LMAPR1400 — Physical & Chemical Kinetics

2014-2015

5.0 credits	30.0 h + 30.0 h	1q

Teacher(s) :	Bailly Christian ; De Wilde Juray (coordinator) ;
Language :	Français
Place of the course	Louvain-la-Neuve
Inline resources:	> http://icampus.uclouvain.be/claroline/course/index.php?cid=MAPR1400
Prerequisites :	LFSAB1101, LFSAB1102, LFSAB1201, LFSAB1202, LFSAB1301, LFSAB1401, LFSAB1302
Main themes :	Chapter 1: Elements of Reaction Kinetics Chapter 2: Kinetics of free radical chain reactions Chapitre 3: Diffusion and chemical kinetics Chapter 4 - Part I: Kinetics of Heterogeneous Catalytic Reactions Chapter 4 - Part II: Kinetic modeling of heterogeneous catalytic reactions Chapter 5 - Part I: Transport Processes with Reactions Catalyzed by Solids - Interfacial Gradient Effects Chapter 6: Noncatalytic Gas-Solid Reactions Chapter 7: Catalyst Deactivation Chapter 8: Gas-Liquid Reactions
Aims :	Contribution of the course to the program objectives Referring to the web page "Compétences et acquis au terme de la formation" du bac EPL" (http://www.uclouvain.be/prog-2014-fsa1ba-competences_et_acquis), the following LOs are aimed at: -- Axe 1: 1.1, 1.2; -- Axe 2: 2.3, 2.4, 2.6, 2.7. Specific learning outcomes of the course Chapter 1: Elements of Reaction Kinetics After successfully completing this course, the student will be able to : -- Define the issues involved and the methodology used in the kinetic modeling of chemical reactions. -- Define reaction rates and rate expressions. -- Calculate the activation energy of a chemical reaction. -- Explain the basis of collision theory and activated complex theory -- Model complex reactions and reaction networks and reduce the size of a kinetic model and the number of independent rate parameters. Chapter 2: Kinetics of free radical chain reactions After successfully completing this course, the student will be able to : -- Explain the elementary steps of free radical reactions and extract the corresponding kinetics. -- Explain kinetic expressions for the following important examples : thermal cracking of ethane, homogenous radical polymerization, hydroperoxidation, combustion/explosion of H_2 in presence of O_2. -- For free radical polymerization, explain the molar mass distribution and the influence of molecular diffusion on polymerization kinetics. Calculate reaction kinetics based on mechanism for similar cases as seen during exercise sessions. Solve a non isothermal free radical polymerization problem with Tromsdorff effect with the help of numerical simulation tools in the frame of a group miniproject. Chapitre 3: Diffusion and chemical kinetics After successfully completing this course, the student will be able to : -- Derive Fick's law for a perfect gas with the help of simplified model ; make the link to Fourier's law. -- Explain the fluctuations-dissipation theorem and Stokes 'Einstein relationship for Brownian particles. -- Derive the diffusion equation (second Fick's law) from microscopic and macroscopic arguments.

