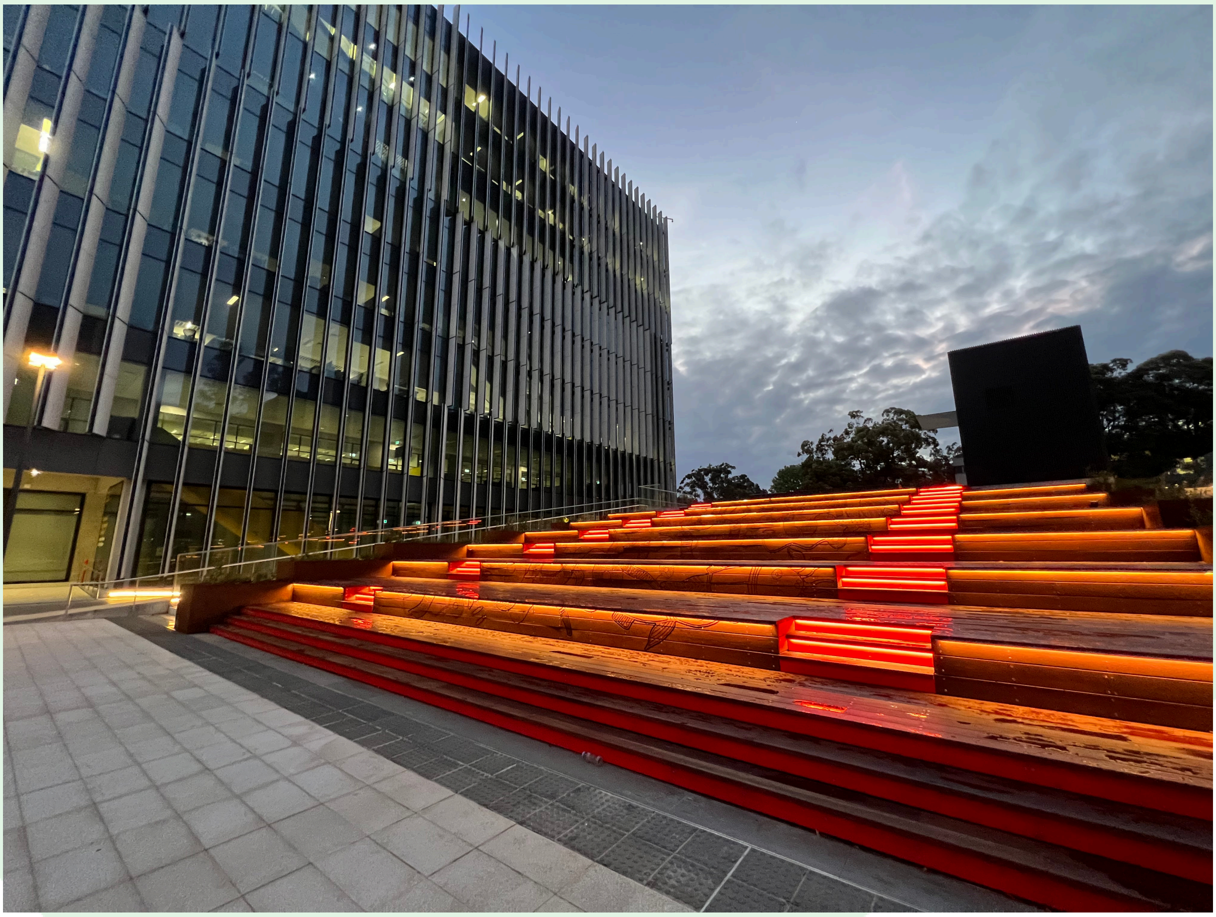
School of Chemical Engineering

UNSW Engineering

CEIC3000

Process Modelling and Analysis

Term 1, 2022



Course Overview

Staff Contact Details

Convenors

Name	Email	Availability	Location	Phone
Stuart Prescott	s.prescott@unsw.edu.au	Just ask!	Science and Engineering Building E8, Room 316a Hilmer	via Teams or email

Lecturers

Name	Email	Availability	Location	Phone
Priyank Kumar	priyank.kumar@unsw.edu.au	just ask!	Science and Engineering Building E8, Room 334	via Teams or email

School Contact Information

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.

For course administration matters, please contact the Course Coordinator.

