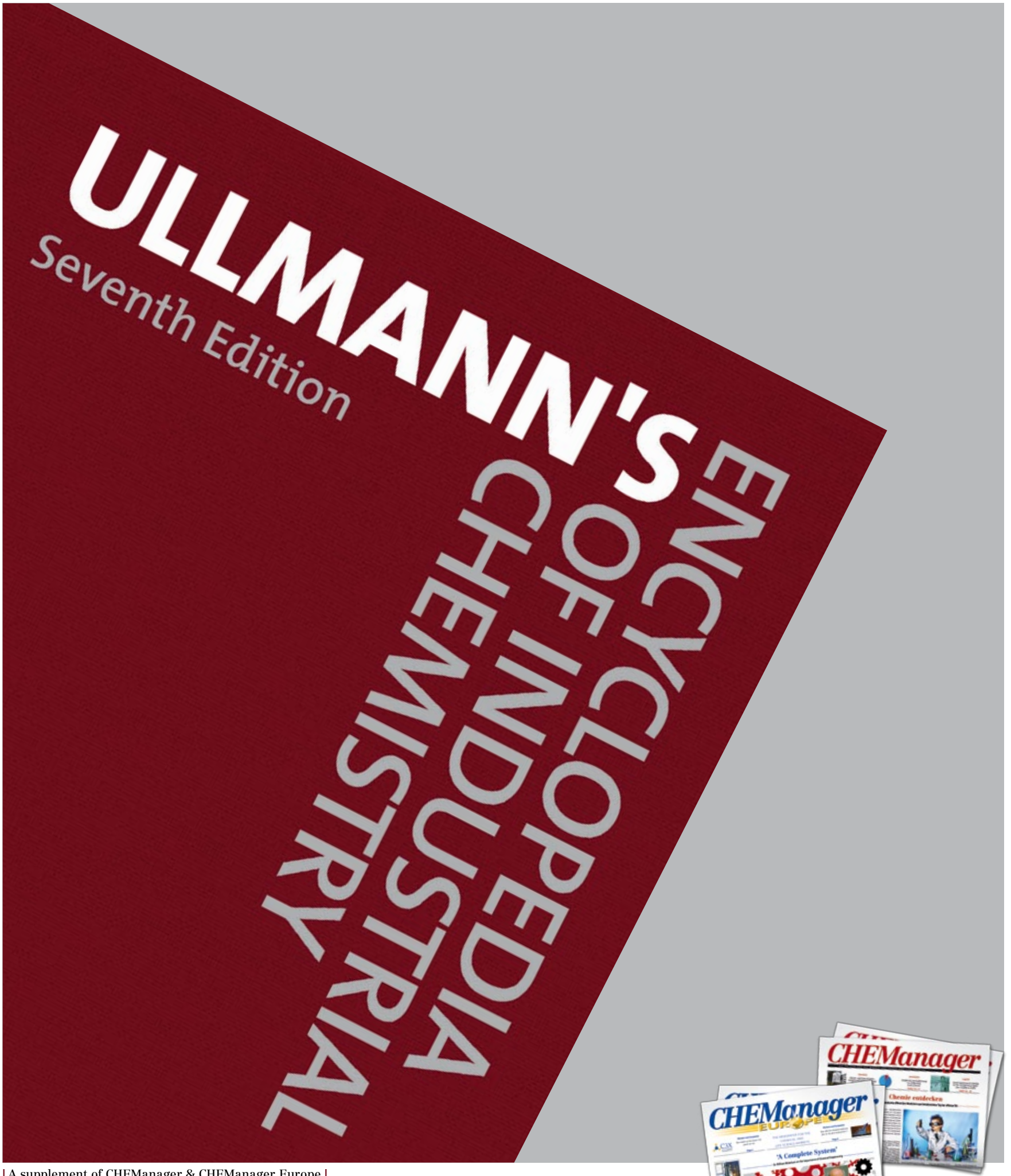
We are delighted to present you with this supplement for the **ACHEMA 2012**. On the next eight pages, we invite you to discover a one-of-a-kind reference, our leading resource, the **ULLMANN'S** Encyclopedia of Industrial Chemistry.
Turn the page to find out more about the advisory board, read extracts from key articles, and much more. **Enjoy browsing!**



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GIT VERLAG

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First published in 1914 by Professor Fritz Ullmann in Berlin, the Enzyklopädie der Technischen Chemie (as the German title read) quickly became the standard reference work in industrial chemistry.

