to characterize in situ and in real time, the microscale structure parameters of solid surfaces such as porosities, thicknesses and gas sorption behaviour in thin supported membrane layers. Atomic force microscopy is used to finely analyse surface structures at microscale.

A technique involving high-speed images of bubble flow, coupled with simultaneous passive acoustic measurements, helps us to understand local and time-depending hydrodynamics in catalytic bubble columns.

It is even possible to dream and to imagine intelligent micro and nanotransmitters that measure every molecular process and model parameter at any location and any time, i.e, with the help of optical techniques using laser beams, such as laser space time resolution fluorescence spectroscopy. This should be particularly applied to real media (particulate or opaque). When will micro-or nano electronic transmitters be implanted directly on particles or catalytic sites to evaluate local parameters values? When will piezo-electrical polymers, that generate a turbulence wake, be able to continuously clean the surface of a membrane?

Breakthroughs in computational tools and capacities

The considerable breakthroughs in computation technology and microelectronics are highlighted in Figure 8. Today, computers are of greatest importance to the engineer or researcher in chemical and process engineering. They are essential for design, control and operation of processes. If the effective speed of electronic hardware and software development, roughly doubled every year over the past 30 years (Moore's law), this acceleration in computing chip power is expected to continue over the coming decade. However, experts predict that around 2010 the magneto-resistive storage technology used will have reached its limit, with a storage density of 10–15 gigabytes/cm^2. The storage limit today is 0.25 gigabytes/cm^2. Holographic memory technology may substitute the magneto-resistive technology with potential storage densities of 150 gigabytes/cm^2. Manipulating individual atoms is now envisioned and considerable perspectives in molecular simulation are anticipated because the present difficulty for its use is the computer required calculation time, which is approximately proportional to N^2, where N is the number of atoms. This limits the size of the molecules and the number of compounds in a mixture.

These rapid increases in computational capabilities enable the handling of more complex mathematics, which permits the exhaustive solution of more and more detailed models. This will help chemical and process engineers to model process physics, process (bio) chemistry and process microbiology from the molecular and cellular scale to the full process plant scale. In addition, the developments in expert systems and artificial intelligence will enable process engineers to have empirical, qualitative information available virtually at their fingertips in a structured and easily accessible fashion. Also, fuzzy logic is of great help in process control, in neural networks for diagnosing on-line defects, for analyzing trends and for the design and modelling of new processes.In many cases, the complexity of phenomena is such that it might take too long to obtain a complete model or all of the necessary experimental parameters.

And, finally, it must be emphasized that powerful computational tools and capabilities largely contribute to the breakthroughs in signal and image processing for the visualization and validation of models at different scales. Operation

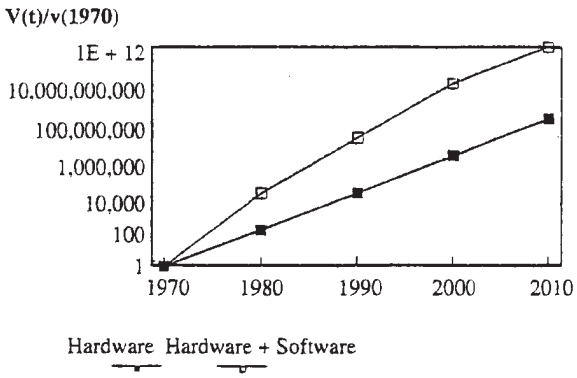

Fig. 8 – *Computing speed acceleration*
Slika 8 – *Ubrzanje brzine računanja*

in real media (particulate or opaque) and/or in complex multiphase flow conditions, are a recent example, as is the use of sophisticated techniques like particle image velocimetry, laser doppler anemometry, laser-induced fluorescence, computed tomography and computed- automated radioactive particle tracking.[13,14]

Chemical and process engineering: quo vadis?

The previous considerations on the future of chemical engineering, involved an integrated multidisciplinary and multi-scale approach to molecular processes, product and process engineering. This approach concerns four main parallel objectives for engineers and researchers.

