EUROKIN

20th Anniversary Symposium

Eurokin is an industrial-academic consortium in the area of chemical reaction kinetics. Its aim is to transfer knowledge in reaction kinetics from the academic domain to the industrial domain, thereby expediting the implementation of the state-of-the-art. In many cases, this has resulted in the development of user-friendly tools to allow, for example, more efficient assessment of experimental conditions.

Financed by the industrial members, Eurokin achieves its goals by funding projects on various kinetics' topics using a mixture of experts drawn from its own academic members and the wider academic world as well as various consultants in the field. Founded in early 1998, Eurokin currently numbers twelve industrial members (companies) and seven academic members (European universities). You may find more information about the Eurokin consortium at http://www.eurokin.org.

To celebrate its 20th anniversary, a special symposium will be held at which experts in the field of reaction kinetics, who have previously hosted Eurokin projects, will return to make presentations in keynote areas of reaction kinetics relevant to the industrial world. The symposium is non-confidential and, unlike other Eurokin symposia, is open to both Eurokin and non-Eurokin members. The symposium will also include a review of the work of Eurokin over the last decade by way of introduction. The details of the symposium are given below.

The meeting will be hosted by SABIC and DSM. Their financial support to realise this symposium is highly appreciated.

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Dates
The two-days' meeting will be held on Tuesday and Wednesday October 16th and 17th, 2018 (see the symposium programme on pages 5 and 6).

Venue

The venue of the symposium will be Kasteel Vaalsbroek (The Netherlands). Kasteel Vaalsbroek is wonderfully located on an estate in the gentle hills of the beautiful Limburg landscape, near the point where the Netherlands, Germany and Belgium meet and near Maastricht and Aachen. It offers a balanced, high-quality mix of relaxation, urban inspiration and rural peace. Stay in one of the 130 atmospheric and spacious rooms in the adjacent hotel or, if you would prefer even more luxury, in one of our tastefully furnished suites with a wonderful view of the gently rolling Limburg landscape. Enjoy a delicious breakfast in the adjacent castle. The à la carte restaurant at Kasteel Vaalsbroek, 'In de Oude Watermolen', is renowned for its local ingredients and seasonal dishes. After a day enjoying the city or nature, relax in our Spa & Wellness Centre Vaalsbroek. Bilderberg Kasteel Vaalsbroek has everything you need to ensure a wonderfully relaxing stay. We have our own free parking spaces for guests.

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Location

- Vaals is close to Aachen (20 minutes by taxi from central station at which there are always enough cabs available) and hence good to reach by train from Düsseldorf (DUS Airport), Cologne (CGN Airport) and Brussels (Zaventem, BRU). There are always enough cabs at Aachen main station.
- If you travel via Amsterdam Airport (Schiphol, AMS) you should take the train to Heerlen (this takes 2 h 40 min.; you can check the schedule at ns.nl). Since there are less cabs available here we can keep a list of who's coming via Heerlen, and connect those on the list for sharing cabs (please inform us at what time you plan to arrive at Heerlen train station).

Open symposium

The Eurokin 20th Anniversary Symposium is open to both Eurokin members and non-members and therefore an excellent opportunity to meet colleagues and experts in the field of reaction kinetics. You are kindly requested to forward this invitation to colleagues within your own company or institution as well as to other contacts who might be interested in this symposium. Although there appears to be much interest for this symposium there are still quite some places available.

Registration and hotel booking

You are requested to register for this symposium by sending an e-mail to Rob Berger (r.j.berger@tudelft.nl). Since the numbers attending is limited, we recommend you to do this at your earliest convenience to guarantee participation. Following registration you will be receive an invoice by e-mail that should be paid as soon as possible.

Please also indicate your registration e-mail your full address (as you want to see it on the invoice).

We have reserved a large number of rooms at the Bilderberg Vaalsbroek Kasteel Hotel. You need to make the hotel reservation by yourself via the link: www.bilderberg.nl/lcr/dsm.

The booking will be at DSM rate, which is € 117,50 per room per night, no breakfast included (breakfast buffet available at € 19,50 p.p.p.d). Tourist tax of € 1,48 and service charge of € 2,20 p.p.p.n. will also be charged.

