Annexe A: New/Revised Course Content in OBTL+ Format

Course Overview

| Course Over view | |
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| Expected Implementation in Academic Year | AY2024/2025 |
| Semester/Trimester/Others (specify approx. Start/End date) | Semester 2 |
| Course Author * Faculty proposing/revising the course | Edwin Yeow and Atsushi Goto |
| Course Author Email | edwinyeow@ntu.edu.sg; agoto@ntu.edu.sg |
| Course Title | CHEMICAL KINETICS & DYNAMICS |
| Course Code | CM4042 |
| Academic Units | 3 |
| Contact Hours | 39 |
| Research Experience Components | Not Applicable |

Course Requisites (if applicable)

| Pre-requisites | CM3041 or by permission |
|-----------------------|-------------------------|
| Co-requisites | |
| Pre-requisite to | |
| Mutually exclusive to | |
| Replacement course to | |
| Remarks (if any) | |

Course Aims

On completing this course, you will employ advanced mathematical and physical ideas for understanding a range of chemical phenomena. You will enhance the knowledge of the kinetics of major chemical processes on a mathematical basis. You will appreciate the power of kinetic ideas in chemical research and industry activities.

Course's Intended Learning Outcomes (ILOs)

Upon the successful completion of this course, you (student) would be able to:

| ILO 1 | Describe the rate laws of chemical reactions. |
|--------|--|
| ILO 2 | Derive the various integrated rate laws for first-order, second-order, third-order and general-order reactions, and be able to explain and apply their corresponding concepts. |
| ILO 3 | explain elementary reactions. |
| ILO 4 | Explain the concept of reversible reactions. |
| ILO 5 | Explain the concept of parallel reactions. |
| ILO 6 | explain the concept of consecutive reactions. |
| ILO 7 | Explain the kinetic reason why the steady-state approximation can be applied. |
| ILO 8 | Explain the concept of Lindemann mechanism. |
| ILO 9 | Explain the concept of chain reactions in small molecular and polymeric systems. |
| ILO 10 | Explain the concept of enzymatic reactions. |
| ILO 11 | interpret the viscosity as a transportation of momentum (Newton's law of viscosity). |
| ILO 12 | Explain how the viscosity is related to the flow rate (Poiseuille formula). |
| ILO 13 | interpret the diffusion as a transportation of molecule. |
| ILO 14 | Explain how the diffusion is related to the concentration gradient (Fick's law of diffusion). |
| ILO 15 | Explain how the diffusion is related to the concentration changes with respect to time and displacement (Fick's second law of diffusion). |
| ILO 16 | Describe the mean value and root-mean-square value of the average distance that molecules diffuse in a given period of time. |
| ILO 17 | Explain the concept of Brownian Motion (Langevin equation). |
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| ILO 18 | explain how the diffusion coefficient is related to the viscosity (Stokes-Einstein equation). |
|--------|---|
| ILO 19 | explain the concept of diffusion-controlled and chemically-controlled reactions. |
| ILO 20 | Explain how the diffusion controlled reaction rate is described (Smoluchowski equation). |
| ILO 21 | Explain the concept of static and dynamic quenching of fluorescence molecules. |
| ILO 22 | Explain how the fluorescence quenching rate is described (Stern-Volmer equation). |
| ILO 23 | Explain and apply the concept of Förster energy transfer model. |
| ILO 24 | Explain the factors governing the efficiency of energy transfer. |
| ILO 25 | explain and apply the concept of Marcus electron transfer model. |
| ILO 26 | Explain the factors governing the efficiency of electron transfer. |
| ILO 27 | explain and apply the concept of through-bond interaction. |
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Course Content

(1) Rate laws. 1.1 Rates of reactions 1.2 First-order reactions 1.3 Second-order reactions 1.4 Pseudo first-order reactions 1.5 Third-order reactions 1.6 Reactions of general order 1.7 Temperature dependence of rate constants (2) Reaction mechanism. 2.1 Elementary reactions 2.2. Reversible reactions 2.3. Parallel reactions 2.4. Consecutive reactions 2.5. Steady-state approximation 2.6. Unimolecular decomposition: Lindemann Mechanism 2.7. Chain reactions 2.8. Enzyme catalysis (3) Transport properties. 3.1. Viscosity 3.2. Diffusion (4) Reactions in liquid solutions. 4.1. Smoluchowski equation. 4.2. Stern-Volmer equation. (5) Electronic energy transfer. 5.1. Förster energy transfer 5.2. Förster critical distance 5.3. Spectral overlap integral 5.4. Orientation factor 5.5. Energy transfer efficiency and rate of energy transfer (6) Electron transfer 6.1. The Rehm-Weller equation 6.2. Adiabatic and non-adiabatic interactions 6.3. Free energy of activation 6.4. Inner and outer-sphere reorganization energy 6.5. Marcus electron transfer theory 6.6. Through-bond interactions 6.7. Applications in photosynthesis and dyesensitized solar cells.