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 targetted 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 exists now ability to engineer novel structures at the molecular and supramolecualar levels via nanostructure synthesis. This leds to the creation of nanoporous and nanocristalline 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 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.[15] Specifically, 10 nm anatase crystallites due to their greater redox potential presents 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.[15]

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 selective oxidation of hydrocarbons. 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 startup and transient periods. Noble metal catalysts exhibit excellent light-off behaviour at 400 °C, but suffer from deactivation by 700 – 800 °C. To achieve high-temperature stability, the 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 $m^2 g^{-1}$ at 1 300 °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 retain a crystal size of 20-nm even at 1100 °C and allow methane light-off by 400 °C.[16] 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.[17]

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 surface functionalization of inorganic structures and extension of supramolecular templating to organic systems. 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 of 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,[18] and for high-value-per gram materials such as bio-implant materials, high-temperature super conductors and nanostructured materials.[19] The gas-phase combustion synthesis (GPCS) 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.[20]

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**

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.[21]

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.

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 would be 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 requi-

res 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. Obviously, the successful management of the information exchange between the process and the man in the framework of sustainability, implies a parallel effort in training operators and chemical and process engineers and, therefore, it is not only a matter of research in chemical and process engineering!

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 novel design equipment based on scientific principles.

Process intensification using multifunctional reactors

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 is such the case**. 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 azeotrope, 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 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.[22] Catalytic distillation combines reaction and distillation in one vessel, using structured catalysts as the enabling element.[23] 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.[24]

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 reformate fractions; for the production of isopropyl alcohol by hydration of propylene; for the selective production of ethylenglycol, 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.[25]

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.[26]

The liquid-liquid two phase reactor involving simultaneous reaction and liquid-liquid phase separation is encountered also. In extractive reaction (or reactive extraction), a second liquid phase containing a solvent is deliberately imposed on the system. The solvent selectively extracts an intermediate or a product, thereby preventing its further reaction. This results in a higher yield or simply removes the product from the dilute phase.[27] In metal processing, the recovery of metal ion from an aqueous solution is often accomplished by reaction and extraction into an added organic phase. The reaction rate and product selectivity in catalytic liquid-phase hydrogenation can benefit from the introduction of an extractant phase. This has been used for the selective hydrogenation of benzene to

cyclohexene using Pt or Ru catalysts. Surrounding the catalyst particles with an aqueous layer is found to increase the selectivity towards the desired cyclohexene, which distributes preferentially into the added phase and is thus prevented from further hydrogenation to cyclohexane.

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*[28] have shown how to crystallize desired solid products selectively 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 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.[29] 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.[30] Many books and a great number of papers have been published on membrane reactors, which combine a molecular separation with a chemical reaction. The paper by *Drioli* and *Romano*[31] 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 removal of product from the reaction site in order to increase conversion of product-inhibited or thermodynamically unfavorable reactions. With such membrane bioreactors, provided that membranes of suitable molecular weight cut off are used, 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 the 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 eniantospecific 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. 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 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.[32]

For more general applications, material scientists must first 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 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. Greater use of membranes in multifunctional operations would advantageously combine reaction and separation in the same vessel.

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 re-

actors incorporating several "functions" in one reactor been formally classified as being multifunctional. The great benefits obtained in integrating the progress of knowledge at different scale and time-lengths have been acknowledged by the process industries. This was illustrated by the first international symposium on multifunctional reactors[33] 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[34] 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.

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*[35] and illustrated in a recent survey by *Krishna*.[36]

The use of hybrid technologies encountered in a great number of multifunctional reactors in general is limited by the resulting problems with control and simulation. The interaction between simultaneous 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.[37]

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, countercurrent flow and induced pulsing flow in trickle beds, 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.[35]

Some attractive options for improved catalytic reactor performance via novel modes of operation are 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 down flow mode. 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.[38] Also, improving the product selectivities in a parallel-series reactions by feeding one reactant through the reactor by stage wise reactant dosing, will be applied.[39]

Process intensification using microengineering and microtechnology

Current production modes will be increasingly challenged by decentralization, modularization and miniaturization. Microtechnologies recently developed, especially in Germany (i.e., IMM, Mains and Forschnungszentrum, Karlsruhe) and in 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 micro-total-analysis-system (μTAS)[40] 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 μTAS techniques with microreaction technology promises to yield a wide range of novel devices for reaction kinetics and micromechanism studies, as well as on-line monitoring of production systems, as explained by *Jensen*[41] in a publication on the state of art on microreaction engineering.

