Diffusion and Kinetics

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Course Staff

<table>
<thead>
<tr>
<th>Dr Kevin J Laws</th>
<th>Room 301, School of Materials Science and Engineering (Building E10)</th>
<th>Consultation hours: by appointment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Course Coordinator Lecturer</td>
<td>Phone: 9385 5234 <a href="mailto:k.laws@unsw.edu.au">k.laws@unsw.edu.au</a></td>
<td></td>
</tr>
<tr>
<td>Assoc. Prof. Jason Harper</td>
<td>Room 223 Dalton Building (F12) School of Chemistry</td>
<td>Consultation hours: by appointment</td>
</tr>
<tr>
<td>Lecturer</td>
<td>Phone: 9385 4692 <a href="mailto:j.harper@unsw.edu.au">j.harper@unsw.edu.au</a></td>
<td></td>
</tr>
<tr>
<td>Dr Rakesh Joshi</td>
<td>Room 448, School of Materials Science and Engineering (Building E10)</td>
<td>Consultation hours: by appointment</td>
</tr>
<tr>
<td>Lecturer</td>
<td>Phone: 93854324 <a href="mailto:r.joshi@unsw.edu.au">r.joshi@unsw.edu.au</a></td>
<td></td>
</tr>
</tbody>
</table>
Course Objective
In this course you will be introduced to the fundamentals of kinetics and diffusion mechanisms pertinent to engineering materials. When successfully completed, you will be able to apply these fundamentals to quantify transport phenomena that occur in various materials processing applications.

Your Course at a Glance

<table>
<thead>
<tr>
<th>Week</th>
<th>Course Lecture Program (Lecturer)</th>
<th>LABS*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Kinetics - Introduction &amp; Reaction Rates (JH)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Kinetics - Temperature Effects &amp; Reaction Order &amp; Mechanisms (JH)</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Kinetics - Temperature Effects &amp; Reaction Order &amp; Mechanisms (JH)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Kinetics – Catalysis, Enzymes &amp; Molecular Reactions (JH)</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Kinetics - Tutorial Session &amp; Practice Exam Questions (JH)</td>
<td>Kinetics Exam (25%)</td>
</tr>
<tr>
<td>4</td>
<td>Diffusion Fundamentals - Introduction to Diffusion (RJ)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Diffusion Fundamentals - Diffusion in Liquids 1 (RJ)</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Diffusion Fundamentals - Diffusion in Liquids 2 (RJ)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Diffusion Fundamentals - Diffusion in Gasses (RJ)</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Diffusion Fundamentals - Diffusion in Solids (RJ)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Diffusion Fundamentals - Diffusion in Thin Films (RJ)</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Diffusion Fundamentals - Tutorial &amp; Practice Exam (RJ)</td>
<td>Diffusion Fundamentals Exam (30%)</td>
</tr>
<tr>
<td>8</td>
<td>Applied Diffusion &amp; Kinetics - Introduction (KJL)</td>
<td>LA1</td>
</tr>
<tr>
<td></td>
<td>Applied Diffusion &amp; Kinetics - Everyday Diffusion &amp; Kinetics Cases (KJL)</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Applied Diffusion &amp; Kinetics - Nucleation, Crystallisation &amp; Growth (KJL)</td>
<td>LA2</td>
</tr>
<tr>
<td></td>
<td>Applied Diffusion &amp; Kinetics - Nucleation, Crystallisation &amp; Growth (KJL)</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>Applied Diffusion &amp; Kinetics - Recrystallisation &amp; Transformation (KJL)</td>
<td>LA3</td>
</tr>
<tr>
<td></td>
<td>Applied Diffusion &amp; Kinetics - Grain Boundary &amp; Interface Diffusion (KJL)</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>Applied Diffusion &amp; Kinetics – Segregation &amp; Homogenisation (KJL)</td>
<td>LA4</td>
</tr>
<tr>
<td></td>
<td>Applied Diffusion &amp; Kinetics - Segregation &amp; Homogenisation (KJL)</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>Applied Diffusion &amp; Kinetics - Tutorial &amp; Practice Exam (KJL)</td>
<td></td>
</tr>
</tbody>
</table>

* You need to attend only one of these identical laboratory sessions
### Timetable