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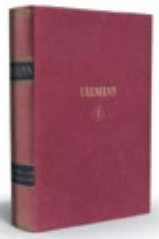

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The 25 volumes of the fourth edition, published between 1972 and 1984, were divided into an alphabetically ordered series of 18 volumes and a general series of six volumes which gave an account of the principles and methods of chemical engineering and process technology.

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The wealth of information provided by Ullmann's can be retrieved from the electronic version (available online with quarterly updates, and on DVD with annual updates) and from the 40 volumes of the 7th print edition published in August 2011. More information on the different editions of Ullmann's is found on page 7.

To keep Ullmann's always up-to-date, articles are revised as soon as new aspects have to be included, and new keywords are incorporated as soon as they have gained industrial relevance. In this respect we, the editors, very much rely on the expertise and the supervision of our Editorial Advisory Board. We are delighted that we could recently welcome several new Advisory Board members from across the globe with expertise in the fields of Food and Feeds, Organic Bulk and Fine Chemicals, Pharmaceuticals, and Biochemistry. Read their exciting self-introductions on page 3!

Yours cordially,
Dr. Barbara Elvers, Editor-in-Chief

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Heike Faulhammer is since 15 years with Arkema, a global chemical company and France's leading chemicals producer.
She completed her studies of Macromolecular Chemistry at the University of Freiburg, Germany, with an post-doctoral stay at the CNRS with Ludwik Leibler at the Unité Mixte de Récherche "Systèmes Macromoleculaires Hétérogènes". Her industrial career started at Arkema in the Technical Polymer Division in an R&D, then process engineer position for long chain polyamides, Rilsan® and Pebax®. A milestone in the following period, as production manager for Rilsan® fine powder, was her participation on a restructuration and modernization plan of the production facilities. Staying in the same division, she was then called to marketing and business for two product lines, serving such diverse markets as automotive, technical textiles, electronics, medical and optical. Her position also included a project of industrial restructuration, this time on world-wide basis. Since 2010 she is as a Director responsible for Arkema's R&D centre with 4 R&D poles: thiochemicals & fine chemicals, carbon nanotubes, polymers & additives, and mineral chemistry.
Heike lives near Pau, France with her husband and 3 children.

Dr. Joydeep Mukherjee has a bachelor's degree in Pharmacy (Birla Institute of Technology, Ranchi, India) and master's degree in Biotechnology from Jadavpur University, Kolkata, India. During his doctoral work in Jadavpur University (1993–97), Dr. Mukherjee was awarded a fellowship of the Council of Scientific and Industrial Research, Government of India to investigate the L-asparaginase from Enterobacter aerogenes as a potential anti-leukemic agent. He was also awarded the "Deutscher Akademischer Austauschdienst" (DAAD) scholarship to work on the bioprocessing aspects of the production of this enzyme as well as fluorescence monitoring during the growth of the producing bacteria with Prof. Thomas Scheper at the University of Hannover, Germany. During the next two-year postdoctoral stay (1998-2000) at the University of Hannover, he worked on the application of oxygen vectors to Claviceps purpurea fermentation and directed biosynthesis in Claviceps purpurea, a fungus producing ergot alkaloids, an important therapeutic agent for neuronal disorders. Dr. Mukherjee started working as an independent researcher in Jadavpur University in 2001. The biotechnological applications of the microbial biodiversity of the Sundarbans were unheard of till his research group ventured into this mysterious realm. His investigations have started opening up the unknown microbiology of the world's largest tidal mangrove forest. This work was appreciated during his sabbatical stay at the Australian Institute of Marine Science (Jan 2007 to Dec 2007), financed by the Department of Biotechnology, Government of India. His other research interests include marine microbial biofilms, marine sponge associated microbial diseases and bioconversion of waste materials.
Dr. Mukherjee is an Associate Professor at the School of Environmental Studies, Jadavpur University, Kolkata. He teaches Ecology and Ecosystems, Environmental Microbiology & Biotechnology and Environmental Health & Toxicology to Master of Philosophy (Environmental Science) and Master of Technology (Environmental Biotechnology) students.