Microreaction technology is expected to have a number of advantages for chemical production.[42] 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 direct fluorination of aromatic compounds, could be pursued because if the microreactor fails, the small amount of chemicals released accidently could be easily 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 screening of small molecules and systems for nucleic acid synthesis and detection have already revolutionized drug discoveries in pharmaceutical companies.[43] Similarly rapid screening of small molecules and systems for nucleic acid synthesis pathways could lead to 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.[44,45] Moreover, scale-up to production by replication of microreactors 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.

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 μTAS 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.

Chemical processing advantages from increased heat and mass transfer in small dimensions are demonstrated by *Jensen,*[41] with model gas, liquid, and multiphase reaction systems: thin-walled microreactors (created by MEMS microelectromechanical systems) for heterogeneous gas-phase reaction; membrane microreactors for hydrogenation or dehydrogenation reactions; packed-bed microreactors with high gas-liquid interfacial area, high surface-to-volume ratios, and low pressure drop; and microfabricated liquid-phase reactors integrating laminar mixing, hydrodynamic focusing, rapid heat transfer, and temperature sensing. These case studies also serve to illustrate the benefits of integrating sensors for flow, temperature, and chemical composition with microfluidic reaction and control components.

Also, de *Bellefon* et al.[46] propose 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. They describe a new concept to achieve HTS of polyphasic fluid reactions for 2 test reactions, a liquid-liquid isomerization of allylic alcohols and a gas-liquid asymmetric hydrogenation. The principle used for the test microreactor is a combination of pulse injections of the catalyst and the substrate, a IMM micromixer with negligible volume and residence time less than 10^{-2} s, and a tubular stainless steel capillary reactor shown in Figure 9. The two scanning electron microscopy images in Figure 10 show the micromixer, in which 2 × 15 inter-digitated microchannels (25 μm width) with corrugated walls are clearly illustrated in Figure 10. 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. Application of this principle is possible by using a static micromixer mounted in a dynamic microactivity test. The catalyst library was then screened. The results of this technique lead to the selection of the best catalyst showing activity towards a large class of allylic alcohols. Similar results obtained in a microreactor as well as in a traditional well mixed batch reactor (40 cm^3) proves the validity of the concept. The comparisons are shown in Figure 11.

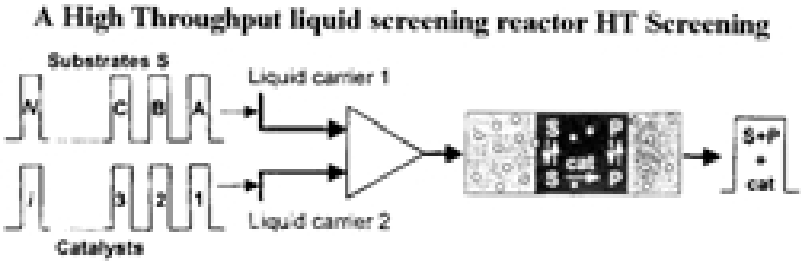

Fig. 9 – *Schematic of the principle used for high-throughput sequential screening of i catalysts and N substrates. The substrate S is treated to form the product P.*[46]

Slika 9 – *Shematski prikaz principa korištenog za brzo detektiranje značajki i katalizatora i N substrata. Obrađivan je substrat S da bi se dobio produkt P.*[46]

