UCLouvain

lfyki1303

2026

Chemical Engineering : Thermodynamics and Kinetics

5.00 credits	30.0 h + 30.0 h	Q2

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 : • Quantitative chemistry (thermodynamics and kinetics), such as taught in course **LEPL1302**; • Organic chemistry, such as taught in course **LFYKI1203**.
Main themes	**Part I : Chemical Thermodynamics and Phases Equilibria** Chapter 1: Practical Applications of Phases Equilibria – Introduction to Chemical Engineering Chapter 2: Equilibre des phases - Systèmes réels à un ou plusieurs constituants Chapter 3: Introduction à l'industrie du raffinage **Part II : Chemical and Physical Kinetics** Chapter 1: Elements of Reaction Kinetics & Kinetics of Complex Reactions Chapter 2: Kinetics of Heterogeneous Catalytic Reactions Chapter 3: Transport Processes with Reactions Catalyzed by Solids - Interfacial Transfers & Intraparticle Transport Chapter 4: Noncatalytic Gas-Solid Reactions Chapter 5: Catalyst Deactivation Chapter 6: Gas-Liquid Reactions
Learning outcomes	**At the end of this learning unit, the student is able to :** **Contribution of the course to the program referential** Referring to the Learning Outcomes (LOs) referential of the "Civil engineering bachelor's degree" the following LOs are aimed at: • Axis 1: AA1.1, AA1.2 • Axis 2: AA2.2, AA 2.3, AA 2.4, AA 2.5, AA 2.6, AA 2.7 • Axis 4 : AA 4.2, AA 4.3, AA 4.4 **Specific learning outcomes of the course** **After successfully completing this course, the student will be able to :** • Model a basic process in the Aspen+ simulator, choose the appropriate thermodynamic method, optimize certain process parameters and critically analyze the results. **Chapter I.1: 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 temperature-pressure 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. **Chapter I.2: 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 I.3: Introduction to the Refining Industry

- Explain the elements characterizing the worldwide demand for crude oil and refined products, as well as its past and future historical evolution.
- Describe the notion of « refining margin », how it is computed and the parameters that influence it.

Chapter II.1: Elements of Reaction Kinetics

- Description of the kinetics of complex reactions and methods for reducing the complexity of kinetic models.

Chapter II.2: Heterogeneous Catalysis

- Different steps in a heterogeneous catalytic reaction, chemisorption, elementary steps in heterogeneous catalytic reactions, Hougen-Watson Langmuir-Hinshelwood and Eley-Rideal approach for deriving rate expressions based on rate-determining steps, methodologies for kinetic modeling, introduction to advanced methods.

Chapter II.3-I: Interfacial Mass and Heat Transfer

- Effect on observed reaction rates, transfer coefficient concept, modeling of the mass and heat transfer coefficient, criteria for evaluating the importance of interfacial transfer limitations.

Chapter II.3-II: Intra-Particle Transport

- Effect on observed reaction rates, porous properties of catalytic particles, continuum description of a catalytic particle and the concepts of porosity, tortuosity, and effective diffusivity, experimental methods to determine porosity and tortuosity of catalysts, types of diffusion, modeling diffusion-reaction within the catalyst and calculating concentration profiles, Thiele modulus concept and effectiveness factor, generalized Thiele modulus concept, criteria for evaluating the importance of intra-particle diffusion limitations.

Chapter II.4: Introduction to Fluid-Particle Reactions

- Modeling approaches.

Chapter II.5: Catalyst Deactivation

- Different types of deactivation, catalyst poisoning and modeling approach, coke formation and modeling approaches.

Chapter II.6: Gas-Liquid Reactions

- Transport phenomena, two-film diffusion-reaction model, examples of concentration profile calculations within films for simple reactions and for the general case, Hatta number concept.

Evaluation methods

At the examination, students are evaluated individually according to in advance explained rules. Intermediate dispensatory interrogation(s) on part(s) of the course is/are possible.

For Part I, a small-scale process simulation project is rated and incorporated into the final examination mark. Some reports on projects or exercises can be marked and the mark included in the final examination mark.

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 (<=8/20) 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.

Teaching methods

The physical concepts and theory are explained in the theoretical sessions.

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.

For part II, 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.

Content

Part I : Chemical Thermodynamics and Phases Equilibria

Chapter 1: Practical Applications of Phases Equilibria – Introduction to Chemical Engineering

Chapter 2: Equilibre des phases - Systèmes réels à un ou plusieurs constituants

Chapter 3: Introduction à l'industrie du raffinage

	Part II : Chemical and Physical Kinetics Chapter 1: Elements of Reaction Kinetics & Kinetics of Complex Reactions Chapter 2: Kinetics of Heterogeneous Catalytic Reactions Chapter 3: Transport Processes with Reactions Catalyzed by Solids - Interfacial Transfers & Intraparticle Transport Chapter 4: Noncatalytic Gas-Solid Reactions Chapter 5: Catalyst Deactivation Chapter 6: Gas-Liquid Reactions
Inline resources	To be defined
Bibliography	Pour la partie I: • Chapitre 2 du livre : Separation Process Principles, Third Edition, Henley, Seader and Roper, Editeur John Wiley & Sons, 2011, ISBN-13: 978-0470646113. Pour la partie II: • 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 BSE. ______________ For Part I: • Chapter 2 of book “Separation Process Principles”, Third Edition, Henley, Seader and Roper, Editor John Wiley & Sons, 2011, ISBN-13: 978-0470646113. For Part II: • Book "Chemical Reactor Analysis and Design" by G.F. Froment, K.B. Bischoff, and J. De Wilde, 3rd 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.
Other infos	In EPL/FYKI, this course is a prerequisite for the courses "Chemical Reactor Analysis and Design" (**LMAPR2330**), as well as “Fluid-fluid separations” (**LMAPR2118**).
Faculty or entity in charge	FYKI

Programmes containing this learning unit (UE)

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		