<table>
<thead>
<tr>
<th>Week</th>
<th>Day</th>
<th>Time</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – 6</td>
<td>Monday</td>
<td>14:00 – 16:00</td>
<td>Webster Theatre B (G15)</td>
</tr>
<tr>
<td></td>
<td>Thursday</td>
<td>11:00 – 13:00</td>
<td>Tyree Energy Technology G16 (H6)</td>
</tr>
<tr>
<td>7 – 12</td>
<td>Monday</td>
<td>14:00 – 16:00</td>
<td>Webster Theatre B (G15)</td>
</tr>
<tr>
<td></td>
<td>Thursday</td>
<td>11:00 – 13:00</td>
<td>Tyree Energy Technology G16 (H6)</td>
</tr>
</tbody>
</table>

### Laboratory

MATS2006 Laboratories are scheduled as below at Chemistry Lab Room 162 West (Chemistry teaching lab). Students must attend one of the four (identical) laboratory classes run on weeks 8, 9, 10 and 11. A lab report must be submitted at the end of the lab class.

#### Kinetics Laboratory Schedule

You need to attend only one of the laboratory sessions. You must attend your allocated laboratory. Laboratories slots are fixed, and if you do not attend your allocated session, or do not bring appropriate PPE you will not be able to re-take the laboratory class and receive a zero grade.

<table>
<thead>
<tr>
<th>Week</th>
<th>Day</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>LA1</td>
<td>Friday</td>
<td>9:00 – 12:00</td>
</tr>
<tr>
<td>LA2</td>
<td>Friday</td>
<td>9:00 – 12:00</td>
</tr>
<tr>
<td>LA3</td>
<td>Friday</td>
<td>9:00 – 12:00</td>
</tr>
<tr>
<td>LA4</td>
<td>Friday</td>
<td>9:00 – 12:00</td>
</tr>
</tbody>
</table>

### Course Content

**Kinetics** - Reaction rate definition, the rate law, rate constant and order. Experimental determination of the rate law: the method of initial rates, methods using integrated rate equations for 1st order and 2nd order reactions; rate constants, half-life. Effect of temperature on reaction rates: the Arrhenius equation, activation energy and frequency factor. Elementary reactions, mechanism, rate determining step; relation to the rate law. Complex reactions: opposing, consecutive and parallel reactions; catalysis and catalysts; enzyme catalysis, Michaelis-Menten mechanisms, molecular reaction kinetics and collision theory.

**Diffusion Fundamentals** - Introduction to diffusion in gasses, liquids, membrane transport, Facilitated diffusion, osmosis, diffusion in solids and thin films, Fick’s first and second laws, factors affecting diffusion

**Applied Diffusion & Kinetics** – Introduction to nucleation and growth in liquid-solid and solid-solid systems, diffusion based recrystallisation and phase transformations, role of kinetics on phase retention (quenching) grain boundary and interface diffusion; role of processing variables on diffusion/kinetics based processes.

### Laboratory work

Laboratory work in the course is designed to directly complement the lecture material and to provide practical understanding and experience in reaction kinetics. Students should note that:

Attendance at laboratory classes is compulsory.
Prior to selected laboratories, students will receive OHS information (such as risk assessments) and will be required to sign a declaration that they have read and understood this information.

Appropriate footwear must be worn by students in laboratories at all times. Safety glasses and laboratory coats must be worn in laboratories. These items will not be provided by the School – students are expected to provide their own. Any student not wearing these items will not be permitted in the laboratory and will not be allowed to retake the laboratory at another time and will receive a mark of zero for that laboratory.

