UCLouvain

lmapr2330 — Reactor Design

2023

5.00 credits	30.0 h + 30.0 h	Q2

Teacher(s)	De Wilde Juray ;
Language :	English > French-friendly
Place of the course	Louvain-la-Neuve
Main themes	The different types of chemical reactors and their modeling are addressed

Learning outcomes

At the end of this learning unit, the student is able to :

Contribution of the course to the program objectives

Referring to the LOs of the KIMA diploma, the following LOs are aimed at:

- Axe 1: 1.1, 1.2, 1.3;
- Axe 2: 2.2, 2.4, 2.5;
- Axe 3: 3.2;
- Axe 4: 4.1, 4.4;
- Axe 5: 5.3, 5.5, 5.6;
- Axe 6: 6.1, 6.3.

Specific learning outcomes of the course

a. Scientific / Engineering

(Reference is made to the chapters and sections of the text book that is used - see below.)

Chapter 7: The Modeling of Chemical Reactors

After successfully completing this course, the student will be able to :

- Describe the different aspects of mass, heat and momentum balances.
- Derive the fundamental continuity equations for species and energy, both in the general form and in specific simplified forms.

Chapter 8: The Batch and Semibatch Reactors

After successfully completing this course, the student will be able to :

- Derive the continuity equations for isothermal and nonisothermal batch reactors.
- Use the continuity equations for isothermal and nonisothermal batch reactors for reactor simulation and design.
- Explain different optimal operation policies and control strategies.

1

Chapter 9: The Plug Flow Reactor

After successfully completing this course, the student will be able to :

- Derive the continuity equations for adiabatic and nonadiabatic, isothermal and nonisothermal plug flow reactors.
- Use the continuity equations for plug flow reactors for reactor simulation and design.

Chapter 10: The Perfectly Mixed Flow Reactor

After successfully completing this course, the student will be able to :

- Derive the mass and energy balances of a perfectly mixed flow reactor.
- Use the mass and energy balances for reactor simulation and design.
- Make a choice between a plug flow reactor and a completely mixed flow reactor for a given application based on different criteria (conversion, selectivity, heat of reaction, etc..).
- Analyze the stability of a perfectly mixed flow reactor and study the eventual transient behavior.

Chapter 11: Fixed Bed Catalytic Reactors

PART ONE INTRODUCTION

After successfully completing this course, the student will be able to :

- Describe the different types of fixed bed reactors.
- Describe some of the important applications of fixed bed reactors.
- Describe and apply the different factors involved in the preliminary design of fixed bed reactors.
- Describe the different types of models that are used for the simulation and design of fixed bed reactors and their assumptions.

PART TWO PSEUDOHOMOGENEOUS MODELS

After successfully completing this course, the student will be able to :

- Derive the basic one-dimensional model for fixed bed reactors.
- Apply the basic one-dimensional model for the simulation and design of fixed bed reactors.
- Describe runaway in a fixed bed reactor.
- Explain the use of a multibed adiabatic reactor and the way to calculate the number of beds required (including the graphical method) and their size.
- Explain the use of a multitubular reactor and the way to calculate its size, the number of tubes, and the temperature of the heat exchanging medium.
- Derive the model equations for the case of a fixed bed reactor with heat exchange between the feed and effluent or between the feed and reacting gas.
- Describe autothermal operation.
- Describe the phenomenon of catalyst deactivation and the related nonsteady-state behavior of fixed bed reactors.
- Explain the use of a one-dimensional model with axial mixing and derive the model equations.
- Explain the use of two-dimensional pseudohomogeneous models for fixed bed reactors.

PART THREE HETEROGENEOUS MODELS

After successfully completing this course, the student will be able to :

- Derive the one-dimensional model for fixed bed reactors that allows accounting for interfacial gradients and to apply this model for reactor simulation and design.
- Derive the one-dimensional model for fixed bed reactors that allows accounting for interfacial and intraparticle gradients and to apply this model for reactor simulation and design.

Chapter 12: Complex Flow Patterns

After successfully completing this course, the student will be able to :

- Explain macro- and micro-mixing in reactors.
- Qualitatively explain the different types of models explicitly accounting for mixing.
- Explain the concept, potential and limitations of residence time distribution (RTD) methods.
- Calculate the RTD of a perfectly mixed vessel.
- Experimentally determine the RTD of a reactor.
- Derive information on the flow pattern from the RTD.
- Derive the RTD for series of n completely stirred tanks.
- Apply the RTD to the simulation and design of reactors, with direct application to

* First order reaction(s) in isothermal completely mixed reactors, plug flow reactors, and series of completely stirred tanks.

* Second order bimolecular reaction in isothermal completely mixed reactors and in a succession of isothermal plug flow and completely mixed reactors: completely macro-mixed versus completely macro- and micro-mixed.

- Describe the concept of multi-zone models.
- Describe the concept of axial dispersion and tanks-in-series models and to derive and apply the continuity equations.

