height. The back mixing in a bubble column is calculated by the injection of a tracer in both the liquid and the gaseous phase. The calculated dispersion coefficients increase with increasing superficial gas velocity.

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Symbols used

a	[m^{-1}]	interfacial area density
C_D	[–]	drag coefficient
c	[–]	molar concentration
D_S	[m]	diameter
D	[$m\,s^{-2}$]	diffusion coefficient
d	[m]	bubble diameter
E	[$m^2\,s^{-1}$]	dispersion coefficient
Eo	[–]	Eotvos-number = $g\,\Delta\rho\,d/\sigma$
g	[$m\,s^{-2}$]	acceleration due to gravity
h	[m]	column height
j	[$m\,s^{-1}$]	superficial velocity
k	[$m^2\,s^{-2}$]	turbulent kinetic energy
$\dot{M}$	[$kg\,m^{-3}\,s^{-1}$]	mass flux
$\dot{m}$	[$kg\,m^{-2}\,s^{-1}$]	mass flux density
$\dot{N}$	[$mol\,m^{-2}\,s^{-1}$]	molar dispersion flux density
$\dot{n}$	[$mol\,m^{-2}\,s^{-1}$]	molar flux density
p	[$kg\,m^{-1}\,s^{-2}$]	pressure
Re	[–]	Reynolds-number = ud/ν
Sh	[–]	Sherwood-number = $\beta d/D$
r	[$m^3\,s^{-1}$]	coalescence kernel
t	[s]	time
u,v,w	[ms^{-1}]	cartesian velocity component
v_i	[m^3]	bubble volume
Z	[–]	dimensionless breakage frequency

Greek symbols

α	[–]	volume fraction
β	[$m\,s^{-1}$]	mass transfer coefficient
ε	[$m^2\,s^{-3}$]	turbulent kinetic energy dissipation rate
η	[$kg\,m^{-1}\,s^{-1}$]	dynamic viscosity
μ	[$kg\,kmol^{-1}$]	molecular weight
ρ	[$kg\,m^{-3}$]	density
ν	[$m^2\,s^{-1}$]	kinematic viscosity
ξ	[–]	mass fraction
σ	[$kg\,s^{-2}$]	surface tension
ω	[s^{-1}]	angular frequency

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Sustainable Growth and Chemical Engineering

By *Jan Venselaar**

1 Growth

Growth is needed. Not so much for ourselves here in the Western world, but because of the needs of the other half of the world population, still growing rapidly, which is entitled to their share of wealth and happiness. In this world, with its globalized communication and globalized economic interdependencies, a sound and stable global economic system will not be obtained with sufficient equity in income, well-being, rights, and mutual respect. Poverty is the basis of conflicts and economic instability [1].

At the same time there is concern about our resources, the environment, and its effects on human health, which are presently connected with economic growth. Many of the problems are being solved, however, it becomes increasingly visible that the methods and technology applied are not always without problems themselves nor do they suffice on the long term. New approaches, including new technologies and new ways to use technologies, are to be developed. This is a challenge for society as a whole, industry, and science and engineering in particular.

Chemistry and chemical engineering play an essential role. Our economy and wealth and to a large extent our wellbeing, depend on material resources. Chemistry transforms the resources into the materials and products we need: energy,

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housing, clothing, food, transport, appliance, clean water, etc. Economic growth presently implies growth in use of resources. That cannot be sustained on the long run. Actually, even the present use of resources is already too large in some cases and, therefore, 'Decoupling' is needed. This must drive innovation in chemistry and chemical engineering and asks for novel approaches.

The article presents some ideas, concepts, and approaches that are essential for sustainable development. It will define a direction and show the outlines of the agenda for sustainable chemical engineering development that is evolving world-wide.