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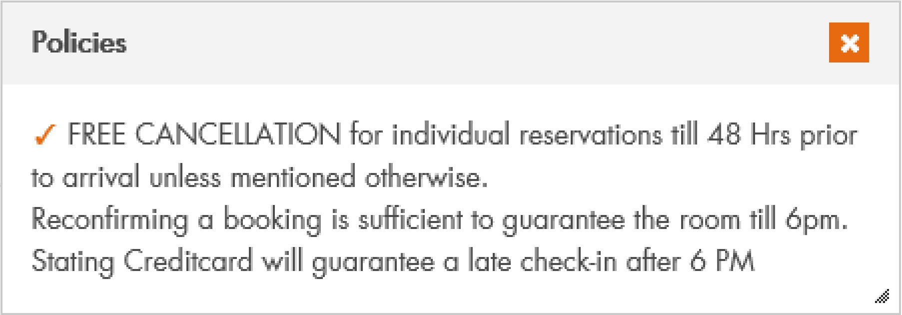

Policies

✓ FREE CANCELLATION for individual reservations till 48 Hrs prior to arrival unless mentioned otherwise.
Reconfirming a booking is sufficient to guarantee the room till 6pm.
Stating Creditcard will guarantee a late check-in after 6 PM

Registration fee and payment

The registration fee amounts to € 200,- per attendee for both days. There is no reduction if you attend only part of the programme. The registration fee covers the symposium dinner and catering during the meeting and includes a subsidy by SABIC and DSM.

Please pay the registration fee by bank transfer: remit the €200, under reference "Eurokin 20th Anniversary Symposium", to:

VDI Technologiezentrum GmbH, VDI-Platz 1, 40468 Düsseldorf
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(Bank: Deutsche Bank AG, Königsallee 45 -47, 40189 Düsseldorf)

Eurokin’s 20th Anniversary Symposium: Programme

Tuesday October 16th

10.00 – 10.30	*Welcome coffee*
10.30 – 10.45	**Opening/Welcome** Hugh Stitt (Johnson Matthey; Chairman Eurokin consortium)
10.45 – 11.30	**Initiation and propagation by Eurokin: a decade of developments in reaction pathway analysis** Linda Broadbelt (Northwestern University)
11.30 – 12.15	**Eurokin - 20 Years of catalyst performance testing** Freek Kapteijn & Jacob Moulijn (Delft University of Technology)
12.15 – 13.45	*Lunch*
13.45 – 14.30	**What progress in catalyst deactivation?** John Birtill (Consultant in Catalyst Technology at Highcliffe Catalysis Ltd.)
14.30 – 15.15	**Large-scale production of fuels and chemicals: coping with complex feedstocks and chemistry** Guy B. Marin (Ghent University)
15.15 – 15.45	*Coffee / Tea break*
15.45 – 16.30	**Turbulent mixing with chemical reactions: from fundamentals to CFD models** Rodney Fox (Iowa State University)
16.30 – 17.15	**Recent advances in microstructured catalysts** Enrico Tronconi (Politecnico di Milano)
17.15 – 18.00	**Multiscale catalysis modelling goes operando: A perspective on the nature of the surface of operating catalysts** Karsten Reuter (TU Munich)
19:30	*Symposium Dinner*

Wednesday October 17th

09.15 – 09.45	**Chemical reaction kinetics at the academic-industrial interface** Jan Verstraete (IFPEN)
09.45 – 10.30	**Porous media for transport and reaction applications: what is a “good” model?** Marc-Olivier Coppens (University College London)
10.30 – 11.00	*Coffee / Tea break*
11.00 – 11.45	**Structured catalytic reactors for steam methane reforming: from lab to commercial scale through detailed kinetic and fluid dynamics modelling** Juray de Wilde (Université catholique de Louvain)
11.45 – 12.30	**First Principles Multiscale Modelling to design Pt-based bimetallic catalysts for (de)hydrogenation reactions** Marie-Françoise Reyniers (Ghent University)
12.30 – 14.00	*Lunch*
14.00 – 14.45	**Kinetic modelling and analysis of catalytic redox cycles** De Chen (NTNU)
14.45 – 15.30	**Diffusion and effective diffusivity in porous media:** ***the importance of nuclear magnetic resonance*** Mick Mantle (University of Cambridge)
15.30 – 16.00	*Coffee / Tea break*
16.00 – 16.45	**Single pellet string reactors revisited - Obsolete or pioneering technology?** Olaf Hinrichsen (TU Munich)
16.45 – 17.30	**Dynamic methods for catalytic kinetics** Yves Schuurman (IRCELyon)
17.30	*Closure*

Initiation and propagation by Eurokin: a decade of developments in reaction pathway analysis

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Reaction pathway analysis is a powerful tool to identify optimal processing conditions, suggest catalyst design strategies, and design novel routes to chemicals. We have developed methods for the assembly of kinetic models of substantive detail that link the atomic and process scales. We have applied our methodology to seemingly very disparate chemistries, yet applying a common methodology reveals that there are many ubiquitous features of complex reaction networks for chemical and biological systems.

