Course Unit	Advanced Chemical Reaction Engineering	Field of study	Chemical Enginnering Processes
Master in	Chemical Engineering	School	School of Technology and Management
Academic Year	2023/2024	Year of study	1
Level	2-1	ECTS credits	6.0
Type	Semestral	Semester	1
Code	6362-756-1102-00-23		

Workload (hours)	Contact hours	T	TP	PL	TC	S	E	OT	O
162		30	-	30	-	-	-	-	-

T - Lectures; TP - Lectures and problem-solving; PL - Problem-solving, project or laboratory; TC - Fieldwork; S - Seminar; E - Placement; OT - Tutorial; O - Other

Name(s) of lecturer(s)	Maria Olga de Amorim Sá Ferreira

Learning outcomes and competences

At the end of the course unit the learner is expected to be able to:
1. Characterize the flow in real reactors: Apply the residence time distribution theory. Understand the concepts of earliness of mixing, segregation and micro/macrofluid.
2. Model the flow and design the behaviour of real reactors by applying flow models based on the association of ideal reactors, the dispersion model, the tanks-in-series model and the laminar flow model.
3. Analyse and design catalytic reactions and reactors: Evaluate situations of pore diffusion, film diffusion and reaction in catalysts and its effects on the performance of the catalytic reactor.
4. Analyse and design non-catalytic heterogeneous reactions: Identify the shell-progressive and shrinking-core models. Design reactors in chemical, external diffusion and internal diffusion regimes.

Prerequisites

Before the course unit the learner is expected to be able to:
1. Know the fundamentals of the basic sciences of chemical engineering and engineering sciences.
2. Establish material and energy balances and the design of ideal reactors.
3. Use informatics tools for engineering calculations (MSExcel, MATLAB).

Course contents

Flow modelling and characterization and design of real reactors. Residence time distribution theory (RTD). Prediction of conversion in real reactors. Fundamentals in heterogeneous catalysis and characterization of catalysts. Analysis and design of catalytic reactions and reactors. Analysis and design of non-catalytic heterogeneous reactions and reactors.

Course contents (extended version)

1. Real reactors: Residence-time distribution.
   - Introduction to the study of real reactors. Non-ideal flow. Residence-time distribution.
   - Pulse and step tracer experiments: E(t) and F(t) curves. Relation between E(t) and F(t) curves.
   - Transfer function concept, G(s). Transfer functions of ideal flow reactors.
   - Relation between G(s), E(t) and F(t). Moment-generating function.
   - Conversion in real reactors. Earliness and lateness of mixing.
   - State of aggregation.
2. Real reactors: Compartment models.
   - Real reactors representation through compartment models.
   - Active and dead volumes. Active, by-pass and recycle flows.
   - Representation of several compartment models and the correspondent E(t) and F(t) curves.
   - Diagnosis of real reactors behaviour.
3. Real reactors: The dispersion model
   - Convection versus axial dispersion. Peclet number.
   - Plug diffusion reactor material balance.
   - Transfer function, RTD and moments for a dispersion reactor.
   - Axial dispersion and chemical reaction. Analytical solution for a 1st order irreversible reaction.
   - Correlations for axial dispersion in tubes and packed beds.
4. Real reactors: Tanks-in-series model.
   - Material balance equation. Transfer function, RTD and moments of the tank-in-series model.
   - Comparison between the dispersion model and the tanks-in-series model.
   - Chemical reaction in a tank-in-series cascade.
5. Real reactors: Laminar flow model.
   - Laminar flow model with a parabolic velocity profile. RTD for a laminar flow model.
   - Chemical reaction in laminar flow reactors.
6. Catalytic reactions: Reactions catalysed by solids.
   - Introduction to heterogeneous reactions.
   - Chemical reaction versus pore diffusion resistance. Thiele modulus.
   - Catalyst efficiency. Catalyst particles: slab, cylinder and sphere geometries.
   - Exothermic reaction with pore diffusion and heat conduction.
   - Chemical reaction with pore diffusion and external diffusion (at the film).
7. Non-catalytic reactions: Fluid-solid non-catalytic reactions.
   - Fluid-solid reaction kinetics.
   - Shell-progressive and shrinking-core models.
   - Chemical reaction, film diffusion and ash diffusion regimes.
   - Non-catalytic heterogeneous reactors design.

Recommended reading

1. Scott Fogler, Elements of Chemical Reaction Engineering, 6th Edition, Pearson, 2021.
2. Gilbert Froment and Kenneth Bischoff, Chemical Reactor Analysis and Design, 3rd Edition, John Wiley&Sons, 2010.
3. Octave Levenspiel, Chemical Reaction Engineering, 3rd Edition, John Wiley&Sons, 1999.
4. Online Resources developed by H. Scott Fogler associated to "Elements of Chemical Reaction Engineering (2020)": http: //websites. umich. edu/~elements/5e/index. html
5. J. L. Figueiredo e F. Ramôa Ribeiro, Catálise Heterogénea, 2ª edição Fundação Calouste Gulbenkian, 2007.

Teaching and learning methods

Theoretical explanation of concepts and techniques of analysis and design of real reactors and heterogeneous reactions: analysis and discussion of application

Teaching and learning methods

examples. Independent study and homework exercises, using MS Excel or MATLAB. Application work in the chemical reaction engineering area, assessed and carried out in collaboration with the curricular unit of Applied Mathematics.

Assessment methods

1. Alternative 1 - (Regular, Student Worker) (Final)
   - Intermediate Written Test - 36% (Chapters 1 to 5.)
   - Intermediate Written Test - 54% (Chapters 6 and 7.)
   - Projects - 10% (Presentations and case studies about Chapters 6 and 7.)
2. Alternative 2 - (Regular, Student Worker) (Final, Supplementary, Special)
   - Final Written Exam - 100%

Language of instruction

English

Electronic validation

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04-10-2023	25-10-2023	25-10-2023	31-10-2023