

Network profile

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The Eurokin consortium: origin, topics and aims

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1 Introduction

A large European inventory of the current practice of kinetics research in companies [1] resulted in the establishment of the Eurokin consortium in 1998. This consortium of industrial and academic members, aims at the implementation of best practice in the area of chemical reaction kinetics, particularly in the industrial environment. Our “industrial approach” is well illustrated in our paper from 2001 [2]. In many cases, this has resulted in the development of user-friendly tools to allow, for example, more efficient assessment of experimental conditions. Other work has been aimed at evaluating the software available for processing kinetic data, while a number of leading academics and experts have been commissioned to produce reviews of the state-of-the-art in a number of chemical kinetics topics. The Eurokin approach is illustrated in Figure 1.

Regular meetings are held where progress in the various research areas is presented and experts in the field are invited to lecture on the latest advances in chemical kinetics. Eurokin thus forms the hub of a network of scientists and technologists active in the field focusing on the commercial applicability of the tools and provides the opportunity to swap experience and discuss problems concerning reaction kinetics.

A selection of achievements, to date, is summarized below.

Experimental set-ups:

- Software for the selection of a suitable test reactor for performing kinetics experiments (includes overview of properties of a wide range of experimental reactors).

- Inventory of suppliers of experimental reactors (also for high throughput experimentation).
- Spreadsheets to assess transport limitations in various experimental reactor types. Concerning catalytic reactors, in-depth investigations were performed on the bypass effect of inert bed dilution in fixed beds [3–5] and on the bypass effect in catalyst coated-wall reactors [6, 7].

Kinetic data analysis:

- Assessment of commercially available software packages for kinetic parameter estimation; this includes four test cases, as well as evaluation and performance results of selected packages [8, 9].
- Investigation of the application of sequential experimental design for kinetic model discrimination and parameter accuracy.
- Coping with irreducible transport limitations, including details of experimental techniques and model libraries incorporating transport phenomena.
- A model library to facilitate the implementation of the reactor model equations for the estimation of kinetic parameters.

State-of-the-art reviews and case studies:

- Methods for establishing reaction networks and lumping.
- Kinetics of deactivating catalysts, including overview of phenomena, techniques for their diagnosis and methods for accelerated testing [10].
- Reactors for investigation of fast exothermic heterogeneous reactions, such as annular coated-wall reactors and micro designs.
- Inclusion of chemical kinetics in computational fluid dynamics (CFD).
- Non-steady-state methods for estimating reaction rate parameters [11].

A limited amount of material is made accessible to the public domain on the Eurokin website <http://www.eurokin.org>. One of the free accessible results is a handy tool for a quick assessment of transport limitations in a user-defined, fixed-bed reactor experiment (Figure 2).

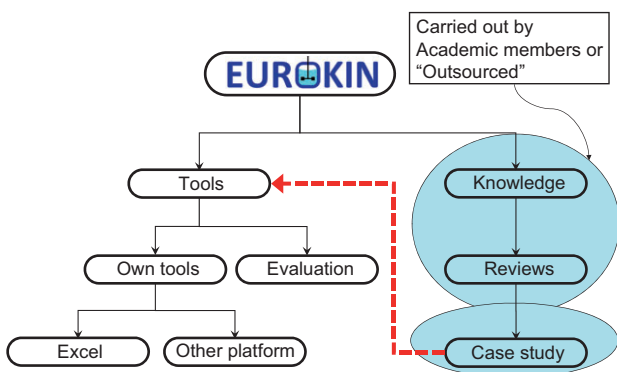


Figure 1 The Eurokin research approach with the final aim to create handy tools facilitating the industrial research; either directly, or, more typical, indirectly via academic reviews and case studies.

2 Membership

The Eurokin consortium currently comprises nine industrial companies: Albemarle, BP, DSM, Eni, Evonik Industries, IFP Energies nouvelles, Johnson Matthey, Linde, and Shell; and seven academic institutions: Delft University of Technology, Ghent University, the Catholic University of Louvain, IRCElyon, Politecnico di Milano, the Norwegian University of Science and Technology (Trondheim), and the Technical University of Munich.

Funding is provided by the industrial members, while the academic members provide support and guidance in the development and execution of the program, which is updated each year. The technical plans for the coming year(s) are regularly defined or adjusted at Main Committee meetings, which are held three times per year, and which are always combined with a workshop focusing on running and completed reviews and tasks.

New members may be admitted to Eurokin at any time, if they are willing to actively contribute to (expanding) the research program. Details on terms and conditions for new members can be obtained from: Dr. Hugh Stitt (Chairman of the EUROKIN Steering Committee), Johnson Matthey, PO Box 1, Billingham, TS23 1LB, United Kingdom, Tel. +44 1642 522704, E-mail: Hugh.Stitt@Matthey.com

3 Current program

The current program has been defined for the next 2 years into a number of tasks, which are grouped in three separate categories. A brief summary is given below.

