THE UNIVERSITY OF NEW SOUTH WALES

School of Chemical Engineering

CEIC3000 Process modelling and Analysis

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Contents

Course Staff

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1. General course information

1.1 Course description

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.

1.2 Outline and 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.

1.3 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) and CEIC3006 (Process Dynamics and Control). 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.

The main UNSW graduate attributes targeted in this course are:

1. an in-depth engagement with the relevant disciplinary knowledge in its interdisciplinary context and,
2. the capacity for analytical and critical thinking and for creative problem-solving.

1.4 Target students and career prospects

This course is essential for all chemical engineering students. However, students from other disciplines such as Bioprocess, Petroleum, Materials or Food Engineering with requisite background will also be considered.

1.5 Course Details

This course is 6 UoC and will take approximately 150 hours of effort over the session.

1.5 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, 10 hours working on the tutorial questions outside of class, 10 hours completing the two assignments, 6 hours completing online quiz, 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 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 tutorial 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 tutorial 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 tutorials. 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.

2. Student Learning Outcomes

At the completion of this course, you should be able to:

• Identify appropriate basis (e.g. assumptions and conditions) for mathematical model building and diagnosis. • Construct and solve mathematical models using both analytical and numerical techniques	
The skills involved in scholarly inquiry	You will be assessed for your ability to formulate a problem statement in the correct mathematical expression. The extent to which you can rightly do this is a reflection of your understanding of the fundamental scientific laws governing the process in question. This attribute underpins the setting of both tutorial and assignment problems.
S4: Able to apply knowledge & skill to problem solving PE1.3: In-depth knowledge of discipline PE2.1: Application of established engineering methods to complex engineering problem solving	

• Interpret and communicate the results of modelling exercise with a view to carrying out further refinement, utilisation for design and optimisation.	
The skills of effective communication	This learning outcome ensures that you not only know the implications of the modeling exercise and how it may be further refined, but that you are also able to adequately express your knowledge-based conviction in ways that not only your peers understand but is also intelligible to the average literate person.
S6: Capable of effective communication PE3.2: Effective oral & written communication	

3. Assessment

In order to verify that the stipulated learning outcomes are being achieved, each student will be assessed as described below:

Component	Due Date	Weight	Rationale
Quiz	Week 3	0%	Student can assess whether they have the required knowledge to succeed in the course and whether they are keeping pace.
2 Assignment tasks	Weeks 6, 10	Asg.1 15% Asg.2 15%	Homework problems are designed to ensure that lecture material is comprehended through personal

			practice and hence achievement of indicated learning outcomes.
Mid-session Exam Old Main Building 230 (K-K15-230) OR Old Main Building G31 (K-K15-G31)	Week 8 Thursday 18:00 - 20:00	25%	The mid-session exam will assess the material presented on the 2/3 of the course. Ensure you attend the correct venue; see your class enrolment.
Final exam	To be announced by UNSW	45%	Assess the overall understanding of the subject material.

Assessment tasks will be graded on the basis of:

- Clear adoption of a structured approach to solving the problem at hand - including indication of adequate and necessary assumptions.
- Implementation of technically sound mathematical and computational steps.
- Adherence to and working within the context of given instructions – for example, application of specific methods and tools as required.
- Communication must be done in grammatically and sensibly correct English.

Assignments are due on the weeks on the table above. Submissions must be done electronically via Moodle by the due date.

4. Course Schedule

Week	**Lecture 1** Tue 9:00-11:00 Electrical Engineering G22 (K-G17-G22)	**Lecture 2** Wed 10:00-12:00 Colombo Theatre C (K-B16-LG05)	**Tutorials** Tut 1: various times, K-F10-M03 Computer lab Tut 2: Thu 16:00-17:00 Weeks 2 to 10 Electrical Engineering G23 (K-G17-G23)	Online
1	Course introduction. How to formulate physicochemical problems I (FT)	How to formulate physicochemical problems II (FT)	MATLAB Refresher (tutorial #1, No tutorial #2)	Intro to modelling
2	Treatment of 1st order nonlinear ODEs – I (FT)	Treatment of 1st order nonlinear ODEs – II (FT)	Flow through a variable cross-sectional circular area Flow through a variable cross-sectional circular area	
3	2nd order nonlinear ODEs – reduction to linear forms (FT)	Newton’s method to solve a system of non-linear algebraic equations. nth order linear ordinary differential equations I – homogeneous and complementary solutions (FT)	Time-dependent temperature variation within a cylindrical tank	
4	nth order linear ordinary differential equations II – Method of Undetermined Coefficients, Inverse Operators & Variation of Parameters (FT)	Coupled simultaneous ODEs (FT)	Batch and continuous stirred-tank reactor (CSTR)	

5	Linear differential equations with variable coefficients I - Introduction to series methods (FT)	Linear differential equations with variable coefficients II - Bessel equation, higher order equations with constant coefficients (FT)	Porous, cylindrical pellets for packed beds catalytic reactors & heat transfer in a solid cylindrical rod	
6	Constructing dynamic models, steady states (SP)	Modelling using linear algebra, eigenvectors, eigenvalues (SP)	Solution of a cylindrical pellet with a convective boundary condition & heat transfer through a Thin, circular metal fins (FT)	Linear algebra revision (SWP)
7	Linear models, stability, eigenvalues, normalisation (SP)	Classifying models, response to impulse (SP)	Stability, classification, impulses.	Transformations (SP)
8	Phase space, characteristic directions, characteristic speeds (SP)	Non-linear models, linearisation, perturbations (SP)	Phase portraits	More sketching phase portraits (SP)
9	Phase space for periodic systems, non-linear systems (SP)	Bifurcations, pitchfork, Hopf, Lorenz model (SP)	Linearisation, more phase portraits	Non-linear phase portraits (SP)
10	Case studies, summary and overview (SP)	Bifurcations, saddle-node, transcritical, multiplicity (SP)	Bifurcations	
11				

(SP) = Stuart Prescott, (FT) = Francisco Trujillo

Tutorials: there are two tutorials per week. On the first tutorial students will work on the assigned problem in small groups on the computer lab. The second tutorial will be supervised by one of the lectures to help students and answer questions.