Werner Klaffke has a 19 years career with Unilever, the global consumer good giant. After an assistant professorship and a postdoctoral stay at Harvard Medical School, he started his career in R&D by turning from the exploration of mammalian surface glycans to the industrial production of bacterial exopolysaccharides. After Unilever divested its Chemicals Coordination he became senior scientist in the Flavour Department and initiated cross organizational projects, one of which was about "reaction flavours" that are produced during cooking and heating of food.
It was then when he also developed into new areas, the academic research of "green chemistry" using renewable starting materials, and the management and implementation of "Open Innovation". The former got him into a full time appointment as a full professor at the University of Münster, Germany, the second secured a major involvement in the change processes that Unilever undertook around the change of the millennium.
Called back to Unilever from the academic post into the Unilever Health Institute, he served as a member of the board and helped setting up the Vitality mission through the advancement of credible health claims obtained through sound research and development. Since then he held both, operational and strategic positions and with the recent reorganization of the global R&D structure, he was promoted R&D Director Discovery carrying responsibility for strategy, quality, and execution of internal and joint programmes.
Werner lives in the countryside outside Münster, Germany, with his wife and two boys.

CERAMICS, BIOCERAMICS

ROBERT B. HEIMANN, Görlitz, Germany

1. Introduction

The development, industrial production, and clinical implementation of bioceramic materials with improved lifetime, reliability, and bioactive functions are high on the agenda of worldwide research and development. Bioceramics are inorganic compounds that are designed to replace a part or a function of the human body in a safe, reliable, economic, and physiologically and aesthetically acceptable manner. They must be mechanically and chemically stable in a biological environment but must also possess biocompatibility. According to the degree of their interaction with living tissue biomaterials are divided into three classes: biotolerant, bioinert, and bioactive (osteoconductive) materials.

For many decades, bioceramics such as alumina, zirconia, hydroxyapatite, tricalcium phosphate, and calcium phosphate dental cements have been used successfully in the clinical practice → *Dental Materials – Metallic → Materials for Implants*. In addition, applications emerge that use biomaterials in the medical device industry. The structure, mechanical properties, and biological interaction of biomaterials, and their clinical applications in joint replacement, bone grafts, tissue engineering, and dentistry is reviewed in [1]. The type and consequences of cellular responses to a variety of today's biomaterials have been dealt in [2–5].

The number of patients receiving biomedical implants to correct skeletal and dental defects, and heal diseases is constantly increasing. Worldwide, large demand exists for load-bearing hip, knee, and dental endoprosthetic implants, but also for bone replacement parts in the maxillar-mandibular area, the ossicular chain of the inner ear, alveolar ridge, and iliac crest augmentation, and several orthodontic and periodontic applications. For example, in the United States and in Europe more than 1×10^6 hip and knee arthroplasties are being performed annually, with increasing tendency. The share of Germany in 2007 was 355×10^3 hip and knee joint implants. The increasing demand for endoprostheses is the result of the wear and tear the hip and knee joints are subjected to during a human lifetime. Since people generally live longer and get increasingly overweight due to overeating and lack of exercise, the protective tissue lining of the acetabular cup eventually wears away, friction increases, and inflammation, pain, and finally immobilization will result. At this point a total hip replacement (THR) is the only reasonable option to maintain mobility, freedom from pain, and, hence, a rewarding life in old age. However, more often younger people require such an operation because their lifestyle including damaging sports activities promotes premature wear on their joints. Here a problem arises since the younger patient will generally outlive the 15–20 years lifetime of contemporary implants so that remediation operations are required with substantial additional cost to the healthcare system of the country involved. Hence, the quest for increasing the lifetime of implants through higher reliability of bioceramic devices such as femoral balls, acetabular cups, and dental fixtures drives the R&D agenda worldwide.

In this contribution, salient properties of bioceramics, their specific reactions with tissue, and clinical application will be discussed. As a prominent example, hip endoprosthetic devices will be highlighted.

1 *T. Kokubo: Bioceramics and Their Clinical Applications, Woodhead Publ., Abingdon, UK 2008, pp. 308.*
2 *L. Di Silvio (ed.): Cellular Response to Biomaterials, Woodhead Publ., Cambridge 2008, pp. 648.*
3 *B. Basu, D.S. Katti, A. Kumar (eds.): Advanced Biomaterials. Fundamentals, Processing, and Applications, J. Wiley & Sons, New York 2009, pp. 720.*
4 *J.A. Planell, D. Lacroix, D. Best, A. Merolli: Bone Repair Biomaterials, Woodhead Publ. Ltd., Cambridge 2009, pp. 420.*
5 *R.B. Heimann: Classic and Advanced Ceramics, Bioceramics, Chap. 10, Wiley-VCH Verlag, Weinheim 2010, p. 552.*

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LIQUEFIED PETROLEUM GAS

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1. Introduction

The term liquefied petroleum gas (LPG) describes hydrocarbon mixtures in which the main components are propane, butane, isobutane, propene, and butenes. Most commonly this term is applied to mixtures of propane and butane. These components and mixtures thereof are gaseous at normal temperature and pressure but can be liquefied by cooling, compression, or a combination of both processes.