2 A Case of Concern

Just an example: Mining activities disturb large areas and leave them often irreparably polluted. Sadly, an example of this is the mining of platinum, essential for the production of car exhaust catalysts intended to reduce pollution. Even more sadly is that the actual reduction of CO and NO_x from traffic is often much less than intended, certainly locally, due to an enormous growth in number of cars and kilometers. Many comparable cases can be shown. This 'end-of-pipe' approach is clearly not effective when growth continues. Furthermore, essential resources are dwindling: nature and biodiversity, but maybe of more concern to engineers: some metals such as copper.

Not just physical factors are involved, but also the 'political' ones. After oil, water might be the next 'casus belli' in coming decades, if that resource is not handled well.

Energy is and will be abundantly available, from fossil and renewable sources. Nevertheless the many side effects of energy-(over)consumption are still an issue of concern due to physical, political as well as social reasons.

Some say that 'things will work out fine on their own, as they have always done' and they point to the past were many 'catastrophes were predicted but never occurred or of which the effects could be handled. But 'things do not work out, change nor develop spontaneously and on their own'. It has always been hard work for many committed people with a sense of responsibility that brought changes necessary to prevent or solve problems. Besides 'results from the past, are no guarantee for the future'. Many things have changed and the world has shrunk in many respects also in its 'buffering' capacity. It is a much more complex one, with much more people and much larger impact on natural systems. The margins for 'things to work out fine' are smaller.

We need to muster all creativity for the challenge ahead and define the direction that development must take.

3 The Challenge for Society and Industry

Sustainable development based on decoupling, leading to sustainable growth and equity, are challenges society has to respond to in the decades to come. At first glance this seems to be an impossible task.

Technology development is a part of the development occurring within so-called socio-economic structures: the 'systems' that take care of the needs we have: food, travel, housing, leisure and all myriad other needs of modern society. They are made up of many components, technical and organizational ones. How such systems are organized and used is strongly influenced by 'culture' with differences between individuals, nations, and larger regions. Such systems are continuously changing. When looking at it from a distance and, in particular, when looking back in time, major changes can be defined which are now coined 'transitions'. Examples are the introduction of steam power, the introduction of cars for mass transport, the introduction of ICT. Technology changed fundamentally along with organization and culture and society looked totally different afterwards: Consider the cultural changes the new modes of telecommunication brought about and the 'shaping of Western society' by electricity and automobility.

Seen as a whole, these developments are 'non-directed'. Changes mostly occur under the influence of ad hoc and short-term incentives. Some parts of it are of course directed, because, on a micro level, there exist specific goals regarding profit or the use of new knowledge, but at the start, there was no intention to end up where we are now.

However, sustainable development is to be – in essential aspects – a 'directed development' of such systems. Not towards a precisely defined image of the future of course. However, a set of conditions can be defined that should be met by future developments. Such directed development is quite a novel approach, which was never tried before, and clearly a controversial issue. Nevertheless, it is regarded as the essential approach for development for a more stable future world society and economy.

Chemistry and chemical engineering will have to respond to it.

Exact description of a sustainable future is of course impossible. To a certain extent one can define the conditions that should be met, whatever form the developments will take. The concept 'sustainability' is best described by its boundary conditions. In general, these are defined as:

a) physical aspects (planet): preventing depletion of essential resources, environmental degradation and loss of biodiversity.
b) human aspects (people): equity, quality of living and work conditions, education, and respect for human rights.
c) economic aspects (profit): sound businesses, also in developing countries, and therefore equity in trading and trading rights and regions. Community must profit from the use of their resources, labor, space, infrastructure, and materials grown or mined.

Development can only be called 'sustainable' if most of these, preferably all, are met and not one of these is deteriorated grossly.

Some conditions can be somewhat quantified. Allowing for an increase of world population (a factor 1,8 till 2 in 40 years) and a justified claim for increased prosperity globally (assume with a factor 5 on average) we would, with present practice, run into problems. Taking into account the already too heavily burdened environment and resources, an efficiency improvement all over is needed in the way that we use our resources with a factor 10 till 20 (so-called 'eco-efficiency'). That concerns use of resources (raw materials, energy, water, space, etc.), emission of pollutants, reduced quality of living-surroundings, and loss of ecological values such as biodiversity etc. [2,3]. The 'people' aspects are less easily to quantify. Their influence on the 'direction' technology development is certainly as large.