5. Resources for Students

Recommended texts

1. Rice, R. G. and Do, D.D., Applied Mathematics and Modelling for Chemical Engineers, John Wiley, 1995.

Reference texts

1. Kreyszig, E., Advanced Engineering Mathematics, John Wiley, 8th edition, 1999.
2. Amundson, N.R., Mathematical Methods in Chemical Engineering, Prentice-Hall, Englewood Cliffs, New Jersey, 1966.
3. Numerical Methods for Engineers by B.M. Ayyub & R.H. McCuen, 1st edition, Prentice-Hall 1995.
4. Problem Solving in Chemical Engineering with Numerical Methods by M.B. Cutlip & M. Shacham, 1st edition, Prentice-Hall, 1999.

UNSW Library also has other useful resources. Assistance may be obtained from:

info.library.unsw.edu.au/web/services/services.html

6. 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.

7. The rationale behind the approach to learning and teaching

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 tutorials, but supplementation will be provided through assignment problems (which will be graded). Solutions will be given in class tutorials. 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.

8. Academic Honesty and Plagiarism

What is Plagiarism?

Plagiarism is the presentation of the thoughts or work of another as one's own. Examples include:

- direct duplication of the thoughts or work of another, including by copying material, ideas or concepts from a book, article, report or other written document (whether published or unpublished), composition, artwork, design, drawing, circuitry, computer program or software, web site, Internet, other electronic resource, or another person's assignment without appropriate acknowledgement;
- paraphrasing another person's work with very minor changes keeping the meaning, form and/or progression of ideas of the original;
- piecing together sections of the work of others into a new whole;
- presenting an assessment item as independent work when it has been produced in whole or part in collusion with other people, for example, another student or a tutor; and
- claiming credit for a proportion a work contributed to a group assessment item that is greater than that actually contributed.†

For the purposes of this policy, submitting an assessment item that has already been submitted for academic credit elsewhere may be considered plagiarism.

Knowingly permitting your work to be copied by another student may also be considered to be plagiarism.

Note that an assessment item produced in oral, not written, form, or involving live presentation, may similarly contain plagiarised material.

The inclusion of the thoughts or work of another with attribution appropriate to the academic discipline does *not* amount to plagiarism.

The Learning Centre website is main repository for resources for staff and students on plagiarism and academic honesty. These resources can be located via:

https://student.unsw.edu.au/plagiarism

The Learning Centre also provides substantial educational written materials, workshops, and tutorials to aid students, for example, in:

- correct referencing practices;
- paraphrasing, summarising, essay writing, and time management;
- appropriate use of, and attribution for, a range of materials including text, images, formulae and concepts.

Individual assistance is available on request from The Learning Centre.

Students are also reminded that careful time management is an important part of study and one of the identified causes of plagiarism is poor time management. Students should allow sufficient time for research, drafting, and the proper referencing of sources in preparing all assessment items.

* Based on that proposed to the University of Newcastle by the St James Ethics Centre. Used with kind permission from the University of Newcastle

† Adapted with kind permission from the University of Melbourne.

9. Course Evaluation and Development

Course delivery is influenced by student feedback in order to ensure continuous improvement. Typically, this is done through the administration of UNSW's MyExperience survey (https://student.unsw.edu.au/myexperience). Several aspects of this course, for example, greater emphasis on treatment of nonlinear 2nd order ODEs have been influenced by previous student feedback. Your constructive suggestions would help in securing better presentation to future students.

10. Other Matters

Calculators are sometimes required in final exams but are no longer supplied by the university. You must provide your own accredited calculator, see university policy at:

https://student.unsw.edu.au/exam-approved-calculators-and-computers

School policy on administrative matters relating to undergraduate students, including matters relating to examination procedures, and what to do in the event of illness or misadventure, may be found on the School's website at:

http://www.engineering.unsw.edu.au/chemical-engineering/policies-procedures

Please also note School policy on special consideration and further assessment at:

http://www.engineering.unsw.edu.au/chemical-engineering/special-consideration-illness-or-misadventure

Information on UNSW Occupational Health and Safety policies and expectations may be found at:

http://www.ohs.unsw.edu.au

Students who have a disability that requires some adjustment in their learning and teaching environment are encouraged to discuss their study needs with the course convener (Dr Francisco J. Trujillo) prior to, or at the commencement of the course, or with the Equity Officer (Disability) in the Equity and Diversity Unit (9385 4734). Information for students with disabilities is available at:

http://www.studentequity.unsw.edu.au

Issues to be discussed may include access to materials, signers or note-takers, the provision of services and additional examination and assessment arrangements. Early notification is essential to enable any necessary adjustments to be made.

10.1 Administrative matters

Students are encouraged to attend all lectures and actively participate in class tutorials. Teaching staff will not be sympathetic to students requiring office consultation if they have been missing lectures, inattentive or disruptive in class. Unruly behaviour in covert or overt forms will not be tolerated.

In the unexpected event of an illness or misadventure causing you to miss a class or assignment due date, please follow the instruction in this link (https://student.unsw.edu.au/special-consideration). Penalty concessions will only be considered if there is unambiguous proof of illness or other misadventure

(see http://www.engineering.unsw.edu.au/chemical-engineering/special-consideration-illness-or-misadventure for School policy on this matter).