Assessment

<table>
<thead>
<tr>
<th>Assessment Task</th>
<th>Fraction</th>
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<tbody>
<tr>
<td>Kinetics Exam</td>
<td>25%</td>
</tr>
<tr>
<td>Wednesday, Week 4, in class, on all kinetics content. Students will be asked to understand simple and complex kinetic systems, determine and apply rate equations, and interpret real data in terms of the theory provided.</td>
<td></td>
</tr>
<tr>
<td>Diffusion Fundamentals Exam</td>
<td>30%</td>
</tr>
<tr>
<td>Wednesday, Week 8, in class based on all diffusion fundamentals content. Students will be asked to understand basic principles of diffusion, fundamental theory, examples of diffusion process, and possible application.</td>
<td></td>
</tr>
<tr>
<td>Applied Diffusion &amp; Kinetics Exam</td>
<td>35%</td>
</tr>
<tr>
<td>TBA - Exam Period based on all applied diffusion and kinetics class content. Students will be asked understand and apply simple fundamental aspects of diffusion and kinetics in commonplace examples and processes.</td>
<td></td>
</tr>
<tr>
<td>Laboratory</td>
<td>10%</td>
</tr>
<tr>
<td>Small group exercise in the laboratory, determining initial reaction rates and correlating concentration dependence to order of the reaction. Concludes with a written report</td>
<td></td>
</tr>
<tr>
<td>Report Due: Conclusion of laboratory period</td>
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References

Kinetics

Diffusion

Learning and Teaching Philosophy Underpinning the Course
(based on UNSW Learning Guidelines)

• Students are actively engaged in the learning process.
  It is expected that, in addition to attending classes, students will read, write, discuss, and engage in analysing the course content.
• Effective learning is supported by a climate of inquiry where students feel appropriately challenged.
  Students are expected to be challenged by the course content and to challenge their own preconceptions, knowledge, and understanding by questioning information, concepts, and approaches during class and study.
• Learning is more effective when students’ prior experience and knowledge are recognised and built on.
  Coursework, tutorials, assignments, laboratories, examinations, and other forms of learning and assessment are intended to provide students with the opportunity to cross-reference these activities in a meaningful way with their own experience and knowledge.
• Students become more engaged in the learning process if they can see the relevance of their studies to professional and disciplinary contexts
  The course content is designed to incorporate both theoretical and practical concepts, where the latter is intended to be applicable to real-world situations and contexts.

Course Information

<table>
<thead>
<tr>
<th>Units of credit</th>
<th>6</th>
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<tbody>
<tr>
<td>How the course relates to other course offerings and overall program(s) in the discipline</td>
<td>This course will give intellectual framework for a number of materials science courses such as phase transformation, materials processing, extractive metallurgy etc taught in years 3 and 4.</td>
</tr>
</tbody>
</table>
| Graduate attributes which will be gained through the course | • Research, inquiry and analytical thinking abilities  
• Capability and motivation for intellectual development  
• Communication  
• Information literacy  
• Capacity for lifelong learning and professional development  
• Professional attitudes |
| Expected learning outcomes | In doing this course, you will learn to:  
• correctly use the language of chemical kinetics including:  
  • rate, rate law, order, molecularity, elementary and overall reaction, half-life; isolation method, pseudo-order, rate determining step, reactive intermediate, steady state approximation; mechanism; activation energy, frequency factor; catalyst; potential energy surface, reaction coordinate, steric factor, transition state. |
- define the (true) rate in terms of the rate of change in any reactant or product
- establish the connection between the observable used to monitor the progress of the reaction and the variable in the rate equation
- use experimental data to propose and/or verify a rate law and determine the rate constant using:
  - the method of initial rates (the isolation method)
  - integrated rate equations for 1st order and simple cases of 2nd order reactions
  - integrated rate equations for such other cases for which the appropriate equations are supplied
- define the half-life of a reactant and, for first and 2nd order reactions, relate it to rate constant
- derive a rate law from a hypothetical reaction mechanism (simple case only)
- define the rate determining step, describe and use the steady state approximation
- relate the equilibrium constant for the overall reaction to rate constants for individual steps
- use the Arrhenius equation to describe the variation of rate constants with temperature
- describe: the role of catalysts in altering the reaction rate
- interpret data for enzyme catalysed reactions in terms of the Michaelis-Menten mechanism
- describe the derivation of expressions for the rate constant according to collision theory and be able to use such expressions to calculate rate constants.
- correctly use the terms: collision cross section, reduced mass, steric factor, reactive cross section, potential energy surface
- Quantify chemical kinetics and mass transfer processes and apply this knowledge in predicting the rates of materials processing operations.
- Quantify time dependent mechanisms that occur in materials processing and synthesis with the help of Fick’s laws of diffusion.
- Appreciate the role of microstructural features such as grain boundaries, dislocations and point defects in diffusion
- Ability to identify, formulate and solve reaction engineering problems from 1st principles
- You will also learn to:
  - Think critically in decision making and problem-solving
  - Communicate with correct terminology

