AIDIC EFCE
ISCRE25 FLORENCE 2018
BRIDGING SCIENCE & TECHNOLOGY
The 25th International Symposium on Chemical Reaction Engineering
20-23 May 2018
Florence, Italy
www.aidic.it/iscre25

Chemical Reaction Kinetics at the Academic-Industrial Interface

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Highlights

- Eurokin, a consortium on kinetics and on chemical reaction engineering;
- Academic-industrial collaboration on reaction kinetics in industrial applications;
- Investigation of pre-competitive topics, evaluating tools and methods.

1. Introduction

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.

Over the last 20 years, the Eurokin consortium on reaction kinetics has been a prime example of this strategy. We will briefly review the areas of cooperation and provide a few examples of results and learnings. 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.

2. The Eurokin Consortium

The Eurokin Consortium was formed in 1998 following a review of current practice of kinetics in companies [1]. It aims at implementing best practice in the area of chemical reaction kinetics [2,3]. The Eurokin consortium comprises 12 industrial companies and 7 academic institutions (see http://www.eurokin.org/).

In the Eurokin Consortium, research funding is provided by the industrial members, while the academic members provide support and guidance in the development and execution of the programme. The actions in the research programme are defined and adjusted at Main Committee meetings, which are held three times per year and focus on running and completing tasks. These meetings are also combined with a workshop, where progress in the various research areas is presented and experts in the field are invited to present the latest advances in chemical kinetics and chemical reaction engineering. Eurokin restricts its projects to pre-competitive topics, such as tools and methods for the study of reaction kinetics.

Through its organization, Eurokin forms a network hub for scientists and technologists active in the field of chemical reaction engineering, providing the opportunity to discuss current developments, to exchange experience and to assess the industrial applicability of various tools.

3. Some of Eurokin's achievements

One of the first topics tackled by the consortium concerned experimental set-ups. In this field, Eurokin's academic-industrial collaboration has resulted in the development of tools to facilitate the assessment of transport limitations in a wide variety of reactors (fixed beds, stirred tanks, slurry reactor, Robinson-Mahoney reactor etc.); provided an overview of the characteristics of a wide range of experimental reactors; developed software for the selection of a suitable test reactor; drawn up an inventory of laboratory equipment and their suppliers; and assessed non-steady state equipment and methods for obtaining kinetic data.

Other work has concerned kinetic data analysis. Here, experimental techniques and equipment to cope with irreducible transport phenomena in systems with very fast reactions have been reviewed; an assessment of available software packages to perform kinetic parameter estimation has been made; sequential design tools have been evaluated; a comparison has been made of data reconciliation techniques; the proper definition of the objective function and best practices in parameter estimation have been reviewed.

Finally, a number of leading academics and experts have been commissioned to write state-of-the-art reviews on several chemical reaction engineering topics. These include topics on catalyst deactivation, microkinetic modelling techniques, ab initio methods, chemical kinetics in computational fluid dynamics (CFD), methods and approaches for describing diffusion in porous particles, the added value of non-steady state methods for assessing reaction rate parameters, theoretical approaches for easier acquisition of liquid-phase kinetics.

4. Ongoing work for industrially-applied reaction kinetics

The current activities in Eurokin build on the vast knowledge that has already been acquired. On the kinetic modelling side, we are currently reviewing techniques to build micro-kinetic models, benchmarking lumped kinetic models against more rigorous models, and reviewing kinetics of reactions involving solids. Concerning experimental tools, we are currently focusing on kinetics in Robinson-Mahoney reactors, and in dynamically operated reactors, on the use of TGA and DSC based equipment and methods, and on the experimental validation of run-away predictions. On the parameter estimation side, the inventory and assessment of kinetic modelling software is currently being updated, while investigating techniques for a posteriori analysis of parameter values and error estimation on model prediction. Another topic focuses on understanding material transport in catalysts through molecular dynamics, reviewing pore network models, and investigating spatially resolved modelling of reaction and transport in catalysts. Several specific applications (hydrocracking, selective oxidation of light hydrocarbons, electrochemical activation of gas-phase reactions, CO_2 conversion etc.) are also under investigation.

5. Conclusions

The Eurokin consortium provides an excellent exchange platform: the industrial members value the access to a wide range of reviews in the field of chemical reaction engineering in a format which is both concise and focused on industrial needs, and a set of tools to use this knowledge. The academic members particularly value the insights into the needs of industry, and connections into the industrial chemical reaction engineering community. After twenty years, the Eurokin consortium continues to generate new projects in the area of reaction kinetics to fulfil the developing needs of industry.

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Keywords:
Eurokin consortium, reaction kinetics, best practice, academic-industrial collaboration.