CH281-15 Chemical Reaction Engineering and Data Analysis

25/26

Department
Chemistry
Level
Undergraduate Level 2
Module leader
Stefan Bon
Credit value
15
Module duration
10 weeks
Assessment
Multiple
Study location
University of Warwick main campus, Coventry

Description

Introductory description

Chemical Reaction Engineering and Data Analysis will familiarise students with the science and engineering concepts needed to transfer chemistry reactions from a university lab to an industrial setting. The module focuses on two integrated parts: reactor scale-up (an introduction to chemical reaction engineering) and data processing and analysis (NLLS parametric regression to a specific model with a set of parameters, and Fourier transformations and analysis). Beside the specific scientific concepts, the module will introduce and build the mathematical skills required to be able to comprehend the material. At the same time, we will teach students using Python as a mathematical and coding tool.

This module will be taught over 10 weeks across 30 peer instruction sessions (30 hours). The core material will be supported with worked-out example problem sets. The interactive lecture sessions will enhance more profound learning and develop a thorough understanding of the material. Students will be divided into teams for each session to discuss tasks and contribute to the delivered material using interactive methods, such as Vevox.

Class participation is stimulated by setting weekly homework assignments. These are part of the formative assessment of the module. A 20% summative assessment in the form of a homework problem set is given (1 question per block, provided during the teaching of each block: 5 questions

in total to be handed in as one complete set after the module has been taught). The remaining 80% is in the form of a written individual exam.

Module aims

This module aims to provide a rigorous foundation of industrial scale-up (chemical reaction engineering) and data processing concepts. It is one of three optional modules for year 2 UG Chemistry students.
The aims are to:
(1) gain a deep understanding of the scientific ideas and concepts associated with chemical reaction engineering and data analysis.
(2) gain a deep understanding of the underlying mathematics.
(2) Apply the gained knowledge in a discussion format to discuss illustrative examples of industrial processes to improve learning.
(3) Apply the knowledge gained to a broader scientific context, linking it to chemistry, chemical engineering, physics, and manufacturing principles.
(4) Develop a skill set to critically process, understand, and communicate/explain scientific principles and phenomena in chemical reaction engineering and data handling.

Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

This module consists of 5 parts. Note that underlying mathematical concepts will be taught at the points needed.

Block 1 (4 interactive lectures + 2 workshops): Basic Chemical Reaction Engineering Concepts

(1) Mass balance, the batch, semi-batch, and flow (CSTR, PFR, PBR) reactors.
(2) Extent of reaction/conversion, recap rate laws and reaction stoichiometry (kinetics). Extension of reaction kinetics.
(3) Residence time distributions in flow reactors.
(4) Reactor sizing.
(5) (2 h) Implement what we have learned thus far.

Block 2: (4 interactive lectures + 2 workshops) Isothermal Reactor Design

(1) Examples of reactions in batch, semi-batch, and a CSTR.
(2) Examples of reactions in CSTR and tubular setups.
(3) Extension to multiple reactor systems (series, parallel).
(4) Examples of complex reactions (such as parallel, reversible, autocatalytic).
(5) (2 h) Implement what we have learned thus far.

Block 3. (4 interactive lectures + 2 workshops): Catalysis and Catalytic Reactors

(1) Catalysts and steps in catalytic reactions.
(2) Rate laws, mechanisms, and rate-limiting steps.
(3) Reactor design in heterogeneous catalysis.

(4) Catalyst deactivation and/or diffusion issues.
(5) (2 h) Implement what we have learned thus far.

Block 4. (4 interactive lectures + 2 workshops): Data Processing I

(1) Uncertainty in data, errors, and error space.
(2) How to carry out NLLS regression, part 1 with examples.
(3) How to carry out NLLS regression, part 2 with examples.
(4) Practical examples: kinetic modeling.
(5) (2 h) Implement what we have learned thus far.

Block 5. (4 interactive lectures + 2 workshops): Data Processing II

(1) Signals and noise in real analytical data.
(2) Harmonic inversion and the Fourier Transform.
(3) Fourier deconvolution.
(4) Filtering and smoothing, linear and non-linear curve fitting.
(5) (2 h) Implement what we have learned thus far.