Course Details

Units of Credit 6

Summary of the Course

This course deals with the formulation of reliable mathematical models for the purpose of process design, control, and optimization. Students will therefore be equipped with skills in the derivation of linear and non-linear ODEs and PDEs based on the application of conservation laws to various chemical and biological processes. Analytical tools for the solution of linear and non-linear ODEs representing initial value and boundary value problems will be discussed. Illustrative examples involving lumped and distributed processes, discrete systems as well as multivariable (matrix) methods are included. Attention will be also given to nonlinear features identification including steady state multiplicity and bifurcation analysis. For situations where closed form solutions are unattainable, approximate methods are sought. Thus, the subject will also cover numerical methods for algebraic and ODEs. The use of numerical differentiation and interpolation in process analysis will also be examined.

Course Aims

The ever increasing global demand for better utilization of raw material and energy resources in an environmentally-sustainable manner means that greater ingenuity must be employed in the development of new processes (or improvement of existing ones). The traditional but time-consuming and expensive practice of first building a small-scale replica of the process for the sole purpose of investigating its dynamic and steady-state behaviour to acquire optimal operating conditions is a luxury that can no longer be afforded. Consequently, a more quantitative approach to process design and operation is now more attractive to industry.

Process modelling and analysis deals with the principles and methods for effectively building and understanding models of processes. This course is a central component of the chemical and process engineering curriculum and leads naturally to the principles of computer-based design and process control.

The objectives of the course are to:

- Acquaint you with the skills to represent physical phenomena in mathematical/computational language by formulating models of different complexities depending of particular engineering needs, as well as with different techniques for mathematical model building, including, phenomenological and empirical approaches.

- Provide you with key mathematical, numerical and computational methods useful for the analysis of wide-ranging chemical engineering problems.

- Integrate results from modelling exercises with known physicochemical features of the system to evolve better process design and operation.

- Acquaint you with the skills to model and understand the dynamic behaviour of physical and chemical processes.

This course offers opportunities to refine your knowledge of other core subjects in a more analytical fashion, making further use of the chemical engineering and mathematics you have already studied. You will be able to consolidate your understanding and even draw extensions to other disciplines.

Course Learning Outcomes

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

Learning Outcome	EA Stage 1 Competencies
1. Identify appropriate basis (e.g. assumptions and conditions) for mathematical model building and diagnosis.	PE1.3, PE2.1
2. Construct and solve mathematical models using both analytical and numerical techniques.	PE1.3, PE2.1
3. Interpret and communicate the results of modelling exercises with a view to carrying out further refinement, utilisation for design and optimisation.	PE3.2

Teaching Strategies

The instructional method employed in this course is informed by the need to stimulate a deep-approach to learning in the students. Recent educational research literature favours this approach, especially for application-oriented concepts frequently encountered in engineering. For that reason, while we will provide the theoretical basis for the relevant analytical or numerical method. Illustrative examples will cut across a range of problems in thermodynamics, transport phenomena, kinetics, reactor design and separation processes. This will ensure that the student develops a knack for the nuances and intrigues unique to each approximation method.

In order to encourage a deep-approach to learning, emphasis is placed on the imbibition of mathematical concepts via problem-solving. Whilst theoretical foundation would be laid using principles illustrated in standard texts, lecture delivery is usually preceded by a qualitative description of why and where the concept(s) in question arise in natural systems and following the mathematical expose; applications to known chemical engineering and/or interdisciplinary processes are subsequently presented. The course is assigned 4 lecture hours per week, and 2 hours per week for problem solving workshops, but supplementation will be provided through assignment problems (which will be graded). Solutions will be given for the workshop questions. Note that supplementation of lecture material through these problem-solving tasks ensures re-iteration of class concepts and/or how they can be manipulated depending on the intrigues of the particular problem. There is no need to worry as some of these twists are self-evident and you will get better at identifying and classifying them with experience – a major incentive for learning rather than mark-hunting!

Significantly, this approach ensures that the stated student learning outcomes can be more readily realised. For instance, our discussion on how ordinary linear and nonlinear differential equations arise in natural systems will enhance your ability to develop similar models for artificially-contrived scenarios in not only chemical engineering operations but also related disciplines – biomedical, materials processing and even finance/stock-broking industry.

Additional Course Information

Requisite knowledge and relationships to other courses

This course is about mathematical model design, implementation and solution. It builds upon the skills base laid in second year mathematics and numerical methods, the conceptual chemical engineering principles from CEIC2001 (Fluid and Particle Mechanics), CEIC2002 (Heat and Mass Transfer) and CEIC2005 (Chemical Reaction Engineering) and the engineering design process from ENGG1000 (Introduction to Engineering Design and Innovation) and CEIC2000 (Material and Energy Systems). The learning from this course is utilised in CEIC3005 (Process Plant and Design), CEIC3006 (Process Dynamics and Control) and CHEN6706 (Advanced Transport Phenomena). The mathematical tools from MATH2019/MATH2018 and MATH2089 are required to simplify and solve differential equations both analytically and numerically.