Liquefied petroleum gas is produced from two distinct sources. The first is by extraction from crude oil and natural gas streams at or close to the point of production from the reservoir and contains propane and butane. The quantities of LPG in the well stream fluid vary greatly, depending on the nature of the reservoir. Production may be (1) of natural gas from a gas reservoir, (2) of gas and light liquid hydrocarbons from a gas condensate reservoir or (3) of crude oil and gas from a combined oil and gas field. LPG typically is one fraction of many (Fig. 1) produced from a given well.

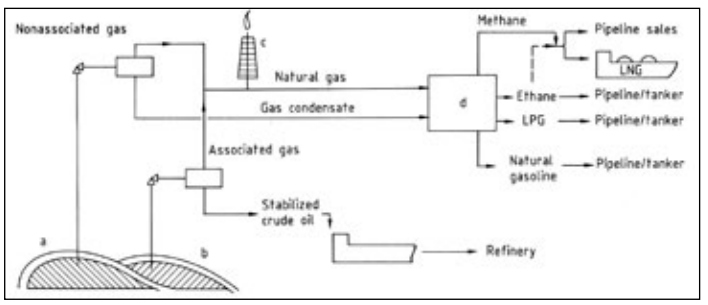

Figure 1. LPG and the other constituents of natural-gas production
NGLP = Natural-gas liquid from gas-processing plants; LNG = Liquefied natural gas; LPG = Liquefied petroleum gas

The extent of recovery of LPG and heavier hydrocarbons from gas depends on the composition of the gas produced and the quality specifications of the gas to be transported to the consumer. Before storage or transportation of crude oil by tanker, its vapor pressure must be lowered so that it can safely be contained in a ship's tank. This reduction, known as stabilization, is achieved by the removal of LPG and lighter species to yield stabilized crude oil and additional natural gas (see Fig. 2). The LPG components in produced oil and gas are predominantly the saturated hydrocarbons propane, butane, and isobutane.

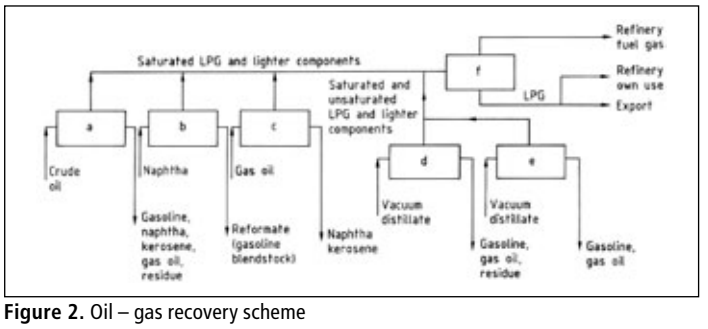

Figure 2. Oil – gas recovery scheme
a) Gas and gas condensate; b) Oil and gas; c) Vent-flare; d) Gas processing plant

Second, LPG is obtained by processing of crude oil in refineries and, in some instances, as a byproduct from chemical plants. The remaining LPG in the stabilized crude oil at the refinery is separated in the crude-oil fractionation column. The constituents of this LPG are propane, butane, and isobutane. Additional LPG is produced in refinery conversion processes such as catalytic reforming, thermal cracking, catalytic cracking, and hydrocracking (see Fig. 3). The composition of this LPG depends on the processing configuration at the refinery but typically includes both saturated (propane, butane, and isobutane) and unsaturated (propene and butenes) components.

So-called bio-LPG, or more specifically biopropane, is technically feasible to produce, and is likely to be commercially available before 2015.

