

CEIC2005

Chemical Reaction Engineering

Term 2, 2022



Course Overview

Staff Contact Details

Convenors

Name	Email	Availability	Location	Phone
Dipan Kundu	d.kundu@unsw.edu.au	via Teams or Email	E10, 222 (Hilmer)	

Lecturers

Name	Email	Availability	Location	Phone
Nicholas Bedford	n.bedford@unsw.edu.au	via Teams or Email	Science and Engineering Building, E8, 422 (Hilmer)	

School Contact Information

Enquiries related to the course (e.g. course content, assessment instructions) should be raised during the scheduled classes, office hours, or in Teams channels/Moodle forums designated for that purpose.

Learning and question etiquette:

- Please be prepared for classes and attend the timetabled classes so that you can ask questions during the class time.
- Please respect that demonstrators and tutors have scheduled the class time to help you learn
 and are likely to be busy with other responsibilities outside those times; questions asked outside
 of class times will take longer to be answered.
- PhD students and other casuals who are teaching classes are normally only expected to look after the timetabled class and not to provide follow-up one-on-one assistance.
- Please don't ask questions in private that could be reasonably asked in a way that everyone can learn from the discussion.
- As a member of a community of learners, please try answering each other's questions!
- Please limit private messages to staff (via email or Teams) to *confidential* matters related to course administration.

For assistance with enrolment, class registration, progression checks and other administrative matters, please see the Nucleus: Student Hub. They are located inside the Library – first right as you enter the main library entrance. You can also contact them via http://unsw.to/webforms or reserve a place in the face-to-face queue using the UniVerse app.

If circumstances outside your control impact on submitting assessments, Special Consideration may be granted, usually in the form of an extension or a supplementary assessment. Applications for Special Consideration must be submitted online.

Course Details

Units of Credit 6

Summary of the Course

Applied physical chemistry, kinetics and reaction engineering. Thermodynamic concepts related to Gibbs free energy as applied to phase equilibria and kinetics are illustrated and expanded. In this course, the student will learn the key concepts of chemical reaction kinetics (such as order of reactions, elemental reactions, reaction mechanisms, steady state kinetics, temperature dependence of chemical reactions, the influence of catalysts on the reaction kinetics etc.) and how these kinetic concepts can be employed to choose and operate a suitable reactor for a certain reaction. Reaction kinetics and thermodynamics are interlinked: One tells you how fast a reaction is, the other tells you whether the reaction will proceed at all. Finally, kinetics and thermodynamics are applied in reaction engineering.

Topics include Introduction to reactor design: ideal batch, steady state mixed flow, steady state plug flow, size comparisons of ideal reactors, optimisation of operating conditions. Multiple reactor systems: reactors series and parallel, mixed flow reactors of different sizes in series, recycle reactors, autocatalytic reactions. Multiple reactions: reactor design for reaction in parallel and reactions in series, series-parallel reactions. Temperature effects: heat of reaction, equilibrium constants, optimum temperature progression, adiabatic and non-adiabatic operation, product distribution and temperature. Kinetics of rate processes: Significance of the rate laws and models for distributed and lumped parameter systems. Experimental measurement and correlation of process rates. Laboratory experiments to illustrate concepts are part of the course.

Course Aims

Chemical Reaction Engineering is one of the core subjects that differentiate chemical engineers and industrial chemists from other engineering disciplines. The majority of chemical processes involve at least one chemical reaction. In this subject students will learn how to use thermodynamics to determine if a given reaction is possible. Students will also learn how to use reaction kinetic models to determine how fast a reaction is and to develop mathematical models, design equations, to simulate the progress of chemical reactions in a variety of reactor types. The course is principally a problem solving course, and requires considerable student interaction and participation.

Course Learning Outcomes

After successfully completing this course, you should be able to:

Learning Outcome	EA Stage 1 Competencies
Apply basic thermodynamic principles to determine if a chemical reaction is feasible.	PE1.3
2. Use mathematical models to simulate the progress of chemical reactions.	PE1.1, PE2.1
Design ideal chemical reactors.	PE2.1, PE2.3

Learning Outcome	EA Stage 1 Competencies
4. Predict the performance of non-ideal reactors.	PE1.3, PE2.2
5. Critically evaluate analyses and designs for chemical reaction systems.	PE3.4, PE3.5, PE3.6, PE3.2, PE2.3

Teaching Strategies

Lectures are used to introduce and highlight key concepts. The focus of this course is on problem analysis and computational aspects and not on rote learning. An extensive set of problems will be used to encourage you to apply analytical and computational techniques introduced in the lectures. The midsession quizzes are to provide assessment and feedback to you on your progress.