Learning outcomes

By the end of the module, students should be able to:

- KNOWLEDGE: The module will provide students with a solid understanding of several fundamental and contemporary aspects of chemical reaction engineering (scale-up), and data analysis. We will discuss basic chemical reaction engineering concepts, isothermal reactor design, catalysis, and catalytic reactions. Data processing by NLLS regression, and Fourier analysis of data. Students will develop specialized knowledge in these areas and integrate this across the broader areas of chemistry, chemical engineering, physics and manufacturing.
- APPLIED LEARNING: This module has active learning activities throughout its delivery and across each block of learning, in which concepts are applied and integrated in an interactive discussion format.
- DIVERSE PERSPECTIVES: Through interactive learning in groups and individual homework sets, students can evaluate diverse points of view embedded within varying frameworks, which may include technological/scientific context, societal and environmental impact, and temporal and trending contexts.
- COMPETENCY SKILLS: Students will engage in critical inquiry and develop their skill set to process, understand, communicate/explain and evaluate scientific principles and their impact.
- COMMUNICATION: Students will be able to communicate effectively in presenting ideas orally (especially in the group-based active learning sessions), and in the format of assessed homework problem sets.
- ETHICAL REASONING: Students can reason ethically when evaluating the design and use of chemical reaction engineering and formulation science principles in modern society and illustrate their learning through the group active learning discussion sessions and homework sets.

Indicative reading list

Reading lists can be found in Talis

Interdisciplinary

This module combines elements from chemistry, physics, engineering, and mathematics.

Subject specific skills

KNOWLEDGE
(See learning outcomes for description)

Transferable skills

APPLIED LEARNING:
DIVERSE PERSPECTIVES:
COMPETENCY SKILLS:
COMMUNICATION:
ETHICAL REASONING:
(See learning outcomes for descriptions.)

Study

Study time

Type	Required
Lectures	20 sessions of 1 hour (13%)
Seminars	10 sessions of 1 hour (7%)
Private study	115 hours (77%)
Assessment	5 hours (3%)
Total	150 hours

Private study description

N/A

Costs

No further costs have been identified for this module.

Assessment

You do not need to pass all assessment components to pass the module.

Assessment group D

	Weighting	Study time	Eligible for self-certification
Take home problem set.	20%	5 hours	Yes (extension)
Throughout the module you will be given 5 short problems to solve, one for each block. You are asked to submit the answers as one set after the module has been taught. These count for 20% of the module mark. Note that in case of a resit, the exam counts as 100%			
Centrally-timetabled examination (On-campus)	80%		No
This is a 1.5-hour open-book exam. To clarify, "open book" here means written notes, books, and printouts are allowed. Electronic devices are not allowed, except for a standard pocket calculator.			

- Answerbook Pink (12 page)
- Students may use a calculator
- Periodic Tables

Assessment group R

	Weighting	Study time	Eligible for self-certification
resit exam	100%		No
1.5 h open book resit exam - 100% . To clarify, "open book" here means written notes, books, and printouts are allowed. Electronic devices are not allowed, except for a standard pocket calculator.			

- Students may use a calculator

Feedback on assessment

homework sets will be marked with group feedback provided within the marking period.

Past exam papers for CH281

Availability

Courses

This module is Optional for:

- UCHA-4 Undergraduate Chemistry (with Intercalated Year) Variants
  - Year 2 of F101 Chemistry (with Intercalated Year)
  - Year 2 of F122 Chemistry with Medicinal Chemistry (with Intercalated Year)
- UCHA-3 Undergraduate Chemistry 3 Year Variants
  - Year 2 of F100 Chemistry
  - Year 2 of F121 Chemistry with Medicinal Chemistry
- UCHA-F110 Undergraduate Master of Chemistry (with Industrial Placement)
  - Year 2 of F100 Chemistry
  - Year 2 of F110 MChem Chemistry (with Industrial Placement)
  - Year 2 of F112 MChem Chemistry with Medicinal Chemistry with Industrial Placement
- Year 2 of UCHA-F107 Undergraduate Master of Chemistry (with Intercalated Year)
- UCHA-F109 Undergraduate Master of Chemistry (with International Placement)
  - Year 2 of F109 MChem Chemistry (with International Placement)
  - Year 2 of F111 MChem Chemistry with Medicinal Chemistry (with International Placement)
- UCHA-4M Undergraduate Master of Chemistry Variants
  - Year 2 of F100 Chemistry
  - Year 2 of F105 Chemistry
  - Year 2 of F110 MChem Chemistry (with Industrial Placement)
  - Year 2 of F109 MChem Chemistry (with International Placement)
  - Year 2 of F125 MChem Chemistry with Medicinal Chemistry
- Year 2 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)