

Teacher(s)	De Wilde Juray ;Mignon Denis ;
Language :	French
Place of the course	Louvain-la-Neuve
Prerequisites	This course assumes that the following notions have been acquired : <ul style="list-style-type: none"> <li>• quantitative chemistry (thermodynamics and kinetics), such as taught in course LEPL1302;</li> <li>• organic chemistry, such as taught in course LMAPR1230.</li> </ul>
Main themes	<p><b>Part I : Chemical and Physical Kinetics</b></p> <p>Chapter 1: Elements of Reaction Kinetics &amp; Kinetics of Free Radical Chain Reactions</p> <p>Chapter 2: Kinetics of Heterogeneous Catalytic Reactions</p> <p>Chapter 3: Transport Processes with Reactions Catalyzed by Solids - Interfacial Transfers &amp; Intraparticle Transport</p> <p>Chapter 4: Noncatalytic Gas-Solid Reactions</p> <p>Chapter 5: Catalyst Deactivation</p> <p>Chapter 6: Gas-Liquid Reactions</p> <p><b>Part II : Chemical Thermodynamics and Phases Equilibria</b></p> <p>Chapter 1: Phases Equilibria – Real Systems with one or more Components</p> <p>Chapter 2: Practical Applications of Phases Equilibria – Introduction to Chemical Engineering</p>
Learning outcomes	<p><b>At the end of this learning unit, the student is able to :</b></p> <p>Referring to the Learning Outcomes (LOs) referential of the “Civil engineering bachelor's degree” the following LOs are aimed at:</p> <ul style="list-style-type: none"> <li>• Axis 1: 1.1, 1.2, 1.3</li> <li>• Axis 2: 2.2, 2.3, 2.4, 2.5, 2.6, 2.7</li> <li>• Axis 5 : 5.3, 5.4 ,5.5</li> </ul> <p><b>Specific learning outcomes of the course</b></p> <p><b>After successfully completing this course, the student will be able to :</b></p> <p><b>Chapter I.1: Elements of Reaction Kinetics &amp; Kinetics of Free Radical Chain Reactions</b></p> <ul style="list-style-type: none"> <li>• Define the issues involved and the methodology used in the kinetic modeling of chemical reactions.</li> <li>• Define reaction rates and rate expressions.</li> <li>• Explain the basis of collision theory and activated complex theory</li> <li>• Calculate the activation energy of a chemical reaction.</li> <li>• Model complex reactions and reaction networks and reduce the size of a kinetic model and the number of independent rate parameters.</li> <li>• Explain the elementary steps of free radical reactions and extract the corresponding kinetics.</li> <li>• Explain kinetic expressions for the following important examples : thermal cracking of ethane and homogenous radical polymerization,</li> <li>1 • For free radical polymerization, explain the molar mass distribution and the influence of molecular diffusion on polymerization kinetics.</li> <li>• Calculate reaction kinetics based on mechanism for similar cases as seen during exercise sessions.</li> </ul> <p><b>Chapter I.2: Kinetics of Heterogeneous Catalytic Reactions</b></p> <ul style="list-style-type: none"> <li>• Define the different steps involved in heterogeneous catalytic reactions.</li> <li>• Make a distinction between ideal and non-ideal adsorption on a catalyst.</li> <li>• Derive Hougen-Watson and Eley-Rideal type rate equations for single and coupled reactions.</li> <li>• Deal with complex catalytic reactions, in particular to generate the reaction network and to reduce the number of independent rate parameters.</li> <li>• Design experimental reactors required for the kinetic modeling of heterogeneous catalytic reactions.</li> <li>• Discriminate between kinetic models and to estimate the rate parameters.</li> <li>• Design experiments in a sequential way, for optimal discrimination between kinetic models or for optimal parameter estimation.</li> </ul> <p><b>Chapter I.3: Transport Processes with Reactions Catalyzed by Solids - Intraparticle gradient effects</b></p> <ul style="list-style-type: none"> <li>• Derive Fick's law for a perfect gas with the help of simplified model ; make the link to Fourier's law.</li> <li>• Derive the diffusion equation (second Fick's law) from microscopic and macroscopic arguments.</li> <li>• Describe multi-component diffusion in a fluid</li> </ul>