Such 'eco-efficiency'- and 'people'-oriented improvement can only be attained by changes in systems as a whole. Just optimizing present practice or introduce improved processes or products alone will not suffice. Growth will counteract their effect (Fig. 1 and Tab. 1) [4].

The challenge for (chemical) industry is to go from the present approach still aiming at improving the existing processes and products to novel processes and products, which are much more efficient and, eventually, play a role in a system change that enables the substantial improvement in eco-efficiency required leading to more equity in prosperity and a stable economical situation worldwide. That role is

- to develop the compounds and materials for new products and activities needed for effective and 'directed' sustainable growth and leading to transitions;
- to make growth possible but in a sustainable manner, implying drastic reduction of resource-use in production and the application of products;
- to come up with products and processes fitting the markets and conditions in developing countries and thereby stimulating growth of wealth and well-being [5].

At the same time, also due to globalization, industry is adapting to the changing market and societal conditions and must continue to do so. It must stay viable and profitable, under conditions that will change substantially and in an ever-increasing pace, an economy that is increasingly competitive and a society that is more demanding in material and immaterial sense.

This leads to fundamental changes in the way chemical industry operates:

- a shift from bulk to fine chemicals,
- a strong increase of very specialized chemicals for specific products and applications;
- shortening of the time-to-market to stay ahead of the competition.

That must be made possible by fundamental changes:

- in the way process and product development is done, e.g., fast screening methods and leading to 'laboratory on a chip' concepts.
- in the way scaleup can be done in the (near) future, not by just increasing the size of equipment, which involves complicated scaleup rules but by changes in process architecture and eventually parallel series of smaller reaction systems and even large assemblies of 'production on a chip' derived from laboratory-on-a-chip devices.

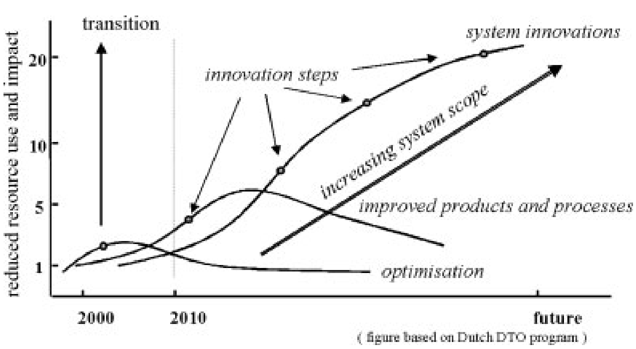

Figure 1. Steps towards improved eco-efficiency.

Table 1. Characteristics of the steps towards improved eco-efficiency.

	Optimization	**Improved**	**Novel system approach**
period yrs	3–5	5–15	10–40
characteristic	good-house-keeping improved operations	process / product innovation	new business concepts, service oriented
improvement	tens of percents	factor 2 till 4	factor 8 till 20
(technical) options, examples	end-of-pipe process optimization	low energy processes, solvent-free products/ processes, waste prevention reduction of production steps	renewable resources and energy, captive use, advanced processes, 'leasing' of compounds
responsible business level	operations and environmental manager	design engineer technology manager	business management
main aspect	organisational, existing technology implementa-tion	new concepts, process-integration	socio-economical requirements, quality of live, product driven
financial	high costs	cost optimization / reduction	opening new markets

It will lead to chemical factories much reduced in size, rather looking like a 'normal assembly hall'. An option is that a specific compound is made on-site where a customer needs it.

Chemical engineering development should be focused on these 'directions' requiring a clear view on the purposes the new processes, products, and molecules must serve, as well as on the constraints and challenges that lie ahead.