This talk will focus developments in reaction pathway analysis in the last decade, with a focus on new methodologies and applications that were initiated and propagated by early work with Eurokin. In particular, examples of the mechanistic modeling of the conversion of a wide variety of hydrocarbon feedstocks will be used to illustrate the evolution and the power of the approach as applied to complex reaction systems.

What progress in catalyst deactivation?

John J. Birtill

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The Eurokin survey on catalyst deactivation was completed in 2004, and the findings were last updated at the meeting in Lyon in 2008. This talk will include an overview of developments during the past 10 years. The target subject matter will include methodology for the measurement and modelling of catalyst performance from experimental work, as well as developments in design and formulation of commercial catalysts, and the monitoring of catalyst performance at industrial scale. Developments in characterization and mechanisms of catalyst deactivation will also be considered.

Eurokin - 20 Years of catalyst performance testing

Freek Kapteijn and Jacob A. Moulijn

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Throughout its existence the Eurokin consortium has been active in developing efficient tools for determining the performance of predominantly heterogeneous catalysts. The general purpose is obtaining intrinsic catalytic information of the active phase, without parasitic influence of transport phenomena, although for instance in reactor design also the performance of commercial catalyst particles is desired.

The development comprised smart experimental testing methods and criteria to test the absence or presence of interfering phenomena on the basis of experimental data. Catalyst testing has been scaled down tremendously during the existence of the consortium. Advances in design and construction of microreactors have been a source of inspiration for the field of catalyst testing. However, there are limits to scaling-down, due to the different scaling dependencies of involved phenomena. A classic challenge is scaling down multiphase systems in beds packed with mm-sized pellets.

The Eurokin consortium is based on a unique cooperation between industry and academia where industry felt a need for a more sound theoretical and practical basis in the field of catalyst performance testing and academic groups enjoyed translating fundamental achievements into a tool kit for kinetic and catalyst performance studies. The cooperation between the industrial and academic members was a big success and Eurokin evolved into a real expertise centre.

An overview will be given of the achievements in the Eurokin consortium regarding performance testing and the challenges where further development is desirable.

Large-scale production of fuels and chemicals: coping with complex feedstocks and chemistry

Guy B. Marin, Joris W. Thybaut, Kevin M. Van Geem

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Major sources of fuels and bulk chemicals consist of complex mixtures of either hydrocarbons or oxygenates. Techniques for the characterization of the latter have progressed tremendously and allow to quantify their composition up to an unprecedented level of detail. Hence, it is possible to account explicitly for the elementary reactions that the feedstock molecules undergo. Very often a limited number of elementary reaction families allows to describe fully the conversion towards fuels or chemicals. The corresponding kinetic parameters have a well-defined chemical meaning and, hence, can in principle be calculated with so-called ab initio techniques. Having identified the relevant elementary reaction families, it is possible to generate the fully detailed reaction network by computer codes. These networks can contain several thousands of elementary reaction. However only a limited number of kinetic parameters are required to implement the reaction kinetics in reactor models allowing to design and optimize the corresponding industrial large-scale production processes.

Turbulent mixing with chemical reactions: from fundamentals to CFD models

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A high-level overview of turbulent mixing of passive scalars will be provided. First, key concepts and modeling approaches from the literature will be reviewed. What is known from fundamental studies, how this knowledge is incorporated in mixing models for reacting flows, and how these models are implemented in computational fluid dynamics codes will all be covered. Finally, open problems requiring further research will be mentioned.

Recent advances in microstructured catalysts

Enrico Tronconi, Gianpiero Groppi, Carlo Giorgio Visconti,
Alessandra Beretta, Mauro Bracconi, Matteo Ambrosetti

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This presentation will first briefly summarize the transport properties of catalysts with micro structured substrates, including honeycomb monoliths, open-cell foams and periodic cellular structures. It will than focus on their potential for facilitating kinetic studies of exothermic high-T reactions, for optimizing the mass transfer – pressure drop trade off in the applications of Environmental Catalysis, and for intensifiying heat-transfer limited processes in non-adiabatic technical tubular reactors for the production of chemicals and energy vectors. The talk will ideally link together, complement and extend a number of contributions provided by our group to Eurokin through the years on related topics.

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Multiscale catalysis modelling goes operando: a perspective on the nature of the surface of operating catalysts

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First-principles electronic structure calculations have emerged as a key contributor in modern catalysis research. Next to the dedicated computation of thermostability, spectroscopic signals and reactivity descriptors, they are increasingly used as basis for predictive-quality multiscale modeling approaches. Corresponding approaches additionally account for meso- and macroscopic aspects like statistical interplay within the catalytic cycle or heat and mass transport in the reactor.

