Nanyang Technological University
Division of Chemistry and Biological Chemistry

Academic Year	AY19/20	**Semester**	2
Course Coordinator	Edwin Yeow (Assoc Prof) Atsushi Goto (Assoc Prof)		
Course Code	CM4042		
Course Title	Chemical Kinetics and Dynamics		
Pre-requisites	CM3041 or by permission		
No of AUs	3		
Contact Hours	Lectures: 39		
Proposal Date	08 January 2020		

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.

Intended Learning Outcomes (ILO)

By the end of this course, you (as a student) would be able to:

Rate laws.

1. Describe the rate laws of chemical reactions.
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.

Reaction mechanism.

3. Explain elementary reactions.
4. Explain the concept of reversible reactions.
5. Explain the concept of parallel reactions.
6. Explain the concept of consecutive reactions.
7. Explain the kinetic reason why the steady-state approximation can be applied.
8. Explain the concept of Lindemann mechanism.
9. Explain the concept of chain reactions in small molecular and polymeric systems.
10. Explain the concept of enzymatic reactions.

Transport properties.

11. Interpret the viscosity as a transportation of momentum (Newton’s law of viscosity).
12. Explain how the viscosity is related to the flow rate (Poiseuille formula).
13. Interpret the diffusion as a transportation of molecule.
14. Explain how the diffusion is related to the concentration gradient (Fick’s law of diffusion).

15. Explain how the diffusion is related to the concentration changes with respect to time and displacement (Fick's second law of diffusion).
16. Describe the mean value and root-mean-square value of the average distance that molecules diffuse in a given period of time.
17. Explain the concept of Brownian Motion (Langevin equation).
18. Explain how the diffusion coefficient is related to the viscosity (Stokes-Einstein equation).

Reactions in liquid solutions.

19. Explain the concept of diffusion-controlled and chemically-controlled reactions.
20. Explain how the diffusion controlled reaction rate is described (Smoluchowski equation).
21. Explain the concept of static and dynamic quenching of fluorescence molecules.
22. Explain how the fluorescence quenching rate is described (Stern-Volmer equation).

Electronic energy transfer.

23. Explain and apply the concept of Förster energy transfer model.
24. Explain the factors governing the efficiency of energy transfer.

Electron transfer.

25. Explain and apply the concept of Marcus electron transfer model.
26. Explain the factors governing the efficiency of electron transfer.
27. Explain and apply the concept of through-bond interaction.

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 dye-sensitized solar cells.

Assessment (includes both continuous and summative assessment)

Component	Course ILO Tested	Related Programme LO or Graduate Attributes	Weighting	Team/Individual	Assessment rubrics
1. Midterm Test 1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10	Competence, Creativity	20%	Individual	Point-based marking (not rubrics based)

2. Midterm Test 2	TBA in class.	Competence, Creativity	20%	Individual	Point-based marking (not rubrics based)
3. Examination (Multiple Choice Questions)	*All*	Competence, Creativity	60%	Individual	Point-based marking (not rubrics based)
Total			*100%*		

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.

Learning and Teaching approach

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.

Reading and References

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

Course Policies and Student Responsibilities

(1) General

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

(2) 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.

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. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Course Instructors

Instructor	Office Location	Phone	Email
Edwin Yeow (Assoc Prof)	SPMS-CBC-03-04	63168759	edwinyeow@ntu.edu.sg
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Planned Weekly Schedule

Week	Topic	Course ILO	Readings/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, 4, 5, 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, 12	Lecture Notes, Chapter 4 in textbook “Chemical Kinetics and Reaction Dynamics” by Paul L. Houston.
6	Diffusion	13, 14, 15, 16, 17, 18	Lecture Notes, Chapter 4 in textbook “Chemical Kinetics and Reaction Dynamics” by Paul L. Houston.
7	Smoluchowski equation	19, 20	Lecture Notes, Chapter 5 in textbook “Chemical Kinetics and Reaction Dynamics” by Paul L. Houston.
8	Stern-Volmer equation	21, 22	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.
11	Midterm test 2 and electron transfer	25	Lectures
12	Electron transfer	25, 26	Lectures
13	Electron transfer	26, 27	Lectures

CBC Programme Learning Outcome

The Division of Chemistry and Biological Chemistry (CBC) offers an undergraduate degree major in Chemistry that satisfies the American Chemical Society (ACS) curricular guidelines and equips students with knowledge relevant to the industry. Graduates of the Division of Chemistry and Biological Chemistry should have the following key attributes:

1. Competence

Graduates should be well-versed in the foundational and advanced concepts of chemical science, be able to evaluate chemistry-related information critically and independently, and be able to use complex reasoning to solve emergent chemical problems.

2. Creativity

Graduates should be able to synthesize and integrate multiple ideas across the curriculum, and propose innovative solutions to emergent chemistry-related problems based on their training in chemistry.

3. Communication

Graduates should be able to demonstrate clarity of thought, independent thinking, and sound scientific analysis and reasoning through written and oral reports to audiences with varying technical backgrounds. They should also be able to effectively engage other professional chemists in collaborative endeavours.

4. Character

Graduates should be able to act in responsible ways and uphold the high ethical standards that the society expects of professional chemists.

5. Civic-mindedness

Graduates should be aware of the impact of chemistry on society, and how chemistry can be applied to benefit mankind. They should also be aware of and uphold the best chemical safety practices.