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Explain diffusional control of chemical reactions and its practical importance..
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Use the mass balance equation to yield Thiele's modulus and the efficiency factor for order 1 reactions.
Chapter 4 - Part I: Kinetics of Heterogeneous Catalytic Reactions
After successfully completing this course, the student will be able to :
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Define the different steps involved in heterogeneous catalytic reactions.
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Make a distinction between ideal and non-ideal adsorption on a catalyst.
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Derive Hougen-Watson and Eley-Rideal type rate equations for single and coupled reactions.
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Deal with complex catalytic reactions, in particular to generate the reaction network and to reduce the number of independent rate parameters.
Chapter 4 - Part II: Kinetic modeling of heterogeneous catalytic reactions
After successfully completing this course, the student will be able to :
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Design experimental reactors required for the kinetic modeling of heterogeneous catalytic reactions.
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Discriminate between kinetic models and to estimate the rate parameters.
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Design experiments in a sequential way, for optimal discrimination between kinetic models or for optimal parameter estimation.
Chapter 5 - Part I: Transport Processes with Reactions Catalyzed by Solids - Interfacial Gradient Effects
After successfully completing this course, the student will be able to :
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Describe the reaction of a component of a fluid at the surface of a solid.
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Model interfacial mass and heat transfer.
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Describe multicomponent diffusion in a fluid.
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Calculate the concentration or partial pressure and temperature differences between a bulk fluid and a surface of a catalyst particle.
Chapter 5 - Part II: Transport Processes with Reactions Catalyzed by Solids - Intraparticle gradient effects
After successfully completing this course, the student will be able to :
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Define and characterize molecular, Knudsen, and surface diffusion in pores.
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Describe diffusion in a catalyst particle by means of a pseudo-continuum model.
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Define the effective diffusivity in a catalyst and the tortuosity of a catalyst, as well as methods to experimentally determine them.
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Give an overview of more fundamental approaches to describe diffusion in a catlyst particle (structure & mp; network models, Molecular Dynamics and Dynamic Monte-Carlo simulations).
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Describe diffusion and reaction in a catalyst particle by means of a continuum model.
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Define and calculate the modulus and the effectiveness factor of a catalyst for a given reaction.
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Identify some major effects of intraparticle diffusion limitations, in particular in falsifying rate coefficients and activation energies and changing the selectivities of coupled reactions.
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Define criteria to evaluate the importance of intraparticle diffusion limitations.
Chapter 6: Noncatalytic Gas-Solid Reactions
After successfully completing this course, the student will be able to :
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Give a qualitative discussion of gas-solid reactions and their kinetic modeling.
Chapter 7: Catalyst Deactivation
After successfully completing this course, the student will be able to :
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Define and characterize the major types of catalyst deactivation: solid-state transformations, poisoning, and coking.
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Model the kinetics of uniform catalyst poisoning.
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Model the kinetics of catalyst deactivation by coke formation.
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Define deactivation functions.
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Describe catalyst deactivation by site coverage only and by site coverage and pore blockage.
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Describe the effect of intraparticle diffusion limitations on the deactivation of a catalyst by site coverage and pore blockage.
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Give an overview of the methods used for the kinetic analysis of catalyst deactivation by coke formation.
Chapter 8: Gas-Liquid Reactions
After successfully completing this course, the student will be able to :
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	Give a qualitative discussion of gas-liquid reactions and their kinetic modeling. -- Derive and apply the two-film theory and the surface-renewal theory. *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 :	At the exam, students are evaluated individually according to in advance explained rules. Intermediate interrogation(s) on part(s) of the course is/are possible. The exam can consist of an oral and a written examination. The written exam consists of a theoretical and an exercise part. The parts taught by each teacher normally count for half of the total mark. Some reports on projects can be marked and the mark included in that of the exam. At the exam, the teachers have the right to reduce the weight of one part of the mark if a deep deficiency (& t;=8/20) is found for the other. Chapters 1 and 4-8 : The exercice part of the exam is written, open book (only the text book used for the course can be used) and counts for 20% of the mark. The theoretical exam is either written or with a written preparation and oral defense/discussion. The miniproject counts for 20% of the total mark and is evaluated based on the group report. Chapters 2 and 3 : Written exam only. The project counts for 1/3 of the mark.
Teaching methods :	The physical concepts and theory are explained in the theoretical sessions. The students are encouraged to ask questions. At the beginning of each theoretical course, the course is placed into context and an overview of what will be studied is given. At the end of each theoretical session, the content is summarized and placed into context again. A session with exercises (or project) follows each theoretical session to practice the theory. The exercises focus where possible on practical problems. In preparation of the exam, a question-answer and discussion session on the content of the course is foreseen.
Content :	Chapter 1: Elements of Reaction Kinetics Chapter 2: Kinetics of free radical chain reactions Chapter 3: Diffusion and chemical kinetics Chapter 4 - Part I: Kinetics of Heterogeneous Catalytic Reactions Chapter 4 - Part II: Kinetic modeling of heterogeneous catalytic reactions Chapter 5 - Part I: Transport Processes with Reactions Catalyzed by Solids - Interfacial Gradient Effects Chapter 6: Noncatalytic Gas-Solid Reactions Chapter 7: Catalyst Deactivation Chapter 8: Gas-Liquid Reactions
Bibliography :	For chapters 1 and 4 to 8: Text book: "Chemical Reactor Analysis and Design" by G.F. Froment, K.B. Bischoff, and J. De Wilde, 3th ed., Wiley, 2010. The book can be purchased via Libris-Agora, Louvain-la-Neuve or directly via the web. Some copies of the book are available in the BSE library. For chapters 1, 2, 3 and 5: Slides and documents available on icampus.
Other infos :	In EPL/FYKI, this course is a prerequisite for the course "Chemical Reactor Analysis and Design" (MAPR2330).
Cycle and year of study :	> Bachelor in Engineering
Faculty or entity in charge:	FYKI