In order to encourage a deep-approach to learning, emphasis is placed on the imbibition of theoretical concepts via problem-solving. Lectures and lecture notes, used to lay the foundation theories, will be sandwiched with a generous dose of illustrative examples from both laboratory and industrial situations. The linkage between thermodynamics, kinetics and reactor design will also be demonstrated by representative reaction systems. Homework assignments and quizzes will also be given to complement class worked examples, serving as pivots for knowledge deepening and application diversification. This approach is taken to encourage, in the student, an enriched learning experience which promotes integration of course material with other aspects of the chemical engineering curriculum.

Additional Course Information

Requisite knowledge and relationships to other courses

This course is about continuing to build your knowledge of reactions and energy, with an application of this knowledge to the design of chemical reactors. It builds upon the skills base from CEIC2000 (Material and Energy Systems), the mathematical underpinning of MATH1131 (Mathematics 1A) and MATH2089 (Numerical Methods and Statistics).

The learning from this course is utilised in CEIC2007 (Chemical Engineering Lab A), CEIC3000 (Process Modelling and Analysis), CEIC3005 (Process Plant and Design), CEIC3006 (Process Dynamics and Control) and CEIC4001 (Process Design Project).

Expectations

Integrity and Respect

The UNSW Student Code of Conduct (https://student.unsw.edu.au/conduct) among other things, expects all students to demonstrate integrity in all the academic work and to treat all staff, students and visitors to the University with courtesy, tolerance and respect.

Time commitment

UNSW expects students to spend approximately 150 hours to successfully complete a 6 UOC course like CEIC2005. Success in CEIC2005 means continual work through the term, completing all online lessons and all the problem solving workshop questions in the corresponding week rather than getting behind and then hoping to catch up.

A typical week in CEIC2005 consists of approximately 12 hours of work on the material in this course:

- 6 h of online lessons, videos, live lectures etc
- 2 h working on the problem solving workshop material (preparation and participation)
- 1 h working on the team assignment
- 2 to 4 h to review, study or work on assignments

Moodle has the activities for each week clearly laid out to help you keep pace.

Don't leave activities until the night before; doing so highly increases the chance of failure either in this course or the next course that assumes that you know the CEIC2005 material. Given the pivotal role of chemical reaction engineering within the chemical engineering curriculum, a solid understanding of this work is absolutely required to permit progression to later theory, laboratory and design courses.

Team project

Work for the team project should be carefully delegated. Be careful not to spend an hour a week talking about what you might do or significant time figuring out who will do what. Do not fall into the trap of all "working together" somewhat inefficiently. Part of the point of this team project is to practice your team management skills. It is not possible to complete these tasks *efficiently* by trying to get each member of the team to work on one "sub-question" within the weekly task and then trying to stitch the fragments together at the end.

Detailed Topics

Applications of physical chemistry, kinetics and reaction engineering. Thermodynamic concepts related to Gibbs free energy as applied to phase equilibria and kinetics are illustrated and expanded. In this course, the student will learn the key concepts of chemical reaction kinetics (such as order of reactions, elemental reactions, reaction mechanisms, steady state kinetics, temperature dependence of chemical reactions, the influence of catalysts on the reaction kinetics etc.) and how these kinetic concepts can be employed to choose and operate a suitable reactor for a certain reaction. Reaction kinetics and thermodynamics are interlinked: One tells you how fast a reaction is, the other tells you whether the reaction will proceed at all. Finally, kinetics and thermodynamics are applied in reaction engineering.

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Assessment

Assessment task	Weight	Due Date	Course Learning Outcomes Assessed
1. Moodle quizzes	10%	Weeks 3, 5, 8, 10 (Friday)	1, 2, 3
2. Homework Assignments	20%	Weeks 5 & 9 (Friday)	2, 3, 5
3. Team Projects	20%	Due Weeks 3, 4, 5, 8, 9, 10 (Wednesday),Assessed Weeks 5 & 10 (Thursday)	5
4. Final Exam	50%	Exam period	1, 2, 3, 4

Assessment 1: Moodle quizzes

Due date: Weeks 3, 5, 8, 10 (Friday)

4 short quizzes through the term (each 2.5%) help measure progress through the content and provide feedback on the learning throughout the term.