- Explain diffusional control of chemical reactions and its practical importance.
- Describe the reaction of a component of a fluid at the surface of a solid.
- Model interfacial mass and heat transfer.
- Calculate the concentration or partial pressure and temperature differences between a bulk fluid and a surface of a catalyst particle.
- Define and characterize molecular, Knudsen, and surface diffusion in pores.
- Describe diffusion in a catalyst particle by means of a pseudo-continuum model.
- Define the effective diffusivity in a catalyst and the tortuosity of a catalyst, as well as methods to experimentally determine them.
- Give an overview of more fundamental approaches to describe diffusion in a catalyst particle (structure & network models, Molecular Dynamics and Dynamic Monte-Carlo simulations).
- Describe diffusion and reaction in a catalyst particle by means of a continuum model.
- Define and calculate the modulus and the effectiveness factor of a catalyst for a given reaction.
- Identify some major effects of intraparticle diffusion limitations, in particular in falsifying rate coefficients and activation energies and changing the selectivities of coupled reactions.
- Define criteria to evaluate the importance of intraparticle diffusion limitations.

#### Chapter I.4: Noncatalytic Gas-Solid Reactions

- Give a qualitative discussion of gas-solid reactions and their kinetic modeling.

#### Chapter I.5: Catalyst Deactivation

- Define and characterize the major types of catalyst deactivation: solid-state transformations, poisoning, and coking.
- Model the kinetics of uniform catalyst poisoning.
- Model the kinetics of catalyst deactivation by coke formation.
- Define deactivation functions.
- Describe catalyst deactivation by site coverage only and by site coverage and pore blockage.
- Describe the effect of intraparticle diffusion limitations on the deactivation of a catalyst by site coverage and pore blockage.
- Give an overview of the methods used for the kinetic analysis of catalyst deactivation by coke formation.

#### Chapter I.6: Gas-Liquid Reactions

- Give a qualitative discussion of gas-liquid reactions and their kinetic modeling.
- Derive and apply the two-film theory and the surface-renewal theory.



#### Chapter II.1: Phases Equilibria – Real Systems with one or more Components

- Describe qualitatively the shape of  $(h,P)$  diagrams of a pure substance and give examples illustrating their usefulness in solving some practical problems encountered in the process industry.
- Define the concept of fugacity, discuss its utility and give a physical interpretation thereof. Show how the fugacity coefficient of a gas can be computed from a measurable value, namely the compressibility factor of this gas.
- Give the shape of the variation of a real gas compressibility and justify this shape on a physical basis.
- Justify the theory of van der Waals according to which the ideal gas equation can be corrected by two parameters in order to take into account the interactions between the molecules contained in the system. Show how these two parameters can be identified.
- Demonstrate how the vapor pressure of a liquid at a given temperature can be derived from the shape of the curve describing the variation of pressure as a function of the molar volume, as expressed by the van der Waals equation.
- Explain the concept and the usefulness of the « equilibrium ratio »  $K$  in the context of problems involving vapor and/or liquid phases at equilibrium.
- Derive expressions of the « equilibrium ratio »  $K$  in terms of fugacity coefficients and activity coefficients.
- Explain how equations of state derived from the van der Waals equation (e.g., Soave-Redlich-Kwong or Peng-Robinson) are used in order to compute thermodynamics properties of vapor-liquid mixtures at equilibrium, in particular the equilibrium ratios  $K$ .
- Explain how correlations for the computation of liquid phase activity coefficients (e.g. Wilson, NRTL, UNIQUAC or UNIFAC) are used in order to compute thermodynamics properties of vapor-liquid mixtures at equilibrium, in particular the equilibrium ratios  $K$ , of non-ideal vapor-liquid mixtures at equilibrium.

#### Chapter II.2: Practical Applications of Phases Equilibria – Introduction to Chemical Engineering

- Explain how to determine which type of thermodynamic model should be used in a practical problem, based on the nature of the present substances and the temperatures-pressures domain being considered.
- Explain the operation principle of a multistage distillation column and explain how the presence of an azeotrope can influence the purity of the distillate and of the residue.
- Explain which are the important operating parameters, which influence the operation of a distillation column and how such an equipment can be controlled in practice.
- Explain the use of multistage distillation in the case of crude oil refining. Also explain which approach is used in process simulation for this operation and which are the operating parameters enabling to control it.
- Explain the principle of liquid-liquid extraction, its usefulness in separation operations and how to choose a good extraction solvent. Enumerate the equipment types used to implement this operation.