4 The Challenges Chemical Engineers Face

The challenges chemical engineers face are therefore:

- define and develop the compounds, materials and products that address the challenges set before meaning highly effective for the intended use, and applicable with minimal environmental impact and risk and easy to recycle;
- in particular, develop the materials and products needed for renewable energy, e.g., highly efficient solar cells, biomass based fuels, fuel cells, etc.;
- find and develop the processes, production paths with the necessary equipment, which are extremely efficient, clean and safe, requiring new production paths completely beyond the optimization of existing ones. Reduction in size of installations is an another goal.
- develop paths to make shifts possible in the resources on which production is based, in particular towards renewable viz biomass based resources for raw materials and energy;
- closing material cycles for the major non-renewable resources by developing the necessary (extremely efficient) recycling paths, processes and necessary equipment on the one hand, and on the other hand by developing the production processes that can be based on those recycled resources;
- the methods to design and test reactions, processes and products, to scale up reaction and production systems: for multiple screening, laboratory-on-a-chip, simulation, and process-architecture design.

All fields of chemical-engineering knowledge are involved. It is evident that in order to attain the ambitious goals described, development in each of the fields can not be isolated, but a coherent development is needed. The structure of such a coherent approach is shown in Fig. 2. It outlines the chain, which links together resources, processes, and products. Also the specific areas and topics within chemistry and chemical engineering, which play a major role for such an integral system approach, are given [4]. Only by using the potential therein, the 'famous' factor 4, 10, or 20 in the overall resource use efficiency, which has to be attained, is possible.

Although, to a large extent, the goals for sustainable development will be set by others, specific methods, indicators, and assessment tools are needed to specifically steer chemical engineering progress towards sustainable development. These are:

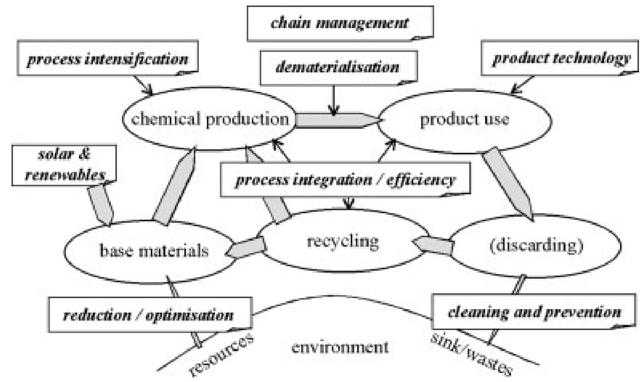

Figure 2. Coherent approach of all fields for sustainable chemical engineering development.

- 'manage' the technology development such that it has a real contribution towards sustainability in the future. Such tools should be used from the moment new research starts.
- determine the actual impact on the environment, safety, etc. of processes and particularly components, materials, and products.

These methods, indicators, and tools have to take into account the effects in whole systems, broadening the view with respect to time, space and actual human behavior. Too easily improvements on the short term and on a local scale prove to be undone or even turn detrimental when looked at in a broader scope.

A crucial point is that technology development is 'need driven'. A process or a material can be 'green' because it is based on renewable resources and the process is efficient, clean and safe. In case it does not contribute to sustainable transition however small, they are not really sustainable.

A good example is the 'case of concern' given above. Cleaner fuels, catalysts etc. do not solve most of the problems coming along with increasing mobility in a 'sustainable manner'.

Cars and even transport systems should be redesigned totally. In the end, the total need for transport should be re-evaluated and organized differently. Such evaluations define the actual demand for new technologies. These will require specific new materials, processes, energy systems etc., which chemical engineering will have to provide. Such assessment capability is also one of the major challenges for chemical engineers.