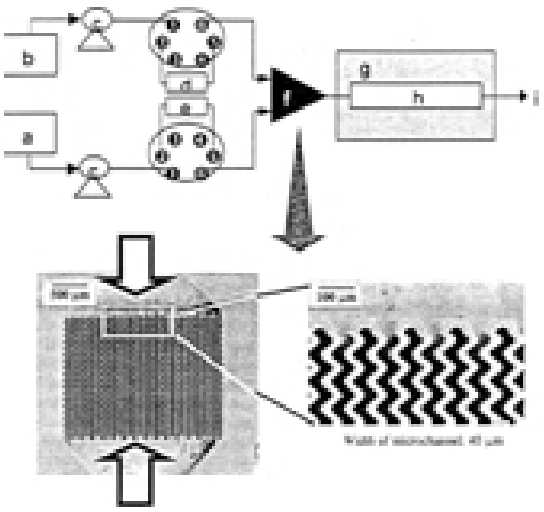

Fig. 10 – *The IMM micromixer for high throughput screening*[46]
Experimental set up: a – water reservouir, b – n-heptane reservoir, c – high pressure liquid pumps, d – HPLC type injection valve equipped with 200 μl loop, e – HPLC injection valve with 1 ml loop, f – micromixer, g – thermoregulated bath, h – tubular stainless steel reactor (0.4 cm i.d, 80 cm lenght), i – outlet analytics, j – SEM image of the mixing microelement showing the 2 × 15 interdigited microchannels (25 μm width) corrugated walls

Slika 10 – *IMM mikromješač za brzo detektiranje*[46]
Eksperimentalni uređaj: a – spremnik za vodu, b – spremnik za n-heptan, c – visokotlačna pumpa za vodu, d – ventil za injektiranje HPLC tipa opskrbljen s 200 μl petljom, e – HPLC ventil za injektiranje s 1 ml petljom, f – mikromješač, g – kupelj, h – cijevni reaktor od nehrđajućeg čelika (0,4 cm nutarnji promjer, 80 cm dug), i – vanjski uređaj za analizu, j – SEM prikaz mikroelementa koji prikazuje 2 x 15 mikrokanale (25 μm široke) s narebrenim stjenkama

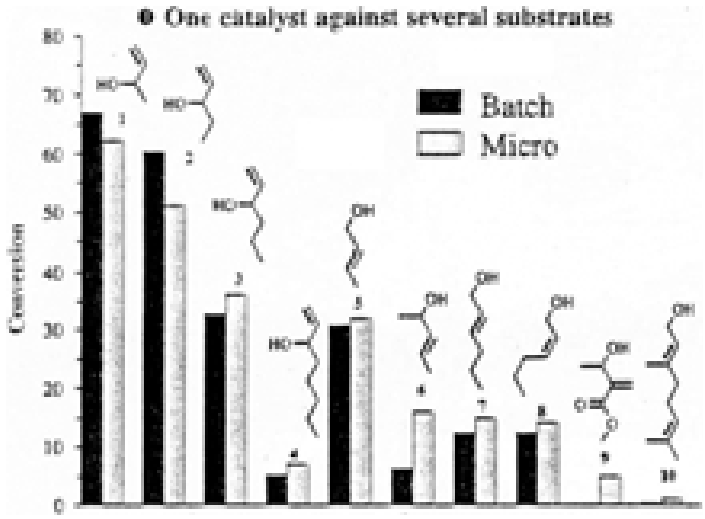

Fig. 11 – *Comparison of results from microreactor with the results given by traditional equipment (batch reactor): one catalyst against several substrates*[46]
Catalyst pulse 0.2 cm^3 of a Rh 0.004 kmol m^{-3} solution equivalent to 80 μg of Rh for each test. Catalyst: $RhCl_3$/TPPTS/NaOH. Rh/TPPTS = 5. Selectivity 95 %. T = 70 °C. Flow rate: Aqueous phase 5 cm^3 min^{-1}, Organic phase 1 cm^3 min^{-1} Substrate 0.1 kmol m^{-3}. Residence time 100 s.

Slika 11 – *Usporedba rezultata dobivenih u mikroreaktoru s rezultatima dobivenim u tradicionalnom uređaju (šaržni reaktor): jedan katalizator za nekoliko supstrata*[46]
Za svaki test injektirano je 0,2 cm^3 Rh, 0,004 kmol m^{-3} otopine ekvivalentno je 80 μg Rh.
Katalizator $RhCl_3$/TPPTS/NaOH. Rh/TPPTS = 5. Selektivnost 95 %. T = 70 °C. Obujamni protok: vodene faze 5 cm^3 min^{-1}, organske faze 1 cm^3 min^{-1} supstrat 0,1 kmol m^{-3}. Vrijeme zadržavanja 100 s.