Reading and References (if applicable)

Recommended textbook: Paul L. Houston, Chemical Kinetics and Reaction Dynamics (2001), Dover Publication; ISBN: 978-0-486-45334-7

Planned Schedule

| Week or Session | Topics or Themes | ILO | Readings | Delivery Mode | Activities |
|-----------------------|--|-----------|--|------------------|------------|
| 1 | Rate laws | 1,2 | Lecture Notes, Chapter 2 in textbook "Chemical Kinetics and Reaction Dynamics" by Paul L. Houston. | | |
| 2 | Elementary reactions, Reversible reactions, Parallel reactions, Consecutive reactions | 3-6 | Lecture Notes, Chapter 2 in textbook "Chemical Kinetics and Reaction Dynamics" by Paul L. Houston. | | |
| 3 | Steady-state approximation, Unimolecular decomposition: Lindemann Mechanism | 7,8 | Lecture Notes, Chapter 2 in textbook "Chemical Kinetics and Reaction Dynamics" by Paul L. Houston. | | |
| 4 | Chain reactions, Enzyme catalysis | 9,10 | Lecture Notes, Chapter 2 in textbook "Chemical Kinetics and Reaction Dynamics" by Paul L. Houston. | | |
| 5 | Viscosity | 11,1 2 | Lecture Notes, Chapter 4 in textbook "Chemical Kinetics and Reaction Dynamics" by Paul L. Houston. | | |
| 6 | Diffusion | 13- 18 | Lecture Notes, Chapter 4 in textbook "Chemical Kinetics and Reaction Dynamics" by Paul L. Houston. | | |
| 7 | Smoluchowski equation | 19,2 0 | Lecture Notes, Chapter 5 in textbook "Chemical Kinetics and Reaction Dynamics" by Paul L. Houston. | | |
| 8 | Stern-Volmer equation | 21,2 2 | Lecture Notes, Chapter 5 in textbook "Chemical Kinetics and Reaction Dynamics" by Paul L. Houston. | | |
| 9 | Electronic energy transfer | 23 | | | Lectures |
| 10 | Electronic energy transfer | 24 | | | Lectures |

| Week or Session | | ILO | Readings | Delivery Mode | Activities |
|-----------------------|--|-----------|----------|------------------|------------|
| 11 | Midterm test 2 and electron transfer | 25 | | | Lectures |
| 12 | Electron transfer | 25,2 6 | | | Lectures |
| 13 | Electron transfer | 26,2 7 | | | Lectures |

Learning and Teaching Approach

| Approach | How does this approach support you in achieving the learning outcomes? |
|---------------------|--|
| Lectures (39 hours) | You will be spending time to learn details for the course content in lecture theatre. Topics in course content will be introduced in lecture. Application questions will be discussed and explained. |

Assessment Structure

Assessment Components (includes both continuous and summative assessment)

| No. | Component | ILO | Related PLO or Accreditation | Weightage | Description of Assessment Component | | Rubrics | Level of Understanding |
|-----|--|---|---------------------------------|-----------|--|------------|----------|---------------------------|
| 1 | Continuous Assessment (CA): Others([quiz/test]) | 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 | Competence, Creativity | 20 | | Individual | Analytic | Multistructural |
| 2 | Continuous Assessment (CA): Others([quiz/test]) | TBA in class. | Competence, Creativity | 20 | | Individual | Analytic | Multistructural |
| 3 | Summative Assessment (EXAM): Others([final examination] Examination (Multiple Choice Questions)) | All | Competence, Creativity | 60 | | Individual | Analytic | Multistructural |

| Description of Assessment Components (if applicable) | | | | |
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Formative Feedback

You will be given feedback in three ways:

- 1. By response to postings on the course discussion board.
- 2. Through the marking of the mid-term.
- 3. General feedback will be provided to the students following the final exam.

NTU Graduate Attributes/Competency Mapping

This course intends to develop the following graduate attributes and competencies (maximum 5 most relevant)

| Attributes/Competency | Level | | |
|-----------------------|----------|--|--|
| Curiosity | Basic | | |
| Decision Making | Basic | | |
| Problem Solving | Advanced | | |

Course Policy

Policy (Academic Integrity)

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values. As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. On the use of technological tools (such as Generative AI tools), different courses / assignments have different intended learning outcomes. Students should refer to the specific assignment instructions on their use and requirements and/or consult your instructors on how you can use these tools to help your learning. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Policy (General)

You are expected to attend lecture classes or watch the recorded lecture videos and take all scheduled tests.

Policy (Absenteeism)

Absence from the midterm without a valid reason will affect your overall course grade. Valid reasons include falling sick supported by a medical certificate and participation in NTU's approved activities supported by an excuse letter from the relevant bodies. There will be make-up opportunities for CA components.

Policy (Others, if applicable)

Diversity and Inclusion Policy

Integrating a diverse set of experiences is important for a more comprehensive understanding of science and engineering. It is our goal to create an inclusive and collaborative learning environment that supports a diversity of perspectives and learning experiences. That honours your identities, including ethnicity, gender, socioeconomic status, sexual orientation, religion, or ability.

To help accomplish this:

- If you are neuroatypical or neurodiverse, have dyslexia or ADHD (for example), or have a social anxiety disorder or social phobia:
- If you feel your performance in the course is being impacted by your experiences outside of class:hi Ai HUa
- If something was said in the course (by anyone, including instructor/supervisor) that made you uncomfortable.

Please e-mail our Associate Chair (Students & Continuing Education) at ac-cceb-stud@ntu.edu.sg about how we can help facilitate your learning experience.

As a participant in course discussions, you should also strive to honour the diversity of your classmates.

You can do this by using preferred pronouns and names, being respectful of others' opinions, actively making sure all voices are being heard, and refraining from the use of derogatory or demeaning speech or actions.

All members of the course are expected to strictly adhere to the student code of conduct (https://www.ntu.edu.sg/life-at-ntu/student-life/student-conduct). If you witness something that goes against this or has any other concerns, please speak to your instructors or a faculty member.

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