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MICROREACTORS – MODELING AND SIMULATION

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1. Introduction

In the field of conventional, macroscopic process technology modeling and simulation approaches are by now used on a routine basis to design and optimize processes and equipment. Many of the models employed have been developed for and carefully adjusted to specific processes and reactors and allow flow, heat and mass transfer to be predicted, often with a high degree of accuracy. In comparison, modeling and simulation approaches for microreactors are more immature, but have great potential for even more reliable computer-based process engineering. In general, the purposes of computer simulations are manifold, such as feasibility studies, optimization of process equipment, failure modeling, and modeling of process data. For each of these tasks within the field of chemical engineering simulation methods have been applied successfully.

Microreactors (→ Microreactors) are developed for a variety of different purposes, specifically for applications that require high heat- and mass-transfer coefficients and well-defined flow patterns. The spectrum of applications includes gas and liquid flow as well as gas-liquid or liquid-liquid multiphase flow. The variety and complexity of flow phenomena clearly pose major challenges to the modeling approaches, especially when additional effects such as mass transfer and chemical kinetics must be taken into account. However, there is one aspect which makes the modeling of microreactors in some sense much simpler than that of macroscopic equipment: the laminarity of the flow. Typically, in macroscopic reactors the conditions are such that a turbulent flow pattern develops, which makes the use of turbulence models [1] necessary. With turbulence models the stochastic velocity fluctuations below the scale of grid resolution are accounted for in an effective manner, without the need to explicitly model the time evolution of these fine details of the flow field. Heat- and mass-transfer processes strongly depend on the turbulent velocity fluctuations, and for this reason the accuracy of the turbulence model is of paramount importance for a reliable prediction of reactor performance. However, currently (2011) there is no model available which is capable of describing turbulent flow phenomena in a universal manner and is computationally inexpensive at the same time. For this reason, simulation approaches for microreactors, which usually do not require turbulence models, offer some potential to make predictions with a degree of accuracy unparalleled by models of macroscopic reactors.

When comparing processes in microreactors with those in conventional systems, a few general differences can be identified:

- Flow in microstructures is usually laminar, in contrast to the turbulent flow patterns on the macroscale
- The diffusion paths for heat and mass transfer are very short, and this makes microreactors ideal candidates for heat- or mass-transfer-limited reactions
- The surface-to-volume ratio of microstructures is very high. Thus, surface effects are likely to dominate over volumetric effects
- The fraction of solid wall material is typically much higher than in macroscopic equipment. Thus, solid heat transfer plays an important role and must be accounted for when designing microreactors

While the absence of turbulence simplifies many modeling tasks, the predominance of surface effects introduces additional complications, especially in the case of multiphase flow. Some of the fundamental mechanism, for example, those of dynamic wetting and spreading phenomena, are not yet well understood, and this adds some degree of uncertainty to the modeling of these processes. As more and more practical applications of microfluidic systems emerge, research in the field of fluidic surface and interfacial phenomena gains additional impetus. Hope fully in the following years refined models for microfluidic multiphase systems will be formulated and will add an additional degree of predictability to flow phenomena in microreactors.

1 *S.B. Pope, Turbulent Flows, Cambridge University Press, Cambridge 2000.*

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UREA

JOZEF H. MEESSEN, Stamicarbon, Sittard, The Netherlands

1. Introduction

Urea *[57-13-6]*, $CO(NH_2)$, $\underline{M}_r$ 60.056, plays an important role in many biological processes, among others in decomposition of proteins. The human body produces 20–30 g of urea per day.

In 1828, Wöhler discovered [1] that urea can be produced from ammonia and cyanic acid in aqueous solution. Since then, research on the preparation of urea has continuously progressed. The starting point for the present industrial production of urea is the synthesis of Basaroff [2], in which urea is obtained by dehydration of ammonium carbamate at increased temperature and pressure:

$$NH_2COONH_4 \rightleftarrows CO(NH_2)_2 + H_2O$$

In the beginning of the 20th century, urea was produced on an industrial scale by hydration of cyanamide, which was obtained from calcium cyanamide:

$$CaCN_2 + H_2O + CO_2 \rightarrow CaCO_3 + CNNH_2$$

$$CNNH_2 + H_2O \rightarrow CO(NH_2)_2$$

After development of the NH_3 process (Haber and Bosch, 1913, → *Ammonia, 1. Introduction – Chemical Properties → Ammonia, Chap. 4*), the production of urea from NH3 and CO_2, which are both formed in the NH_3 synthesis, developed rapidly:

$$2NH_3 + CO_2 \leftrightharpoons NH_2COONH_4$$

$$NH_2COON_4 \leftrightharpoons CO(NH_2)_2 + H_2O$$

At present, urea is prepared on an industrial scale exclusively by reactions based on this reaction mechanism.