	<ul style="list-style-type: none"> <li>• Explain the elements characterizing the worldwide demand for crude oil and refined products, as well as its past and future historical evolution.</li> <li>• Describe the notion of « refining margin », how it is computed and the parameters that influence it.</li> </ul>
Evaluation methods	<p>At the examination, students are evaluated individually according to in advance explained rules. Intermediate interrogation(s) on part(s) of the course is/are possible. Some reports on projects or exercises can be marked and the mark included in the final examination mark.</p> <p>The part taught by each teacher normally counts for a half of the total mark, unless specified otherwise during the course. However, if a deep deficiency (<math>\leq 8/20</math>) is found for one part of the course, the total mark will represent a failure at the examination and be reduced to 8/20 as a maximum.</p>
Teaching methods	<p>The physical concepts and theory are explained in the theoretical sessions. A session with practical exercises (or potentially a project) follows each theoretical session to practice the theory. The exercises focus where possible on practical problems. For the preparation of the examination, a questions-answers session is foreseen, with discussion of the course contents.</p> <p>The exercises related to Part I will be based on the use of a process simulator (ASPEN+) enabling to place the theoretical notions, which have been studied, in a perspective as close as possible to the industrial reality.</p>
Content	<p>Part I : Chemical Thermodynamics and Phases Equilibria</p> <p>Chapter 1: Phases Equilibria – Real Systems with one or more Components</p> <p>Chapter 2: Practical Applications of Phases Equilibria - Introduction to Chemical Engineering</p> <p>Chapter 3 : Introduction to the Refining Industry</p> <p>Part II : Chemical and Physical Kinetics</p> <p>Chapter 1: Elements of Reaction Kinetics &amp; Kinetics of Free Radical Chain Reactions</p> <p>Chapter 2: Kinetics of Heterogeneous Catalytic Reactions</p> <p>Chapter 3: Transport Processes with Reactions Catalyzed by Solids - Interfacial Transfers &amp; Intraparticle Transport</p> <p>Chapter 4: Noncatalytic Gas-Solid Reactions</p> <p>Chapter 5: Catalyst Deactivation</p> <p>Chapter 6: Gas-Liquid Reactions</p>
Inline resources	<p>&gt; <a href="https://moodleuclouvain.be/course/view.php?id=10044">https://moodleuclouvain.be/course/view.php?id=10044</a></p>
Bibliography	<p>Pour la partie I:</p> <ul style="list-style-type: none"> <li>• Copie des supports de présentation disponible sur Moodle.</li> <li>• Chapitre 2 du livre : Separation Process Principles, Third Edition, Henley, Seader and Roper, Editeur John Wiley &amp; Sons, 2011, ISBN-13: 978-0470646113.</li> </ul> <p>Pour la partie II:</p> <ul style="list-style-type: none"> <li>• Livre: "Chemical Reactor Analysis and Design" by G.F. Froment, K.B. Bischoff, and J. De Wilde, 3th ed., Wiley, 2010. Le livre peut être acheté à la librairie Libris-Agora à Louvain-la-Neuve ou directement via le web. Quelques exemplaires du livre sont disponibles dans la bibliothèque ESB.</li> <li>• Syllabus / transparents disponibles sur Moodle</li> </ul> <hr/> <p>For Part I:</p> <ul style="list-style-type: none"> <li>• Copy of presentation material available on Moodle.</li> <li>• Chapter 2 of book : Separation Process Principles, Third Edition, Henley, Seader and Roper, Editor John Wiley &amp; Sons, 2011, ISBN-13: 978-0470646113.</li> </ul> <p>For Part II:</p> <ul style="list-style-type: none"> <li>• 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 in Louvain-la-Neuve or directly via the web. Some copies of the book are available in the BSE library..</li> <li>• Slides and documents available on Moodle</li> </ul>
Other infos	<p>In EPL/FYKI, this course is a prerequisite for the courses "Chemical Reactor Analysis and Design" (LMAPR2330), as well as "Fluid-fluid separations" (LMAPR2118).</p> <p>Prerequisites for taking LMAPR1400:</p> <p>This course assumes that the following notions have been acquired :</p> <ul style="list-style-type: none"> <li>• quantitative chemistry (thermodynamics and kinetics), such as taught in course LEPL1302;</li> <li>• organic chemistry, such as taught in course LMAPR1230.</li> </ul>
Faculty or entity in charge	<p>FYKI</p>

<b>Programmes containing this learning unit (UE)</b>				
Program title	Acronym	Credits	Prerequisite	Learning outcomes
Minor in Applied Chemistry and Physics	MINOFYKI	5		
Specialization track in applied Chemistry and Physics	FILFYKI	5		
Mineure Polytechnique	MINPOLY	5		