Tasks related with experimental methods and reactors to obtain kinetics:

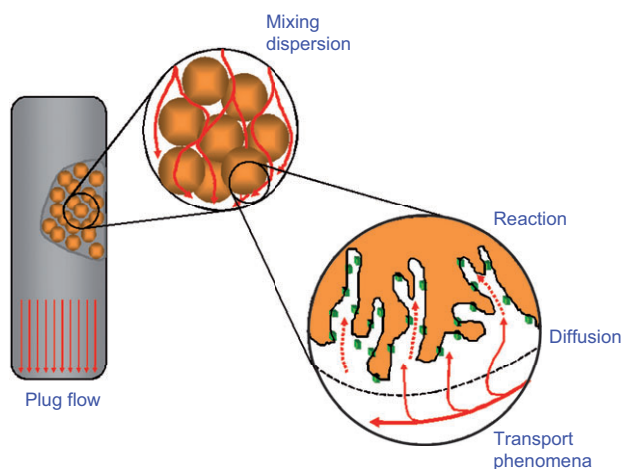


Figure 2 Illustration of potentially rate limiting transport phenomena in a fixed bed, which can be estimated using the Eurokin web tool available at <http://www.eurokin.org>.

- Spreadsheets for evaluating the absence of transport phenomena are continuously maintained and improved based on best practice (fixed beds, stirred tanks, slurry reactor, Robinson-Mahoney reactor).
- Methods and approaches/models for describing the diffusivity in pore systems of catalyst bodies.
- Dynamic methods case studies to analyze the added value of non-steady-state methods over steady-state methods, for obtaining reaction kinetics parameters and other relevant parameters.
- Phase (dis)appearance in gas-liquid-solid (GLS) reactors, focusing on approaches and methods to adequately describe the effect of appearance and disappearance of a liquid phase in fixed beds.

Tasks concerning software to obtain kinetics from experimental data:

- The best practice and new developments of software related with reactor modeling, kinetic parameter estimation and the design of experiments is monitored. This includes data reconciliation and a proper definition of the objective function in the estimation.
- Tools to extrapolate uncertainties in reaction kinetics, catalyst descriptors and physical properties to those in the performance of the industrial reactor.

Tasks on theoretical methods to obtain kinetics:

- Assessment of non-experimental methods and software by means of case studies of specific reaction networks, for estimating relevant parameters (rate constants and activation energies) from databases and theoretical approaches (hydrogenation over a heterogeneous catalyst).

- Liquid-phase kinetics: investigation of theoretical approaches and methods to obtain the reaction

kinetics of liquid-phase reactions in an indirect way, e.g., from kinetics measured in the gas phase.

References

- [1] Bos ANR, Lefferts L, Marin GB, Steijns MHGM. *Appl. Catal. A: General* 1997, 160, 185–190.
- [2] Berger R, Stitt EH, Marin GB, Kapteijn F, Moulijn JA. *CatTech* 2001, 5, 30–60.
- [3] Berger R, Pérez-Ramírez J, Kapteijn F, Moulijn JA. *Chem. Eng. Sc.* 2002, 57, 4921–4932.
- [4] Berger R, Pérez-Ramírez J, Kapteijn F, Moulijn JA. *Applied Catalysis A: General* 2000, 227, 321–333.
- [5] Berger R, Pérez-Ramírez J, Kapteijn F, Moulijn JA. *Chem. Eng. J.* 2002, 90, 173–183.
- [6] Berger R, Kapteijn F. *Ind. Eng. Chem. Res.* 2007, 46, 3863–3870.
- [7] Berger R, Kapteijn F. *Ind. Eng. Chem. Res.* 2007, 46, 3871–3876.
- [8] Berger R, Hoorn J, Verstraete J, Verwijs JW. In *Studies in Surface Science and Catalysis*, Froment GF, Waugh KC, Eds., Elsevier: Amsterdam, 2001, Vol. 133, pp. 631–636.
- [9] Berger R, Hoorn J, Verstraete J, Verwijs JW. Eurokin website (<http://eurokin.tudelft.nl/wp-content/plugins/download-monitor/download.php?id=46>), 2001.
- [10] Birtill J. *Ind. Eng. Chem. Res.* 2007, 46, 2392–2398.
- [11] Berger R, Kapteijn F, Moulijn JA, Marin GB, De Wilde J, Olea M, Chen D, Holmen A, Lietti L, Tronconi E, Schuurman Y. *Appl. Catal. A: General* 2008, 342, 3–28.