UCL Université catholique de Louvain

LMAPR1400

2013-2014

Physical & Chemical Kinetics

5.0 credits	30.0 h + 30.0 h	1q

Teacher(s) :	De Wilde Juray (coordinator) ; Bailly Christian ;
Language :	Français
Place of the course	Louvain-la-Neuve
Prerequisites :	LFSAB1302 or equivalent courses in quantitative chemistry and thermodynamics.
Main themes :	The course is divided in two parts. The first part deals with the kinetics of homogeneous reactions. The molecular basis of chemical reaction kinetics is first presented, i.e. collision theory and Transition State Theory. Next come homogeneous coupled and complex reactions, including their modeling. The detailed reaction mechanisms are taken into account. Some biochemical and radical reactions (in particular oxidations, polymerizations and explosive reactions) are studied as important examples. The second part focuses on heterogeneous reactions. First, we deal with the fundamental aspects of molecular diffusion and the coupling between transfer phenomena and chemical reaction kinetics through the Thiele modulus. Heat and mass transfer at the interface and inside the reactive phase are considered and their modeling is described. Questions linked to catalyst deactivation are next studied. Finally, an introduction to gas-solid and gas-liquid reaction kinetics is presented. Thermal cracking and hydrocarbon processing reactions form the main examples chosen in this part.
Aims :	The course aims at familiarizing the student with the kinetics of chemical and physical transformations of matter, in particular the coupling between chemical reaction kinetics as such and physical transfer and adsorption phenomena. Knowledge of these rates is crucial for the modeling of industrial processes. The main objectives of the course are : (i) understanding the molecular basis of chemical reaction kinetics and diffusion processes, (ii) the identification of rate laws based on detailed reaction mechanisms in homogeneous and heterogeneous cases, (iii) the description of experimental and numerical methods used to obtain them, and (iv) the study of heterogeneous catalytic reactions. *The contribution of this Teaching Unit to the development and command of the skills and learning outcomes of the programme(s) can be accessed at the end of this sheet, in the section entitled "Programmes/courses offering this Teaching Unit".*
Evaluation methods :	Exam: preparation in writing possibly followed by possible oral defense.
Teaching methods :	Lectures, problem-based learning and exercises,
Content :	Chapter 1: Fundamentals of Reaction Kinetics 1.1 Refresher : Chemical Rates and Rate Equations 1.2 Molecular theories: collision theory 1.3 Molecular theories: Transition State Theory 1.4 Coupled Reactions 1.5 Reducing the Size of Kinetic Models 1.6 Bio-Kinetics 1.7 Complex Reactions 1.8 Modeling the Rate Coefficient Chapter 2: Kinetics of Radical Chain Reactions 2.1 Introduction 2.2 Straight Radical Chain Reactions 2.3 Examples : Slow Oxidation of Hydrocarbons and Linde-Bodenstein Kinetics 2.4 Kinetics of Radical Polymerizations 2.5 Branched Radical Chain Reactions Chapter 3 : Diffusion and Reaction 3.1 Microscopic Approach to Fick's Law 3.2 Diffusion Equation 3.3 Introduction to Diffusion in Complex Mixtures 3.4 Chemical Reactions with Diffusion Limitations 3.5 Thiele Modulus Chapter 4: Kinetics of Heterogeneous Catalytic Reactions 4.1 Introduction 4.2 Adsorption on Solid Catalysts 4.3 Rate Equations 4.4 Complex Catalytic Reactions Chapter 5: Transport Processes with Reactions Catalyzed by Solids

	Part One Interfacial Gradient Effects 5.1 Reaction of a Component of a Fluid at the Surface of a Solid 5.2 Mass and Heat Transfer Resistance 5.3 Concentration or Partial Pressure and Temperature Differences Between Bulk Fluid and Surface of a Catalyst Particle Part Two Intraparticle Gradient Effects 5.4 Molecular, Knudsen, and Surface Diffusion in Pores 5.5 Diffusion in a Catalyst Particle 5.6 Diffusion and Reaction in a Catalyst Particle. A Continuum Model 5.7 Falsification of Rate Coefficients and Activation Energies by Diffusion Limitations 5.8 Influence of Diffusion Limitations on the Selectivities of Coupled Reactions 5.9 Criteria for the Importance of Intraparticle Diffusion Limitations Chapter 6: Catalyst Deactivation 6.1 Types of Catalyst Deactivation 6.2 Kinetics of Catalyst Poisoning 6.3 Kinetics of Catalyst Deactivation by Coke Formation Chapter 7: Introduction to Gas-Solid and Gas-Liquid Reactions 7.1 Introduction 7.2 A Qualitative Discussion of Gas-Solid Reactions 7.3 General Model with Interfacial and Intraparticle Gradients 7.4 Heterogeneous Model with Shrinking Unreacted Core 7.5 Models for Transfer at a Gas-Liquid Interface 7.6 Two-Film Theory 7.7 Surface Renewal Theory
Other infos :	Support: Transparencies on i-campus Gilbert F. Froment, Kenneth B. Bischoff, and Juray De Wilde, "Chemical Reactor Analysis and Design", 3th edition, Wiley, 2010. R.W Missen, C.A. Mims, B.A. Saville, « Introduction to Chemical Reaction Engineering and Kinetics », Wiley
Cycle and year of study :	> Bachelor in Engineering
Faculty or entity in charge:	FYKI