### Teaching strategies

- Core concepts, theories and approaches to address kinetic, diffusion and reaction engineering problems will be covered in lectures. Several examples will be discussed to demonstrate the use of kinetics and diffusion in materials science and engineering.
- Grades are distributed between different small formative assessment tasks to encourage students to engage with the course material consistently during the semester, to allow practicing the different skills the course aims to support and provide timely feedbacks.
- State of the art chemical plant operations will be discussed as part as a site visit to Qenos Sydney manufacturing plant.
A seminar will be presented on a topic selected for its relevance to material science students and its technical and applicative significance. The seminars will be presented by a leading expert.

Teaching material, including course outline, notes, problems, assignments, case studies and course announcements are available on the Course Moodle website.

^Based on the professional attributes given in Engineers Australia National Generic Competency Standards - Stage 1 Competency Standard for Professional Engineers and UNSW Graduate Attributes.

Academic Honesty and Plagiarism

What is Plagiarism?

All details regarding plagiarism can be found here: [https://student.unsw.edu.au/plagiarism](https://student.unsw.edu.au/plagiarism)

It is important to understand what plagiarism is. The general concept is plagiarism is using the words or ideas of others and passing them off as your own. Examples of plagiarism, including self-plagiarism, are:

- **Copying**

  Using the same or very similar words to the original text or idea without acknowledging the source or using quotation marks. This includes copying materials, ideas or concepts from a book, article, report or other written document, presentation, composition, artwork, design, drawing, circuitry, computer program or software, website, internet, other electronic resource, or another person's assignment, without appropriate acknowledgement.

- **Inappropriate paraphrasing**

  Changing a few words and phrases while mostly retaining the original structure and/or progression of ideas of the original, and information without acknowledgement.

  This also applies in presentations where someone paraphrases another’s ideas or words without credit and to piecing together quotes and paraphrases into a new whole, without appropriate referencing.

- **Collusion**

  Presenting work as independent work when it has been produced in whole or part in collusion with other people. Collusion includes,
  
  - students providing their work to another student before the due date, or for the purpose of them plagiarising at any time
  - paying another person to perform an academic task and passing it off as your own
  - stealing or acquiring another person’s academic work and copying it
  - offering to complete another person’s work or seeking payment for completing academic work.

  This should not be confused with academic collaboration.

- **Inappropriate citation**

  Citing sources which have not been read, without acknowledging the ‘secondary’ source from which knowledge of them has been obtained.

- **Self-plagiarism**

  ‘Self-plagiarism’ occurs where an author republishes their own previously written work and presents it as new findings without referencing the earlier work, either in its entirety or partially.
Self-plagiarism is also referred to as 'recycling', 'duplication', or 'multiple submissions of research findings' without disclosure. In the student context, self-plagiarism includes reusing parts of, or all of, a body of work that has already been submitted for assessment without proper citation.

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.

Continual Course Improvement

- At the end of the course, students will be asked to provide evaluative feedback through myExperience, the University’s course and teaching evaluation and improvement process.
- Students are encouraged to address any problems regarding teaching of this course at the annual staff-student meeting.
- Student comments on teaching during the session are welcome and will be appreciated.
- At times students may be asked to answer a short questionnaire for feedback on the course.

Administrative Matters

- Students should attend at least 80% of all classes.
- Students unable to submit assignments on time or attend the laboratory or exams on health grounds should make a request for special consideration. Information on this process can be found here: https://student.unsw.edu.au/special-consideration. Medical certificates or other appropriate documents must be included. Students should also advise the lecturer of the situation.
- Unless otherwise specified in the task criteria, all assignments must be uploaded via Moodle prior to the due date for submission.
- Assignments/lab reports submitted after the due date for submission will receive a 10% of maximum grade penalty for every day late, or part thereof.
- Students who have a disability that requires some adjustment in their teaching or learning environment are encouraged to discuss their study needs with the course coordinator prior to, or at the commencement of, their course, or with the Equity Officer (Disability) in the Equity and Diversity Unit: https://student.unsw.edu.au/disability. Early notification is essential to enable any necessary adjustments to be made.

Rules for Exams

Rules governing conduct during exams are given at: https://student.unsw.edu.au/exam-rules