5 An Agenda for Chemical Engineering

These challenges define the paths along which chemical engineering research and development must proceed. Proposals for agendas aiming at this have been made. Examples are those developed in The Netherlands in the last decade. The first one was made by the Dutch Foundation on Sustainable Chemistry Development (DCO) [5]. The Dutch Organization for Process Engineering Research (OSPT) developed its "Green Manifesto" [6]. Recently a consortium of academic research groups, technological institutes and industries developed a coherent research and development program within the framework of the Dutch interdepartmental program knowledge infrastructure strengthening (ICES-KIS). In other countries, such agendas are developed too. Furthermore, European research framework programs incited this also.

All show main areas for development:

1. product development and application
2. process intensification
3. biomass resources

The three areas show considerable overlap of course. Specific 'subareas' of development that serve both get also special attention in most agendas. Those are genomics, catalysis, separation, integration of conversion, and separation in (bio)chemical production and micro-systems technology. Fig. 3 schemes the Dutch ICES-KIS proposal [7].

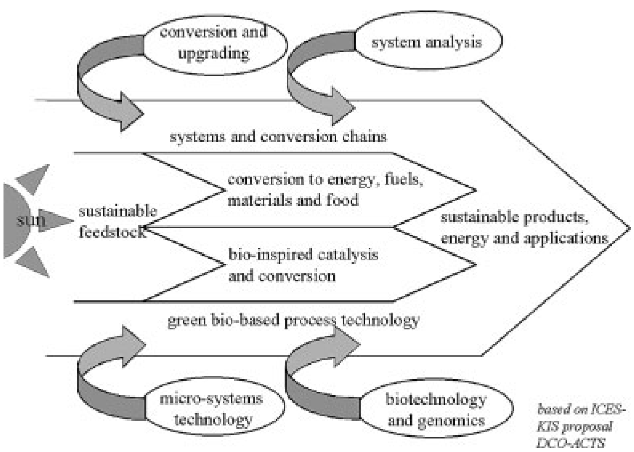

Figure 3. Coherence of programmes for sustainable chemical engineering [7].

5.1 Product Development and Application

The agenda is directed on development of compounds and materials that are optimized for their specific function. They will perform better with less and are able to create extra functionality to improve the performance of the materials and products they are used in.

Dematerialization is the major issue regarding sustainability and higher quality of products and more functionality for better competitiveness. Developing these new and improved products can be (and maybe should be) the major driver for chemical engineering. [9]

Development is aimed at

- new materials with high strength, low weight and being 'self-reparable',
- improved functionality and better performance, for instance enantiomer-specific synthesis,

but also specifically for sustainable energy issues as

- organic material based photovoltaic cells and membranes for fuel cells etc.,
- better energy storage systems to handle the periodic nature of sustainable sources.

and furthermore,

- fast and multiple screening methods through micro-systems (laboratory on a chip),
- software tools for 'designing' and simulating the specific activity and characteristics of molecules.

The knowledge to link together micro- and meso-level by predicting the behavior of molecules, groups of molecules, and submicron particles is growing. Villermaux has named this as one of the new frontiers of chemical engineering [10].

The possibility to create these molecules and clusters, forms the essential basis of many other fields as nanotechnology and microelectronics. A fascinating area of enormous social importance is the development of drugs and additives for so-called functional foods that are much more 'targeted' for a specific activity and even for specific personal characteristics of patients.

5.2 Process Intensification

The agenda is directed on the development of smaller and faster reaction systems with less steps, higher conversion and efficiency due to a better heat and mass transfer.

Extremely efficient use of resources and flexible production facilities reduced in size are the major issues in regard to sustainability and improved competitiveness.

These developments are also closely linked to each other and often not possible without development in the other fields:

- High-efficiency reaction systems, through novel designs, change from batch to continuous, novel methods of energy transfer;
- Integration of different process functions in the reactor (e.g. reaction and separation);
- Improved catalysis, ranging from novel catalysts to combined bio-chemical systems, cascade catalysis and 'one-pot reaction systems';
- Genomics and biochemistry for chemicals, starting with fine chemicals but gradually transferring that knowledge to base chemical production.