This concept has been extended to gas-liquid catalysis with asymmetric hydrogenation of acetamidocinamic methyl ester with Rh/diphos catalyts, with some modification to the experimental setup.[46] The results indicate that the microreactor is working under a chemical regime, and that it compares well to the enantioselectivity obtained and those previously reported for the catalyst under similar conditions.

In terms of catalyst and time consumption per test, the numerous tests for the liquid-liquid isomerization were performed twice to test reproducibility, using only one or two micromoles of metal over a total screening time of one hour. The test for the gas-liquid asymmetric hydrogenation showed 0.2 μmole of catalyst, and 3–5 min per test. Throughput testing frequencies of more than 500 per day are thus achievable, albeit with computer control of the appa-

ratus. Such testing frequencies impose a characteristic time of only 3 minutes for necessary online operations such as injection, collection and analysis by any detector, including mass detection by UV, IR, CD, or fast chromatography with microcapillary columnus. Using these microreactors for dynamic, high throughput screening of fluid-liquid molecular catalysis offers considerable advantages over traditional parallel batch operations by ensuring good mass and heat transport in a small volume, reducing sample amounts (to μg levels), a larger range of operating conditions (temperature, pressure) and fewer, simpler electro-mechanical moving parts.[46]

The examples shown 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. They can provide significant advantages in information generation for high throughput experimentation and process development, and from difficult to obtain operating regimes. In terms of chemical manufacture, they allow distributed, mobile and intensified processing.[47] However, 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 dimension, i.e, not only the high transport rates, but the forces associated with high surface area-to-volume ratio.

Manufacturing end-use properties: development of multidisciplinary product-oriented engineering with a special emphasis on complex fluids and solids technology

This is the answer for today's ever-growing market place demand for sophisticated products that combine several functions and properties: cosmetics, detergents, surfactant 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. This product engineering (synthesis of properties), as previously discussed, is the translation of molecular structure into macroscopic phenomenological laws in terms of state variables. In practice, these technologies mostly concerns 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 application (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 programmed release of active components.

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 structured material, face many challenges in fundamentals (structure-activity relationships on 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).[48]

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 homogeneisation; 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, manufacturing cost, as well as 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 whose growth 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.[49] 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 has to be divided into two substeps : generation of droplet 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. Thus, the kinetics of the molecular process determines whether the desired end-product properties

will really be achieved, even if the required droplet size had been achieved in the first substep.

Complementary in topics such as microemulsions for chemical, food and pharmaceutical industries (drug delivery systems), it should be emphasized recent investigations on monodisperse emulsion formation with micro-fabricated microchannel (MC) array, called straightthrough microchannel, i.e, silicon array of elongated through-holes for monodisperse emulsion droplets.[50] Such oblong straightthrough MC equipment allows to get monodisperse oil in water emulsion droplets with average diameter of 32.5 μm and a coefficient of variation of 1.5 % verifying their excellent monodispersity. Such monosized droplets in emulsions have advantages for control of their physical and functional end-use properties, stability and application to other processings (Figure 12).

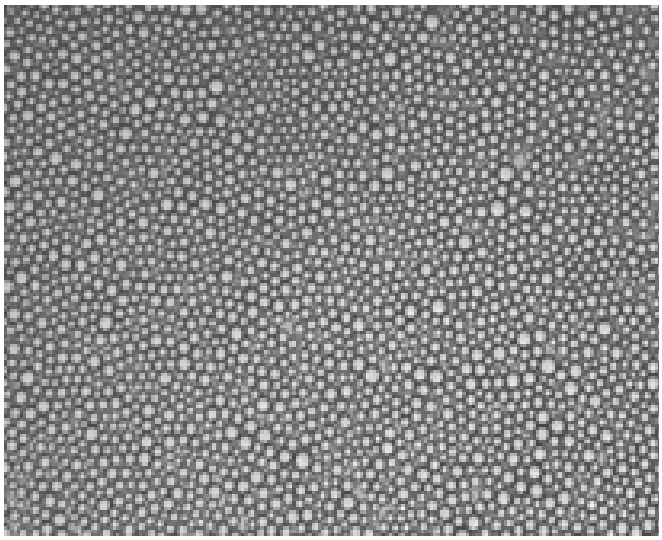

Fig. 12 – *Monodispersed emulsion formed with micro-fabricated microchannel array*