The purposes of the course are to increase the strength of students' mathematical skills and abstract thinking and to help them appreciate process analysis and synthesis. This is the first course in chemical engineering where students really consider processes in unsteady-state. It should be seen as a much more mathematical progression of CEIC2000 and so these courses closely linked. The course will show you mathematical, numerical and computational techniques for creating models of processes.

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 CEIC3000. We expect 60 hours to be spent participating in face-to-face classes/recorded lectures, 10 hours working on the workshop questions outside of class, 10 hours completing the two assignments, 6 hours completing the mid-semester test and the final exam, with the remaining 64 hours provided for private study and preparation for the examinations. Therefore, outside class you should be spending at least 7 hours per week working on CEIC3000.

Competence

Students are expected to enter CEIC3000 having developed competencies in all the material covered in the pre-requisite courses, at least. Little time is available to remediate any deficiencies in your knowledge of those topics. Over the course of the term, you will be developing new competencies and to illustrate the standards we expect, marking rubrics or guidelines will be provided for all assessments. The teaching staff will apply these marking guides fairly and provide you with feedback so you can continue to improve over the term and beyond.

Participation

When you attend face-to-face or synchronous online classes, we expect you to actively participate in the activities organised. This may mean listening, taking notes, asking questions or engaging in peer discussions. It may also mean working by yourself or in groups on workshop exercises.

Students are expected to contribute to online discussions through the course forum on Moodle. You may wish to discuss challenges faced through this course, ask questions about course content, discuss solutions to workshop and practice questions. It is expected that students will help each other, and the lecturers will contribute as required.

Attendance and punctuality

We expect students to be punctual and attend at all lectures and workshops. University commitments take precedence over regular work activities, holidays etc. Students who attend less than 80% of their possible classes may be refused final assessment. If you miss a class, we expect you to catch up in your time, lectures will be recorded and made available through Moodle, but remember that recorded lectures are a poor substitute for being there and participating.

Assessment

Assessment task	Weight	Due Date	Course Learning Outcomes Assessed
1. Assignment 1: developing models	15%	Friday Week 5	1, 2, 3
2. Assignment 2: analysing models	15%	Friday Week 10	1, 2, 3
3. Mid-Session Exam	25%	Friday Week 8	1, 2, 3
4. Final Exam	45%	To be published in the exam timetable.	1, 2, 3

Assessment 1: Assignment 1: developing models

Submission notes: via Moodle
Due date: Friday Week 5

In this assignment, you will develop models and solve them, applying insight from the analyitcal and numerical modelling to simplified design problems. This assignment is designed to let you demonstrate your achievements in the first half of the course, developing models from first principles, simplifying them to make them tractable, applying sophisticated mathematical techniques to find steady state solutions, and using numerical methods to investigate the problem.

Templates for the numerical methods sections of the assignment will be provided.

Assessment 2: Assignment 2: analysing models

Submission notes: via Moodle
Due date: Friday Week 10

In this assignment, you will develop models of systems based on the underlying physics of the situation and analyse them, applying insight from the analysis to simplified design problems. This assignment will allow you to demonstrate your knowledge of the second half of the course in analysing models and how that can be used to understand the real system that they represent.

Templates for the numerical methods sections of the assignment will be provided.

Assessment 3: Mid-Session Exam

Start date: 09/04/2021 03:00 PM
Submission notes: via Moodle
Due date: Friday Week 8

Progress test on course to date. The mid-session examination will cover all of the material from the first 7 weeks of the course. You will be asked to develop models, simplify them, use integration or steady-state approximations to see deeper insights into the model, make approximations to simplify models, and analyse models.

Assessment 4: Final Exam

Submission notes: via Moodle
Due date: To be published in the exam timetable.

In this final examination, with questions assessing the entire course, you'll demonstrate your skills in developing models, simplifying them, integration techniques, model analysis, linearisation, phase portraits and numerical methods.

Attendance Requirements

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

Course Schedule

This course has a combination of timetabled classes and self-paced learning activities. As described earlier, not all the timetabled classes will be needed, but you can use those times to work on some of the self-paced lessons. We'll announce what is happening with classes each week. Completing the relevant self-paced learning activities each week will help you keep up with the material and get the most out of the timetabled classes.