Chapter 13: Fluidized Bed and Transport Reactors

After successfully completing this course, the student will be able to :

- Describe the technological aspects of fluidized bed and riser reactors.
- Describe the most important applications of fluidized bed reactors.
- Describe the most important features of the fluidization and transport of solids.
- Define and model heat transfer in fluidized beds.
- Derive the two-phase model for fluidized bed reactors.
- Derive the basic model for a transport or riser reactor.
- Apply the fluidized bed and riser reactor models for reactor simulation and design.

Chapter 14: Multiphase Flow Reactors

After successfully completing this course, the student will be able to :

- Describe the different types of multiphase flow reactors:

* Packed columns

* Plate columns

* Empty columns

* Stirred vessel reactors

* Miscellaneous reactors.

- Describe (including their assumptions), derive and apply the most frequently used design models for multiphase flow reactors:

* Gas and liquid phases completely mixed

* Gas and liquid phase in plug flow

	* Gas phase in plug flow. Liquid phase completely mixed. b. Other / Transversal After successfully completing this course, the student will be able to : • Look up scientific and technical information in a text book. • Report a technical study in a scientific and concise way (mini-project "Methane steam reforming: reactor simulation and sensitivity study"). • Work in small groups. • Be critical and ask questions. • Verify the units of the different variables and terms appearing in mathematical equations. • To use a corpus of scientific and technical knowledge, allowing to solve given problems in the discipline studied. • To analyze, organize and develop an engineering approach for process development responding to specific needs or a given problem, the analysis of a given physical phenomenon or a system. • To contribute, as a team member, to the realization of a project with a given discipline or multiple disciplines according to a well described approach. • To efficiently communicate by writing and presentation, in English or French, the results of a well-defined project. • To show a rigorous behavior and critical thinking in carrying out scientific or technical tasks with respect for ethical issues.
Evaluation methods	The students are evaluated individually. The demands will be specified explicitly in advance of the exam. The exam consists of a theoretical part and an exercise. The latter is open book (only the text book used for the course can be used) and counts for 20% of the marks. The theoretical exam is with a written preparation and oral defense/discussion. The exercise is written. Evaluation of the mini-project One mini-project on the simulation of a methane steam reforming reactor, including a parametric sensitivity study, is evaluated. It counts for 10% of the marks.
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 follows each theoretical session to practice the theory. The exercises focus where possible on practical problems. One mini-project "3D simulation of a cold-shot type cooling in a fixed bed ammonia synthesis reactor" aims at familiarizing the students with CFD (Computational Fluid Dynamics) type simulation models and different important aspects, such as the modeling of turbulence, boundary conditions, the required grid independency of the results, the interpretation of the results, etc.. In groups of 2-3, the students have to propose their own design of a cold shot cooling system and to evaluate its performance in terms of cooling and temperature uniformity. Besides the development of technical skills, the project aims at teaching the students to work in group and how to report a technical study in a scientific and clear way. One mini-project "Methane steam reforming: reactor simulation and sensitivity study" allows the students to apply a reactor model with detailed reaction kinetics and accounting for intraparticle diffusion limitations to design a commercial steam reformer. Furthermore, the sensitivity of the reactor performance to a number of variables is studied. Apart from developing the technical skills of the students, the mini-project also aims at teaching the students how to work in group (of 2-3) and how to report a typical technical study in a scientific and concise way, both in writing and orally in front of an audience. Lab sessions on fixed bed and fluidized bed reactors are foreseen. They aim at familiarizing the students with these two of the most important reactor technologies and at carrying out measurements of the hydrodynamic behavior and confronting the experimental data with theoretical correlations. In preparation of the exam, a question-answer and discussion session on the content of the course is foreseen.
Content	• The modeling of chemical reactors; • The batch and semibatch reactors; • The plug flow reactor; • The perfectly mixed flow reactor; • Complex flow patterns; • Fixed bed catalytic reactors; • Fluidized bed and transport reactors; • Multiphase flow reactors.
Inline resources	https://moodleucl.uclouvain.be/course/view.php?id=10045
Bibliography	Livre: "Chemical Reactor Analysis and Design" par G.F. Froment, K.B. Bischoff, and J. De Wilde, 3ème edition. Wiley, 2010. Le livre peut être acheté via la librairie Libris-Agora à Louvain-la-Neuve ou directement via le web. Quelques exemplaires du livre sont disponibles dans la bibliothèque BSE.

Other infos	Particular attention is paid to the units of the different variables and terms appearing in the mathematical equations in the course. It is highly reommended to have background in : • Mathematics (Analysis), • Chemistry (basis), • Transport phenomena, • Reaction kinetics
Faculty or entity in charge	FYKI

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Learning outcomes
Master [120] in Chemical and Materials Engineering	KIMA2M	5		🔍
Master [120] in Biomedical Engineering	GBIO2M	5		🔍