Slika 12 – *Monodisperzna emulzija dobivena uporabom niza mikroproizvedenih mikrokanala*

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

Multiple emulsion based on the PPSIT technology (Figure 13) combine protecting and occluding effects of classical W/O emulsions and 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 skin's microrelief, short-, mid-, and long term moisture holding capacity (adaptogenic moisturization) and skin firmness improvement. Such multiple emulsions are manufactured by novel one step manufacturing technology even facilitating industrial scaling up to a large scale (up to 1 t batches).

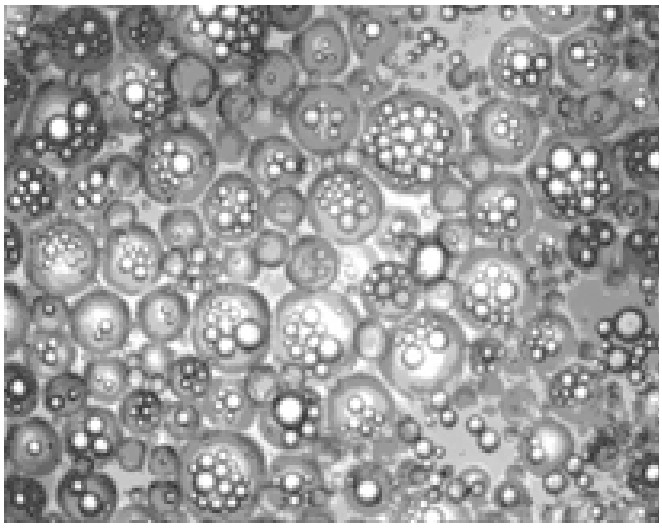

Fig. 13 – *Multidispersed W/L/W emulsion manufactured by PPSI technology*[51]

Slika 13 – *Višedisperzna W/L/W emulzija proizvedena PPSI tehnologijom*[51]

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 solid shell or even can entrap additional solving oil compartments to be as detected active (Figure 14). SLN particles can be manufactured based on proloxamer derivatives as well as non-ethoxylated lipids, such as Compritol or Dynasan. High pressure homogeneization reveals also 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 either be protected against 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

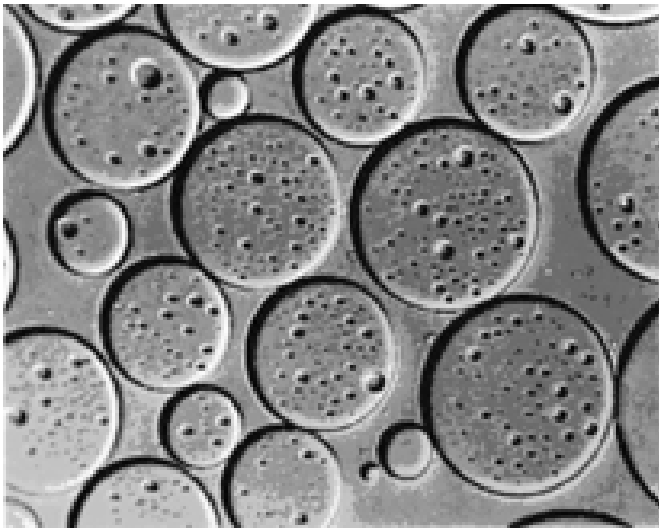

Fig. 14 – *Solid-Lipid-Nanoparticles*

Slika 14 – *Čvrsto-lipidi-nanočestice*

focus of cosmetical 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 get typical sustained release properties.