This provides unprecedented insight into the catalytic function, be that the actual reaction mechanisms or the nature of the surface of the operating catalyst. Particularly with respect to the latter, this insight points at substantial deviations from the standard picture that analyzes catalytic function merely in terms of properties of and processes at active sites as they emerge from a crystal lattice truncation of the nominal catalyst bulk material. Instead, a highly dynamic picture is suggested with continuous reaction-induced complex (surface) morphological changes at (near-) ambient conditions or an evolving, possibly liquid-like phase behavior due to limited heat dissipation channels. Advancing multi-scale catalysis modeling methodology to scrutinize such a picture is the next grand challenge. In my lecture I will survey corresponding methodologies and discuss their capabilities and current limitations.

Chemical reaction kinetics at the academic-industrial interface

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Since its early development, chemical reaction engineering has always strongly benefitted from close cooperation between academia and industrial companies. This has been particularly so in the area of chemical reaction kinetics, where best practice in industry generally lags behind developments in academia. The gap between industrial practice and academic achievement can be closed by a structured and concerted effort to learn from each other's experiences leading to, on the one hand, an increase in industrial capabilities in the area of reaction kinetics and, on the other hand, a source of industrially relevant themes as input to academic research through close contact with the needs of industry. The Eurokin consortium on reaction kinetics has been a prime example of this strategy. The close interaction of the industrial members and academia through the Eurokin consortium has also allowed the identification of gaps-and-needs in the area of reaction kinetics in industrial applications. We will briefly review the areas of cooperation and provide a few examples of results and learnings. After twenty years, the Eurokin consortium continues to generate new projects in the area of reaction kinetics to fulfil the developing needs of industry.

Porous media for transport and reaction applications: what is a “good” model?

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Formulating a geometrical model for porous media is essential for a huge range of applications involving transport and reactions in the pore space and on their internal surface. These applications vary from heterogeneous catalysis to adsorption and membrane separation processes, concrete and other building materials, rocks, soil or food products. But what is a “good” model? Can we and should we include the position of every single atom for the model to be called “good”? Pragmatically speaking, a model should be an adequate representation of the system to permit correct (enough) predictions for the application of interest.

We survey insights gained over the years, thanks to progress in analytical experimental and imaging techniques, statistical and computational methods, and mathematical insights. Whether the medium is isotropic or anisotropic, the degree of heterogeneity, order and disorder in the organisation of solid and pores, and whether the medium changes over time: all affect the level of complexity of the modelling approach required. Both morphological (shape related) and topological (connectivity related) aspects should be considered. Continuum models may not always be adequate, because of fundamental shortcomings, especially related to unrealistic assumptions on pore network topology. Discrete models should be more accurate, as long as topological information is available. A multiscale approach is generally preferred, integrating aspects from the atomistic via the nanoscale to mesoscopic grains and macroscopic particles. However, no model can ever be better than the data available at these different scales; theoretical and experimental analysis, together with information on the formation of the material, where possible, help to determine what is important to include.

Structured catalytic reactors for steam-methane reforming: from lab to commercial scale through detailed kinetic and fluid dynamics modelling

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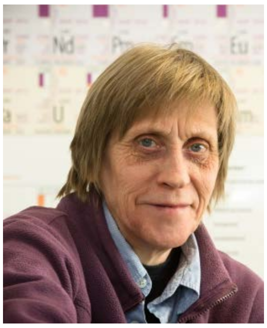
Structured catalytic reactors offer perspectives for combining reduced pressure drop, intensified heat transfer and improved catalyst effectiveness. Focusing on application to steam-methane reforming, different aspects of the development of such reactors are dealt with, such as the catalyst, the detailed modelling of the kinetics and the fluid dynamics, validation of the resulting reactor model through pilot plant tests and scale-up and optimization of the reactor using the validated model.



First principles multiscale modelling to design Pt-based bimetallic catalysts for (de)hydrogenation reactions

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Supported Pt is used in a variety of hydrogenation and dehydrogenation reactions and plays a key role in various industrial and environmentally important processes. Pt-bimetallic catalysts often display catalytic properties that differ from those of the parent Pt-metal and offer the opportunity to obtain new catalysts with enhanced selectivity, activity, and stability. Fundamental kinetic models that include catalyst descriptors obtained from Density Functional Theory (DFT) calculations enable to obtain a better understanding of the origin of the catalytic behaviour of Pt-bimetallics and to provide guidelines for optimal catalyst properties.