Urea is produced worldwide on a large scale; its production volume exceeds 150×10^6 t/a in 2010. The main application of urea is its use as fertilizer. Urea, being the most important member of the group of nitrogenous fertilizers, contributes significantly in assuring world food supply.

2. Physical Properties

Pure urea forms white, odorless, long, thin needles, but it can also appear in the form of rhomboid prisms. The crystal lattice is tetragonal–scalenohedral; the axis ratio a : c=1 : 0.833. The urea crystal is anisotropic (noncubic) and thus shows birefringence. At 20 °C the refractive indices are 1.484 and 1.602. Urea has an mp of 132.6 °C; its heat of fusion is 13.61 kJ/mol.

Physical properties of the melt at 135 °C follow:

ρ	1247 kg/m3
Molecular volume	48.16 m^3/kmol
η	3.018 mPa · s
Kinematic viscosity	2.42×10^{-6} m^2/s
Molar heat capacity, Cp	135.2 J mol^{-1} K^{-1}
Specific heat capacity, cp	2.25 kJ kg^{-1} K^{-1}
Surface tension	66.3×10^{-3} N/m

In the temperature range 133–150 °C, density and dynamic viscosity of a urea melt can be calculated as follows:

$$\varrho = 1638.5 - 0.96\ T$$

$$\text{In}\ \eta = 6700/T\ 15.311$$

The density of the solid phase at 20 °C is 1335 kg/m^3; the temperature dependence of the density is given by 0.208 kg m^{-3} K^{-1}.

1 *F. Wöhler, Ann. Phys. Chem. 2 (1828) no. 12, 253–256.*
2 *A.I. Basaroff, J. Prakt. Chem. 2 (1870) no. 1, 283.*

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by Frank Weinreich, Associate Publisher, Wiley-VCH

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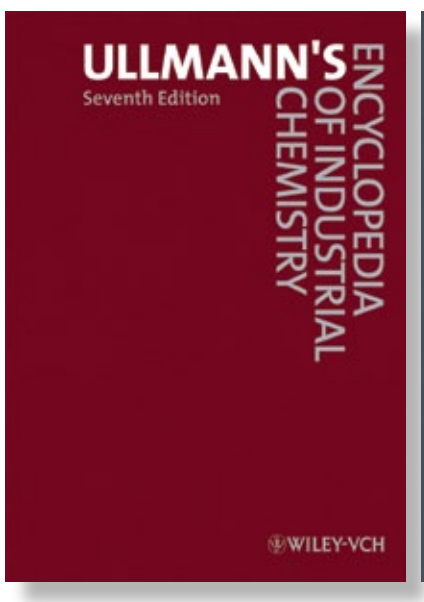

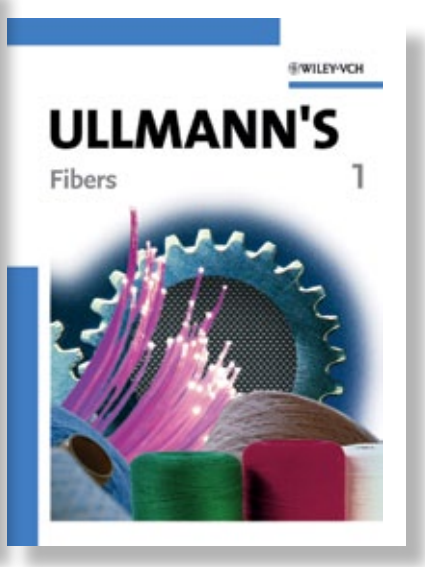

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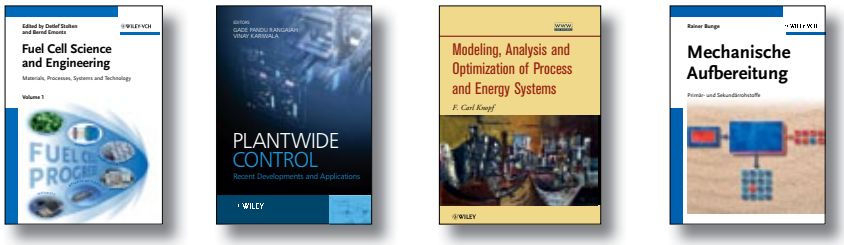

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