Control of the shape and size of crystals in an industrial crystallization process can also be cited as an example. *Wintermantel*[48] 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 crystals 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's 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 in the article by *Wintermantel,*[48] with the results of crystallization from a feed ammonium sulphate solution containing amaranth dye. It was shown that the amaranth molecule is adsorbed onto 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 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 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[52]. In the pharmaceutical industry numerous patents and significant development works revolve around the relationship between active substance level, pore size distribution, and tablet size. However, new approaches offer now the possibility of accurately predicting the effect of solvents or impurities, as explained by *Winn* and *Doherty*[53] who reviewed models for predicting crystal shape of organic materials grown from solution as well as their utility for process and product design.

Recent models recognize the significance of 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.[54]

In general, with respect to the manufacture of chemical-based consumer products, complementary industrial exam-

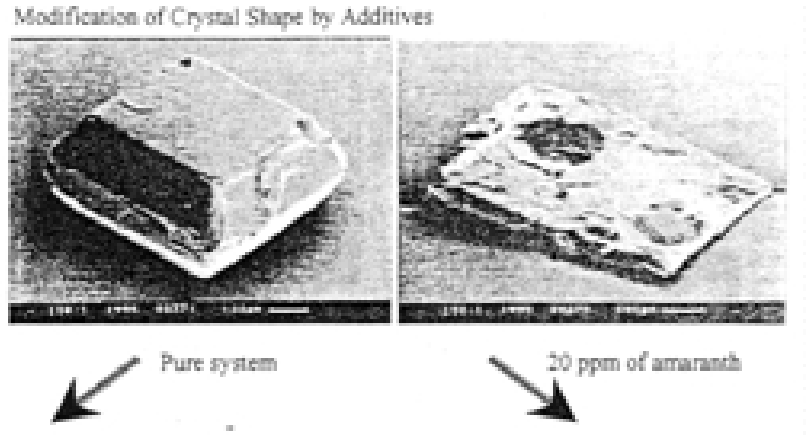

Fig. 15 – *Product-oriented engineering: controlled crystallization process*[48]

Slika 15 – *Kemijsko inženjerstvo orijentirano na razvoj proizvoda (produktno inženjerstvo): kontrolirani proces kristalizacije*[48]

ples oriented on product-centered processing have been proposed by *Wibowo* and *Ng,*[55] 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.,[56] specifically, to illustrate the potential of chemical product engineering.

Finally, we have to 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).

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 explanation 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, and with specialists in physical chemistry, biology, mechanics and mathematics**.** This 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

In the previous sections we have emphasized the necessary multidisciplinary and multiscale integrated approach 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 design and implement the complete manufacturing systems also 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 4). 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 modeling of molecular and physical properties on the microscopic scale. For molecular modeling, 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.

It is clearly impossible to cover all directions of present-day molecular modeling research, as it involves a wide spectrum of problems in the chemical and material sciences. Vapor-liquid equilibria, vapor-liquid-liquid equilibria, liquid-solid equilibria, supercritical solution properties; amphiphiles; polymers at interfaces; adsorption on surfaces and influence of impurities; microporous materials or ceramics structures; freezing of solids; phase transition in pores; partitioning of hydrocarbons in zeolites; determination of zeolites structures; structure and properties of large polymeric molecules; nanoscopic structures in lithographic nanofabrication processes; study of atypical antibody and the key-interactions governing the structure of its binding site; transport properties such as viscosity, diffusivity, and thermal conductivity can be calculated by molecular modelling based on information from thermodynamic, kinetic and rheological data banks. For example, *Sheehan* and *Sharratt,*[57] reviewed the potential benefits of the application of molecular modeling techniques for the prediction of solvent effects on reaction kinetics and liquid-liquid phase equilibria. They show, that when the theoretical model of an equilibrium process to produce an endo and exoproduct and the computational method used to represent this model are carefully choosen, molecular modeling can be a valuable tool for engineering design, i.e, evalua-

ting solvent influence on process performance. There is no doubt that molecular modelling is now playing an increasingly important role in future chemical and process engineering research and practice.[58–60] 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, the consensus seems to be, that simulation is useful in initial screening, but that experimental data are still essential for final design.[61]

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 not generally 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 2, 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 a manufacturing industry such as automotive manufacturing, the component is either in a machine or in a transport device. In the process industry by contrast, 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.[48]

In general, 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.[62]

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 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. The CO-LanN ensures that software tools used by the process industries reaches a level of interoperability that will sustain growth and competitiveness. *Pons* et al.[63] have described the goals and means of the CO-LaN, especially its work process related to testing procedures applied to software components, in order to assess their compliance with the published CAPE-OPEN interface specifications. A recent paper by *Gani*[64] 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.[65] More specifically the bottleneck for good models of multiphase and complex systems is the understanding of the physics, chemistry and biology of interactions, rather than the refinement of numerical codes, whose sophistification is not at all concerned with real-life problems in plants and in industrial practice.