The quizzes are intended primarily as formative assessment, but are counted towards the final mark at a significant level to encourage you to take them seriously and to discourage last-minute cramming. These quizzes will be assessed on the basis of technical accuracy of calculations and evidence of good engineering judgement with assumptions and problem simplification.

Assessment 2: Homework Assignments

Due date: Weeks 5 & 9 (Friday)

There are 2 parts to the assignment (worth 10% each), designed to let you tackle longer and more open ended problems.

These problems will let you explore more deeply aspects of thermodynamics, kinetics and reaction engineering, putting theoretical knowledge into real engineering practice. The emphasis in the marking scheme is not only technical accuracy but contextualisation of the results to the specific engineering problem being investigated.

Assessment 3: Team Projects

Submission notes: via Moodle

Due date: Due Weeks 3, 4, 5, 8, 9, 10 (Wednesday), Assessed Weeks 5 & 10 (Thursday)

Working in a team, you will investigate contexts of chemical reaction engineering, undertaking short case studies of how key concepts from the course can be seen in common industrial settings. There are approximately weekly tasks for this project that are assessed periodically through the term.

Your short team reports will be compiled, reviewed and improved over the course of the term. Note that you will also be required to complete an evaluation of each member of your team, covering the contribution to the team output and the quality and style of interaction with other members in the team.

These team evaluations are used to moderate the final marks from the team project.

Assessment 4: Final Exam

Due date: Exam period

The final exam is designed to ensure that students are able to apply the principles of thermodynamics, kinetics and reaction engineering to design problems where resources, including time, are constrained. The final exam also focuses on individual achievement and competence in the subject matter, in line with our obligations to Engineers Australia.

Attendance Requirements

Students are strongly encouraged to attend all classes and review lecture recordings.

Course Schedule

View class timetable

Timetable

Date	Туре	Content
Week 1: 30 May - 3	Lecture	Online activity/hybrid lecture
June		Thermodynamics: Intro to course, 2nd and 3rd laws of thermodynamics; Gibbs function
	Workshop	Start work on team project
Week 2: 6 June - 10	Lecture	Online activity/hybrid lecture
June		Thermodynamics: Phase diagrams and phase equilibria, colligative properties, internal pressure, J-T coefficients
	Workshop	Applications of thermodynamics to chemical engineering problems
Week 3: 13 June - 17	Lecture	Online activity/hybrid lecture
June		Chemical kinetics: Extent of reaction, kinetics, rates of reaction, reversible reactions, equilibria, collision theory, rate laws, rate order, Arrhenius equation, diffusion controlled reactions
	Workshop	Phase equilibria and phase diagram problems
Week 4: 20 June - 24	Lecture	Online activity/hybird lecture
June		Chemical kinetics: reaction mechanisms, more complex reaction rates, case studies in homogenous and heterogenous catalysis
	Workshop	Reactions, reaction rates, describing reactions problems
Week 5: 27 June - 1	Lecture	Online activity/hybird lecture
July		Chemical kinetics: Enzyme reactions. Polymerisation reaction kinetics. Obtaining rate data. Chemical kinetics in the context of reaction engineering.

	Workshop	Complex reaction mechanisms and reaction kinetics problems
Week 6: 4 July - 8 July	Online Activity	Flexibility Week Revision/consolidation of chemical kinetics and material balances
	Workshop	More kinetics problems
Week 7: 11 July - 15 July	Lecture	Online activity/hybird lecture
		Reaction Engineering: Continuous Stirred Tank Reactors (CSTRs). Levenspiel plots. Residence time distributions.
	Workshop	Batch, semi-batch and CSTR design problems
Week 8: 18 July - 22	Lecture	Online activity/hybird lecture
July		Reaction engineering: Plug Flow Reactors (PFRs). Comparison of CSTRs and PFRs. Residence time distributions
	Workshop	Tubular reactors and plug flow reactor design problems
Week 9: 25 July - 29	Lecture	Online activity/hybird lecture
July		Reaction engineering: Sets of reactors. Relaxing assumptions. Non-ideal reactors. Axial dispersion model.
	Workshop	Using sets of reactors to solve design problems
Week 10: 1 August - 5	Lecture	Online activity/hybird lecture
August		Reaction Enginerering: Diagnosing problems in reactors
	Workshop	Diagnosing faults in reactors and measuring improvement

Resources

Recommended Resources

- Atkins' Physical Chemistry, by Peter Atkins and Julio de Paula, any recent edition (7th onwards). Oxford University Press, New York. This is available in the library and provides an excellent resource for thermodynamics and the fundamentals of chemical kinetics.
- Elements of Chemical Reaction Engineering, by H Scott Fogler, any edition, Wiley. An e-book of this is available in the UNSW Library (see links from Moodle). It provides an excellent introduction to the application of chemical kinetics to the design of reactors, to the design of ideal and non-ideal reactors.

