CH281-15 Chemical Reaction Engineering and Data Analysis

26/27

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 scientific and engineering concepts needed to transfer chemical reactions from a university lab to an industrial setting. The module concentrates on two interconnected parts: reactor scale-up (an introduction to chemical reaction engineering) and data processing and analysis (including numerical root finding and integration, ODE solving, kinetic model development and discrimination illustrated with heterogeneous catalytic reactions, determination of rate coefficients using NLLS, EVM/ODR, and Bayesian MCMC approaches, and Fourier transformations and analyses for signal processing). In addition to the scientific concepts, the module will introduce and develop the mathematical skills necessary to understand the material. Simultaneously, we will teach students to use Python as both a tool for mathematics and a coding language.

This module will be delivered over 10 weeks, comprising 30 peer instruction sessions (30 hours). The core content will be supported by worked examples and problem sets. The interactive lecture sessions aim to promote deeper learning and foster a comprehensive understanding of the subject. Students will be encouraged to organise into teams for each session to discuss tasks and engage with the material through interactive methods.

Class participation is encouraged through weekly homework assignments, which count toward the

module's formative assessment. A 20% individual summative assessment is conducted via short weekly homework multiple-choice quizzes (2 questions per week, 20 questions in total over 10 weeks); the answers must be submitted weekly (e.g., via an assessed Moodle online quiz). The remaining 80% is assessed through a written individual exam.

Module aims

This module aims to establish a rigorous foundation in industrial scale-up (chemical reaction engineering) and data processing concepts. It is one of three optional modules for second-year undergraduate Chemistry students. The aims are to:

(1) Develop a thorough understanding of the scientific principles related to chemical reaction engineering and data analysis.
(2) Develop a solid understanding of the underlying mathematics and a basic understanding of the Python coding language.
(3) Use the acquired knowledge in a discussion format to explore examples of industrial processes, enhancing learning.
(4) Apply the knowledge gained to a broader scientific context, linking it to chemistry, chemical engineering, physics, and manufacturing principles.
(5) Develop a skill set to critically analyse, 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 4 parts. Note that the underlying mathematical and coding concepts will be taught as needed.

Block 1 (6 lectures with active participation): Basic Chemical Reaction Engineering Concepts
(1) Mass/mole balance, the batch, semi-batch, and flow (e.g. CSTR, PFR, PBR) reactors.
(2) Conversion, recap rate laws and reaction stoichiometry (kinetics). Extension of reaction kinetics.
(3) Reactor sizing and Levenspiel Plots.
(4) Space time and Space Velocity

Block 2: (12 Lectures with active participation) Isothermal Reactor Design
(1) Reactors in parallel, series, and potpourri arrangements.
(2) Volume Changes in reactions
(3) Multiple Reactions
(4) Data-Processing I: Numerical root finding and integration, ODE solving.

Block 3. (6 lectures with active participation): Catalysis and Catalytic Reactors
(1) Heterogeneous catalysis and reactor design
(2) Data processing II: Kinetic model development:/discrimination rate laws, mechanisms, and rate-limiting steps.
(3) Data processing III: Determination of experimental parameters through NLLS, EVM/ODR and Bayesian MCMC methods.

Block 4 (6 lectures with active participation). Data Processing IV
(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.

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, EVM/ODR and Bayesian MCMC methods, and Fourier analysis of data for signal processing. 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 the formative assessed homework problem sets.
- ETHICAL REASONING: Students can reason ethically when evaluating the design and use of chemical reaction engineering principles in modern society and illustrate their learning through the group active learning discussion sessions and formative homework sets.

Indicative reading list

Reading lists can be found in Talis

Specific reading list for the module

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	30 sessions of 1 hour (20%)
Seminars	(0%)
Private study	110 hours (73%)
Assessment	10 hours (7%)
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 D1

	Weighting	Study time	Eligible for self-certification
Online weekly multiple-choice quiz	20%	10 hours	No

	Weighting	Study time	Eligible for self-certification
Throughout the module, you will be given weekly multiple-choice questions to solve, two per week (20 in total). You are asked to submit the answers to the online meeting by weekly deadlines. These count for 20% of the module mark. Note that in the 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.			

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

Assessment group R1

	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
- Answerbook Pink (12 page)

Feedback on assessment

Formative 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 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 F105 Chemistry
    - Year 2 of F125 MChem Chemistry with Medicinal Chemistry
- Year 2 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)