Attention should be focused on the systemic analytical models based on the multi-scale integrated approach previously referred to 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. What is needed in models is less anatomy and more physiology.

Conclusions.

Chemical and Process Engineering – a multidisciplinary technology 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 society concern and market demands versus

technology offers.[1,2] Presently, this involves a double challenge. 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 specialities 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 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 entire production site. We have defined it as "molecular Processes-Product -Process" Engineering or 3P Engineering. This approach is necessary for 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, biochemical and food 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. 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: (a) Total multiscale control of the process to increase selectivity and productivity, a good illustration is the nanostructural tailoring of required materials with controlled structure, (b) Process intensification by design of novel equipment based on scientific principles and new production operating methods. Examples concern multifunctional reactors, and the use of micro technology for high-throughput rapid catalyst screening experiments, (c) 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 foodstuff and the control of the shape, size and structure of crystals in crystallization processes encountered in chemical industries, (d) to implement multiscale and multidisciplinary computational modeling and simulation to real-life situations, an understanding of the physics, chemistry and biology of the interactions should be emphasized, rather than the refinement of numerical codes, whose sophistication is not at all related with real-life problems in industrial practice.

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 3P engineering, i.e, application of LCA not only to product design and its use, but also to the plant and the equipment together with the associated services.[66] Thus, this multidisciplinary and multiscale integrated approach will be of great help, in responding to the increasing environmental, societal and economic requirements and to the transition towards sustainability. The 3P Engineering approach will be required to understand the multidisciplinary interactions at different time and length scales necessary for a successful product and process development. This is the reason why chemical engineering will behave more and more as a multisdisciplinary discipline, serving mankind and concerning itself with 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 problem solvers. Indeed, chemical engineering today must both apply and complete Isaac Newton's citation: "solving problems is more important than learning rules". To do this in today's world of chemical and process industries, a great number of challenges must be faced. 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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SAŽETAK

Budućnost kemijskog inženjerstva na globalnom tržištu: zahtjevi tržišta i tehnološka rješenja

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Kemijsko inženjerstvo mora se neprekidno razvijati jer mora odgovoriti na promjenljive potrebe kemijske procesne industrije. U radu je prikazana njegova sposobnost da se nosi sa znanstvenim i tehnološkim problemima. Kemijsko inženjerstvo od velike je važnosti za održivi razvoj, pri čemu treba zadovoljiti kako zahtjeve tržišta za specifičnim proizvodima željenih uporabnih svojstava tako i društvena i ekološka ograničenja koja se postavljaju na industrijske procese. Multidisciplinarni, višerazinski pristup kemijskom inženjerstvu temelji se na modeliranju na razini molekula, razvoju znanstvene instrumentacije i snažnih računalnih alata. Budućnost kemijskog inženjerstva može se sumarno prikazati pomoću četiri glavna cilja: (1) Porast produktivnosti i selektivnosti pomoću intenzifikacije inteligentnih postupaka i višerazinskog pristupa vođenja procesa; (2) Izvedba nove opreme temeljene na znanstvenim principima i novim načinima proizvodnje: intenzifikacija procesa; (3) Primjena kemijsko inženjerske metodologije za dizajn produkta i procesa, koristeći 3P inženjerski pristup (proces na razini molekule-produkt-proces); (4) Implementacija višerazinskog kemijsko inženjerskog modeliranja i simulacije realnih situacija od molekularne do proizvodne razine.

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Prispjelo 25. travnja 2003.
Prihvaćeno 3. lipnja 2003.