Course Evaluation and Development

The School of Chemical Engineering evaluates each course each time it is run through (i) myExperience Surveys, and (ii) Focus Group Meetings. As part of the myExperience process, your student evaluations on various aspects of the course are graded; the Course Coordinator prepares a summary report for the Head of School. Any problem areas are identified for remedial action, and ideas for making improvements to the course are noted for action the next time that the course is run. Focus Group Meetings are conducted each term. Student comments on each course are collected and disseminated to the Lecturers concerned, noting any points which can help improve the course.

All of the activities in this course from the online lessons through to the team project have been designed in response to student feedback.

Submission of Assessment Tasks

In the School of Chemical Engineering, all written work will be submitted for assessment via Moodle unless otherwise specified. Attaching cover sheets to uploaded work is generally not required; when you submit work through Moodle for assessment you are agreeing to uphold the Student Code.

Some assessments will require you to complete the work online and it may be difficult for the course coordinator to intervene in the system after the due date. You should ensure that you are familiar with assessment systems well before the due date. If you do this, you will have time to get assistance before the assessment closes.

All submissions are expected to be neat and clearly set out. Your results are the pinnacle of all your hard work and should be treated with due respect. Presenting results clearly gives the marker the best chance of understanding your method; even if the numerical results are incorrect.

Marking guidelines for assignment submissions will be provided at the same time as assignment details to assist with meeting assessable requirements. Submissions will be marked according to the marking guidelines provided.

Late penalties

Unless otherwise specified, submissions received after the due date and time will be penalised at a rate of 5% per day or part thereof (including weekends). For some activities including Moodle quizzes and Team Evaluation surveys, extensions and late submissions are not possible.

Special consideration

If you have experienced an illness or misadventure beyond your control that will interfere with your assessment performance, you are eligible to apply for Special Consideration prior to submitting an assessment or sitting an exam.

UNSW has a <u>Fit to Sit / Submit rule</u>, which means that if you attempt an exam or submit a piece of assessment, you are declaring yourself fit enough to do so and cannot later apply for Special Consideration.

For details of applying for Special Consideration and conditions for the award of supplementary assessment, please see the information on UNSW's <u>Special Consideration page</u>.

Please note that students will need to provide some documentary evidence to support absences from any assessments missed because of COVID-19 public health measures such as isolation. UNSW will **not** be insisting on medical certificates for COVID-related absences of 7 days or less, with the positive PCR or RAT result being sufficient. Longer absences due to self-isolation or COVID-related illness will still need documentation such as a medical certificate.

Applications for special consideration **will still be required** for assessment and participation absences related to COVID-19. Special consideration requests should not be lodged for missing classes if there are no assessment activities in that class.

Academic Honesty and Plagiarism

Academic integrity is fundamental to success at university. Academic integrity can be defined as a commitment to six fundamental values in academic pursuits: honesty, trust, fairness, respect, responsibility and courage (International Center for Academic Integrity, 'The Fundamental Values of Academic Integrity', T. Fishman (ed), Clemson University, 2013). At UNSW, this means that your work must be your own, and others' ideas should be appropriately acknowledged. If you don't follow these rules, plagiarism may be detected in your work.

Further information about academic integrity and plagiarism can be located at:

- The Current Students site
- The ELISE training site

The Conduct and Integrity Unit provides further resources to assist you to understand your conduct obligations as a student: https://student.unsw.edu.au/conduct.

Referencing is a way of acknowledging the sources of information that you use to research your assignments. You need to provide a reference whenever you draw on someone else's words, ideas or research. Not referencing other people's work can constitute plagiarism. Further information about referencing styles can be located at https://student.unsw.edu.au/referencing.

For assessments in the School of Chemical Engineering, we recommend the use of referencing software such as Mendeley or EndNote for managing references and citations. Unless required otherwise specified (i.e. in the assignment instructions) students in the School of Chemical Engineering should use either the APA 7th edition, or the American Chemical Society (ACS) referencing style as canonical author-date and numbered styles respectively.

Academic Information

To help you plan your degree, assistance is available from academic advisors in <u>The Nucleus</u> and also in the <u>School of Chemical Engineering</u>.