Face-to-face workshop sessions cannot be recorded. Online workshops may not be suitable for recording, for example where break-out rooms are used.

[View class timetable]

Timetable

Date	Type	Content
O-Week: 7 February - 11 February	Online Activity	1. Welcome video with important course info 2. Get yourself set up for numerical methods with either Python or Matlab 3. Revise material from CEIC2002 (heat transfer and mass transfer), CEIC2005 (kinetics and reaction engineering), MATH2089 (numerical methods for ODEs, linear algebra, plotting functions), MATH2018/2019 (advanced integration), MATH1231 (linear algebra), ENGG1811 (functions and loops)
Week 1: 14 February - 18 February	Lecture	(Monday) Process modelling: Introduction and basic ingredients
	Online Activity	More on basic ingredients for modelling
	Workshop	Application of basic ingredients to situations Brief revision and refamiliarisation with numerical methods in Python
Week 2: 21 February - 25 February	Lecture	(Monday) How to formulate physicochemical problems
	Online Activity	Different physicochemical scenarios
	Workshop	Setting up and formulating example problems
Week 3: 28 February - 4 March	Lecture	(Monday) Simple analytical solutions to physicochemical problems

	Online Activity	Selected 1st and 2nd order ODEs in process modelling
	Workshop	Building models, solving and analysing them
Week 4: 7 March - 11 March	Lecture	(Monday) Advanced solutions to physicochemical problems
	Online Activity	Special and numerical solutions to process models
	Workshop	Building models, solving and analysing them
	Homework	Work on Assignment 1 (see details in Assessments section)
Week 5: 14 March - 18 March	Lecture	(Monday) Case studies: some chemical engineering process models
	Online Activity	Additional case studies
	Lecture	(Tuesday) Constructing dynamic models. Approach to steady state.
	Workshop	More complex problems and modelling real processes
Week 6: 21 March - 25 March	Lecture	No lectures in Flexibility Week - this is a chance for extra revision and consolidation of material from CEIC3000 and also its prerequisite courses.
	Online Activity	Revision of some linear algebra for analysing models
	Workshop	Setting up and solving complex models
Week 7: 28 March - 1 April	Online Activity	Using linear algebra for modelling
	Lecture	(Monday) Linear systems analysis. Stability. Normalisation.
	Online Activity	1. More on formulating problems with linear algebra 2. Linear algebra and 'transformations'
	Workshop	Stability, classification, impulses.
Week 8: 4 April - 8 April	Lecture	(Monday) Phase space, characteristic directions, characteristic speeds.
	Online Activity	More sketching phase portraits
	Workshop	Sketching phase protraits and interpreting their meaning
	Online Activity	1. Linearisation of nonlinear problems

		2. Perturbations 3. Phase portraits for non-linear systems
	Assessment	Mid-session exam (see details in Assessments section)
Week 9: 11 April - 15 April	Online Activity	Getting more detailed qualitative informatio from phase portraits
	Lecture	(Monday) Bifurcations 1. Pitchfork, Hopf bifrucations. Lorenz model of convection.
	Workshop	Linearisation and more complicated phase portraits
	Homework	Work on Assignment 2 (see details in Assessments section)
Week 10: 18 April - 22 April	Lecture	(Monday) Bifurcations 2. saddle-node and transcritical bifurcations. Multiplicity.
	Lecture	(Wednesday) Case studies, summary, reflections on process modelling, final exam discussion.
	Workshop	Bifurcation examples, finding bifurcations, analysing problems aroud bifurcation points
	Homework	Work on Assignment 2 (see details in Assessments section)

Resources

Prescribed Resources

1. Rice, R. G. and Do, D.D., Applied Mathematics and Modelling for Chemical Engineers, John Wiley, 1995. (e-book available from library, see links in Moodle)
2. Modelling and Analysis CEIC3000 Course Notes, S.W. Prescott, J. Bao, and B.W. Bequette. (e-book available via Moodle)

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 analysed; 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.

Recent changes made to the course are described on Moodle.

Laboratory Workshop Information

This course makes extensive use of numerical methods. You can complete it using Python (with the numpy/scipy packages) or Matlab. These are available via either CoCalc.com or myAccess.

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 Fit to Sit / Submit rule, 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 Special Consideration page.

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 The Nucleus and also in the School of Chemical Engineering.

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 NSW health or government authorities. Current alerts and a list of hotspots can be found here. 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

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	
PE3.6 Effective team membership and team leadership	