Venue

The combined seminar on Mathematics in Chemical Kinetics and Engineering and Eurokin workshop will be held in IFP-Lyon, a major center for research and industrial development, for the oil, natural gas and automotive industries.
IFP is pleased to invite you to attend this seminar on Monday 23 May in IFP-Lyon, France.
Participation in the seminar is free.

Hotel

Please inform us about hotel needs before 15 May 2005. Hotel is to be paid directly by the attendees once at the hotel. You will be charged in case of no-show. Rooms are booked at the following address (outside Lyon city):
Hôtel Soleil et Jardin
44 rue de la République - 69360 Solaize, France
Phone: +33 4 78 02 44 90 / Fax +33 4 78 02 09 26

Location

Lyon is two hours from Paris by high-speed train (TGV). IFP-Lyon is about 15km south of Lyon. To get to the conference with taxi or rental car:
. from Lyon: take the A7 motorway south towards Vienne-Marseille, exit at Solaize, follow the sign Institut Français du Pétrole
. from the airport: take the A43 motorway towards Lyon, then the ring road ("boulevard periphérique") towards Marseille, then the A7 motorway
. by train (SNCF): get-off at the Lyon Perrache station (best) or Lyon Part Dieu, then take a taxi.

Invitation

Mathematics in Chemical Kinetics and Engineering

Mackie
Eurokin

Combined 2005 seminar & workshop

IFP-Lyon, France
23 - 24 May 2005
http://www.mackie-workshops.com
http://www.eurokin.org

Program

Monday 23 May (Open seminar & workshop)

- 10:00 Coffee and registration
- 10:45 Introduction
- 11:00 Method of homogenization applied to dispersion, convection and reaction in porous media, *Andro Mikelic*
- 12:00 State-by-state transient screening of industrial catalysts: from model-free kinetic characterization to the detailed mechanism, *Gregory S. Yablonsky*

- 12:45 Buffet

- 13:45 Methods for total energy calculations in chemical systems, *Philippe Sautet*
- 14:45 Non-experimental methods for estimating reaction rate parameters, *Linda J. Broadbelt*
- 15:30 Coffee break
- 16:00 Kinetic modeling of CO conversion over copper based catalysts, *Yves Schuurman*
- 16:30 Microstructured reactors for multiphase chemistries, *Claude de Bellefon*
- 17:00 Visit of IFP-Lyon (optional)

Transfers to the hotel

- 20:00 Dinner in Lyon

Tuesday 24 May (Eurokin members only)

- 9:00 Eurokin main committee meeting
- 15:00 End

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Abstracts

Method of homogenization applied to dispersion, convection and reaction in porous media, ***Andro Mikelic, Institut Camille Jordan Université Lyon 1, France***

The homogenization technique, which is a rigorous method of averaging by multiple scale expansions, is applied to the transport of reacting solute in a porous medium. We focus our attention on situations when Peclet's and Damkohler's numbers are important. Starting from the pores, with the usual convection-diffusion equation for the solute and a first-order chemical reaction for the solute particles at the pore boundaries, we give a derivation of the 3D dispersion tensor for solute concentration. For particular pore geometry and particular scaling, we find the well-known Taylor dispersion formula. Our approach allows handling higher Peclet numbers than in the literature. For important Damkohler's number, our method gives important corrections in the upscaled transport and reactive term.

State-by-state transient screening of industrial catalysts: from model-free kinetic characterization to the detailed mechanism, ***Gregory S. Yablonsky, Dpt. of Chem. Eng. Washington Univ., St. Louis, USA***

A new approach, “state-by-state transient screening”, is presented. According to the approach, the detailed kinetic mechanism is extracted from primary non-steady-state kinetic data. The key idea is to kinetically test a catalyst with a particular composition (e.g. amount of surface oxygen) that changes insignificantly during the test. A complete screening experiment includes the sequence of such tests performed over a catalyst with different composition prepared separately and scaled (e.g. oxidation degree). The approach is based on three experimental principles: a) insignificant catalyst change during a single-pulse experiment; b) control of reactant amount stored/released by catalyst in a multi-pulse experiment; c) uniform chemical composition within the catalyst zone. The approach is illustrated using selective butane, butadiene and furane oxidation over a VPO catalyst.

Methods for total energy calculations in chemical systems, ***Philippe Sautet, Laboratoire de Chimie, UMR CNRS 5182, Ecole Normale Supérieure de Lyon, France***

The calculation of total energy and atomic forces is of great importance for several problems in chemistry, such as the prediction of molecular structures, the description of elementary reaction steps, or the simulation of molecule electronic properties. In principles this “simply” requires to solve the Shrödinger equation. However, analytic solutions can only be obtained when the system contains a single electron, and the difficulty begins as soon as electron-electron interaction terms are considered. In this talk, we will present the various methods for the determination of the total energy, with a special emphasis on the Density Functional Theory. Applications will be presented in the case of molecular reactivity at the surface of a catalyst.

Non-experimental methods for estimating reaction rate parameters", ***Linda J. Broadbelt, Dpt of Chemical Engineering Northwestern University, USA***

Computational methods and other sources for estimating parameters used in calculating reaction rates that can replace or enhance experimental procedures will be reviewed. In particular, familiar quantities such as reaction rate constants, adsorption constants and equilibrium constants commonly found in rate expressions for non-catalysed, heterogeneously catalysed and homogeneously catalysed reactions will be discussed. Commercial and freely-available databases for both thermodynamic quantities and rate coefficients will be enumerated. Group additivity schemes and quantum mechanical methods for calculating thermodynamic quantities will also be described. The use of quantum mechanical methods to calculate rate coefficients using transition state theory will also be reviewed. Finally, correlations for calculating kinetic quantities from properties that are easier to measure such as the Evans-Polanyi relationship and the UBI-QEP method will be reviewed. An emphasis will be placed on which methods can be used for which types of chemical systems and applications.

Kinetic modeling of CO conversion over copper based catalysts, ***Yves Schuurman, Institut de Recherche sur la Catalyse, Villeurbanne, France***

Interest has been renewed for the water-gas shift reaction in the light of the production of hydrogen for fuel cell applications. This catalytic reaction converts CO into CO_2 by the reaction with water and provides additional hydrogen. Current industrial catalysts are not suited for onboard applications. Therefore a low-pyrophoric monolith supported copper catalysts have been developed. In order to assist catalyst development kinetic modeling of the reaction data has been performed and compared to a Cu/Zn/Al reference catalyst. Whereas a discrimination based on “classical” Langmuir-Hinshelwood kinetic models was not possible, microkinetic modeling provided detailed information into the reaction mechanism. The data can be described adequately by a relatively simple rate equation based on a two-step redox mechanism.

Micro-structured reactors for multiphase chemistries, ***Claude de Bellefon, V. Meille, D. Schweich, CNRS ESCPE Lyon, France***

The design, set-up and use of micro-structured reactors for high throughput experimentation, kinetic investigations and other laboratory applications is reported. Concepts for the proper design of gas-liquid contacting in very small reaction volumes in micro-reactors are presented. Three type of micro-structured components have been used: a micro-mixer displaying 25 to 40 µm width channels, a falling film reactor displaying a 100x300 µm channel and a multiphase contactor equipped with a metallic mesh with openings of 5 µm diameter. Using these components, catalyst screening or kinetic studies can be performed with precious metal inventory down to 1 µg, with a throughput of ca. 200 tests per day using automated injector/collector, hydrogen pressure up to 46 bar and temperature up to 80°C. Examples in the field of asymmetric hydrogenations, gas-liquid selective oxidation and triphase hydrogenations will be given.