Additional support for students

- Current Student Gateway
- Engineering Current Student Resources
- Student Support and Success
- Academic Skills
- Student Wellbeing, Health and Safety
- Equitable Learning Services
- IT Service Centre

Course workload

Course workload is calculated using the Units-Of-Credit (UOC). The normal workload expectation for one UOC is approximately 25 hours per term. This includes class contact hours, private study, other learning activities, preparation and time spent on all assessable work.

Most coursework courses at UNSW are 6 UOC and involve an estimated 150 hours to complete, for both regular and intensive terms. Each course includes a prescribed number of hours per week (h/w) of scheduled face-to-face and/or online contact. Any additional time beyond the prescribed contact hours should be spent in making sure that you understand the lecture material, completing the set assignments, further reading, and revising for any examinations.

On-campus class attendance

Physical distancing recommendations must be followed for all face-to-face classes. To ensure this, only students enrolled in those classes will be allowed in the room. Class rosters will be attached to corresponding rooms and circulated among lab demonstrators and tutors. No over-enrolment is allowed in face-to-face class. Students enrolled in online classes can swap their enrolment from online to a **limited** number of on-campus classes by Sunday, Week 1.

In certain classroom and laboratory situations where physical distancing cannot be maintained or the staff running the session believe that it will not be maintained, face masks will be designated by the course coordinator as **mandatory PPE** for students and staff. Students are required to bring and use their own face mask. Mask can be purchased from IGA Supermarket (Map B8, Lower Campus), campus pharmacy (Map F14, Middle Campus), the post office (Map F22, Upper Campus) and a vending machine in the foyer of the Biological Sciences Building (Map E26, Upper Campus).

Your health and the health of those in your class is critically important. You must stay at home if you are sick or have been advised to self-isolate by <u>NSW health</u> or government authorities. Current alerts and a list of hotspots can be found <u>here</u>. Do not come to campus if you have any of the following symptoms: fever (37.5 °C or higher), cough, sore throat, shortness of breath (difficulty breathing), runny nose, loss of taste, or loss of smell. If you need to have a COVID-19 test, you must not come to campus and remain in self-isolation until you receive the results of your test.

You will not be penalised for missing a face-to-face activity due to illness or a requirement to self-

isolate. We will work with you to ensure continuity of learning during your isolation and have plans in place for you to catch up on any content or learning activities you may miss. Where this might not be possible, an application for fee remission may be discussed. Further information is available on any course Moodle or Teams site.

For more information, please refer to the FAQs: https://www.covid-19.unsw.edu.au/safe-return-campus-faqs

Note: This course outline sets out description of classes at the date the Course Outline is published. The nature of classes may change during the Term after the Course Outline is published. Moodle should be consulted for the up to date class descriptions. If there is any inconsistency in the description of activities between the University timetable and the Course Outline (as updated in Moodle), the description in the Course Outline/Moodle applies.

Image Credit

Dr Peter Wich

CRICOS

CRICOS Provider Code: 00098G

Acknowledgement of Country

We acknowledge the Bedegal people who are the traditional custodians of the lands on which UNSW Kensington campus is located.

Appendix: Engineers Australia (EA) Professional Engineer Competency Standard

Program Intended Learning Outcomes	
Knowledge and skill base	
PE1.1 Comprehensive, theory based understanding of the underpinning natural and physical sciences and the engineering fundamentals applicable to the engineering discipline	✓
PE1.2 Conceptual understanding of the mathematics, numerical analysis, statistics, and computer and information sciences which underpin the engineering discipline	
PE1.3 In-depth understanding of specialist bodies of knowledge within the engineering discipline	✓
PE1.4 Discernment of knowledge development and research directions within the engineering discipline	
PE1.5 Knowledge of engineering design practice and contextual factors impacting the engineering discipline	
PE1.6 Understanding of the scope, principles, norms, accountabilities and bounds of sustainable engineering practice in the specific discipline	
Engineering application ability	
PE2.1 Application of established engineering methods to complex engineering problem solving	✓
PE2.2 Fluent application of engineering techniques, tools and resources	✓
PE2.3 Application of systematic engineering synthesis and design processes	✓
PE2.4 Application of systematic approaches to the conduct and management of engineering projects	
Professional and personal attributes	
PE3.1 Ethical conduct and professional accountability	
PE3.2 Effective oral and written communication in professional and lay domains	✓
PE3.3 Creative, innovative and pro-active demeanour	
PE3.4 Professional use and management of information	✓
PE3.5 Orderly management of self, and professional conduct	1
PE3.6 Effective team membership and team leadership	✓