High-efficiency reaction systems make use of completely novel reaction designs, totally deviating from the 'classic' forms. In particular, in highly exothermic reactions, a change from batch to continuous in such novel design systems have proven to be very effective and at the same time economically profitable due to a factorial reduction in energy use, less use of material and therefore less waste. A characteristic example is the Helix reactor in the form of a twisted tube, which was optimally designed for exothermic/endothermic reactions, in which selectivity issues play an important role [11]. Further advantages are that such plants are safer, have a higher capacity and are much smaller because downstream processing is reduced too.

Development in catalysis aims at the transformation of multi-step processes using separate catalysts in the subsequent reactions into single-step processes applying more catalysts at the same time, as well as enzymes as chemocatalysts. That resembles the biochemical activities that take place in a living cell ('bio-mimicking'). Total process chains can be 'shrunk' to one or a few steps. Fig. 4 gives an overview on the developments aimed at. The potential is very large [12].

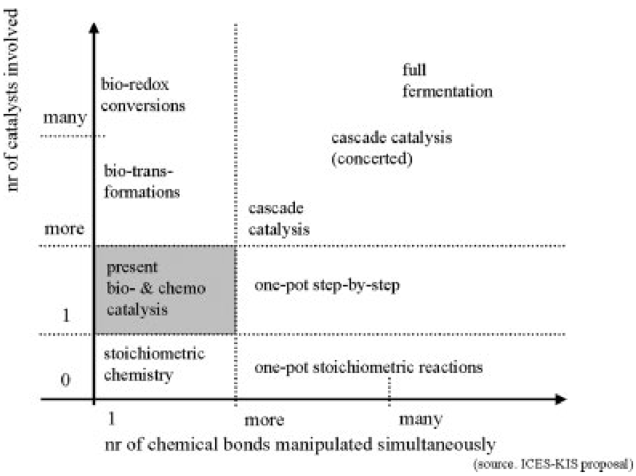

Figure 4. Developments in catalysis [8,12].

Examples for combining functions in one reaction system are the application of membranes to remove a reaction-limiting compound, e.g., a product in fermentation processes. Another example is the combined reaction and solid/liquid separation that can be done in a membrane slurry reactor [11]. Applications can be found in hydrogenation processes using heavy metal based catalysts in the pharmaceutical industry. Particles can be made very small reducing diffusion limitation and, nevertheless, can be easily recovered.

5.3 Biomass Resources for Energy and Chemical Production

In this agenda, two 'lines of thought' come together. One starts from the knowledge that exist in this field already for specific niches and developing it further to more general use for fine chemical production and from there to bulk chemical production. The other one concerns the economic feasibility; starting with the use of available biomass resources for energy purposes. The so developed infrastructure and 'base use' can form a sound economical basis for chemicals production.

To come to a feasible application of biomass a number of issues, not only technological, have to be treated:

- the complexity and variability of biomass resources,
- bulk conversion to 'simple' intermediates with high efficiency,
- but also: new synthesis paths and production routes will have to be considered aiming at a shift from hydrocarbon-based chemistry towards carbohydrate-based chemistry, for optimal use of the resource,
- logistics aspects due to its bulk, perishability and seasonal character,
- 'tuning and linking' of agricultural and chemical industry operations,
- economics, in relation to its higher costs of production compared to present fossil resources,
- ethical aspects, competition with use for food and other necessary human use.

Process routes based on biomass can take two paths:

- thermal
- biological

Both involve a range of quite different reaction systems, lead to different types of intermediates and require other downstream processing steps. In both paths, process intensification is to be implemented too. A good example of a well developed agenda is [13].

Major developments in thermal processing aim at pyrolysis (without oxygen) resulting in a liquid product: 'Biocrude', or total gasification (with limited amount of oxygen/air) to 'Biosyngas'.

Biocrude can be treated as oil and separated, modified, and used as fuel or a base material for further synthesis steps. Converting locally available biomass to such liquid material could offer for instance advantages for handling and transport.