Kinetic modelling and analysis of catalytic redox cycles

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The oxidation reaction is one of the most important catalytic processes, playing an important role in numerous industrial, environmental and energy applications. All these reactions involve redox reactions where both reactants and catalysts undergo electron transfer reactions through reduction and oxidation. For a selective oxidation reaction, the main reaction mechanism is the Mars and van Krevelen mechanism, and the redox catalytic cycles can be simplified as:

[CatO] + R-C → RC-O + [Cat]
[Cat] +1/2 O_2 → RC-O

Where [CatO] represents the oxidized catalyst surface and [Cat] its reduced state. The active sites or oxidation state are entirely dynamic in nature and depend on the relative re-reduction and re-oxidation rates. The oxidation state of the catalysts and amount of lattice oxygen determine the activity, selectivity and stability. Many redox reactions involving C, Cl, N, and S follow similar simplified mechanism on metal carbide, chlorides, nitrides and sulfides. However, despite the importance of redox reactions, an efficient method for diagnosing or monitoring, kinetic modeling and controlling the catalytic cycles is still missing. Here we report a new approach for developing kinetic model by taking into account the dynamic changes in active sites. The new kinetic model can properly describe not only the reactant kinetic behavior, but also the oxidation state changes in the redox cycle. The application of the new approach in ethylene oxychlorination on $CuCl_2$ [1-2] will be discussed.

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Diffusion and effective diffusivity in porous media: *the importance of nuclear magnetic resonance*

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The talk will describe how pulsed field gradient nuclear magnetic resonance (PFG-NMR) and nuclear magnetic resonance relaxometry has been instrumental in furthering our physical and chemical understanding of how molecules move and interact within porous particles that are typically found in hydrocarbon processing and heterogeneous catalysis operations. In particular the talk will show how PFG-NMR can distinguish between many different types of diffusive mass transport over many different length scales.

For example, we will show how it is possible to measure both inter and intra- particle diffusion in micro porous zeolites and surface diffusion in meso porous materials. Examples will also be given from our recent work describing PFG-NMR experiments performed at high temperatures and pressures to better understand the reaction mechanisms during ethylene oligomerisation; a reaction used in the production of synthetic liquid fuels.

The second part of the talk will focus on how magnetic resonance T1 and T2 relaxometry can be used to study the strength of surface interaction between reactants, products and solvents with the internal surfaces of the solid catalyst material. The combination of both T1 and T2 relaxometry with PFG-NMR therefore provides us with a deeper physical insight into catalytic reactions mechanisms, the role of solvents in catalysis, and catalyst deactivation phenomena.

Single pellet string reactors revisited - obsolete or pioneering technology?

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Introduced in the 1970s, single pellet string reactors (SPSR) are a special type of packed bed, where the confining walls have an only slightly larger diameter than the catalytic pellets. CFD simulation results for SPSRs, varying for example diameter ratio, pellet number, reactor scale and gas properties, are presented aiming at characterising this reactor type for exploring chemical reaction kinetics. Residence time distribution and conversion of an isothermal irreversible 1st order gas phase reaction are compared to ideal plug flow behaviour. Existing design criteria for fixed-bed reactors are evaluated and new criteria for SPSRs proposed. Conversion in SPSRs deviating less than 5 % from plug flow results can be achieved readily. Hence they are a reliable, risk-reducing and cost-effective alternative for catalyst testing and kinetic measurements which deserve a revival after falling into oblivion decades ago.

Dynamic methods for catalytic kinetics

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Heterogeneous catalysis plays an important role for energy and chemicals production. Challenges in the near future in catalysis coincide with those in the energy transition and the need for sustainability in the chemical industry. Better catalysts have to be designed to reduce energy consumption, to reduce waste and to convert new feedstocks into fuels and chemicals. Catalysis is a kinetic phenomenon. Kinetics of catalytic processes give insight into the reaction mechanism. Kinetics are also used for reactor design and process optimization. In this case the kinetics are usually determined in lab scale reactors under steady-state conditions, as the large majority of industrial catalytic processes are operated at steady-state. Transient experiments can provide more information than steady-state experiments and are particularly useful in unraveling complex reaction networks. However, the experiments are more complicated to perform and more time and effort for data treatment/modeling is required than for steady-state experiments. A large variety of different transient kinetics methods have been developed, each with its own characteristics. This presentation will give an overview of different approaches of transient kinetics in heterogeneous catalysis. It will give specific examples on how qualitatively and quantitatively transient kinetics can provide more information than steady-state experiments and how a link can be made to catalyst development.