Biosyngas can be the starting point for a range of products (fuels, chemical intermediates, bulk and fine chemicals). The technology exists. In Malaysia, for instance, production of a very clean diesel fuel is based on it. Studies, as done by TNO, have shown that a conversion to methanol as first step improves the technical and economical feasibility of this type of biobased synthesis routes.

Biotechnology-based routes use fermentation, which can produce a broad range of products and intermediates. A well-known candidate is ethanol. Research aims at broadening the possible resources by methods to convert all types of cellulose-type raw materials to fermentable sugars. Further, routes are developed to base bulk products on ethanol. Biothene, ethylene from biobased ethanol, is quite close to being economical. Commercial bulk production of propanediol through fermentation is done by Dupont.

Genomics research is high on the agenda and has break-through potential. It focuses on the development of new bio-based conversion methods based on the broader and deeper insight into the metabolism of living cells and the underlying genetic information. Main feedstock will be carbohydrates and vegetable oils, which are amply available also from residues and wastes. Combining molecular biotechnology with advanced bioprocess and 'normal' chemical technology (and process intensification) makes biomass-based production of fine and bulk chemicals feasible in process routes consisting of a few or even a single one. Development of such routes for commercial production of caprolactam and phenylalanine is already advanced. A good overview is given in [14].

Two approaches are envisaged to resolve the issue of biomass for chemicals or food and the adverse economics:

'biocascade' and 'biorefinery'. Both intend the use of all plant components and are able to optimize the use of residues and low-value biomass resources. Biocascade selects the use for each component on the basis of the highest economic yield [15]. In biorefinery, biomass is separated in its chemical components, as proteins, carbohydrates, and specific metabolites, which could act as precursors for fine chemicals and food additives.

The ethical aspects involved regarding the use for food or chemical feedstock, leads to the general accepted opinion that only real biomass residues should be used in particular for bulk applications. There seems enough of that for present uses. Even spoiled wastes, still containing enough cellulosic materials can be converted to intermediates for further processing.

6 Epilogue: The Age of Chemistry?

Sustainable chemical engineering is aimed at making needed growth possible, even in the future and do so 'with less' and by taking 'rebound effect in consideration'. It is the new frontier and drive for chemical engineering. It is a new perspective and might be an answer to the concerns often uttered about the future of chemistry, and for instance the dwindling numbers of students and its still poor image.

A sustainable future requires safe products and materials with a high functionality. Furthermore, the envisaged growth of nanotechnology, microelectronics, pharmaceutics etc. is wholly based on molecules and handling of molecules. In that sense, molecules will shape the future. This cannot work without new chemistry and chemical engineering. In retrospect, past ages are characterized sometimes by a field in which much development has taken place and so shaped society:

- 19^{th} century: the age of mechanization
- 20^{th} century: the age of electricity and electronics

Could it be that, in view of the need for sustainable growth and radical reduction in use of resources, the 21th century should become the age of chemistry?

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Influence of Reaction Kinetics on the Performance of a Chromatographic Reactor

By *Ralf Herbsthofer* and *Hans-Jörg Bart***

1 Introduction

Chromatography is a widely used separation and purification method. Especially in analytic applications chromatography is represented in any laboratory as discontinuous process tool. However, the economic use of preparative chromatography in pharmaceutics, life science and biotechnology on an industrial scale demands continuous processes. The preparative continuous annular chromatography (CAC) is a developing technology that allows truly continuous chromatographic separations. With the annular chromatograph it is possible to separate multicomponent mixtures with a control of feed and eluent flow rate and rotation speed [1–3].

In terms of process intensification combinations of reactors and separators give multifunctional reactors which, in general, have several advantages. Applied to irreversible reactions with the separation of an inhibitor from the system the selectivity and reaction rate of irreversible reactions can be improved [4,5]. Applied to reversible reactions the reverse reaction can be reduced because of the intrinsic separation of the products and, therefore, the yield increases [6–8], which is also true for other unit operations [9].

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