

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

Course Overview

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|--|--------------------------------------|
| Expected Implementation in Academic Year | AY2025-2026 |
| Semester/Trimester/Others (specify approx. Start/End date) | Semester 2 |
| Course Author * Faculty proposing/revising the course | Dr Alex van Herk |
| Course Author Email | alex.vanherk@ntu.edu.sg |
| Course Title | Polymeric Materials Circularity & AI |
| Course Code | MS6015 |
| Academic Units | 3 |
| Contact Hours | 39 |
| Research Experience Components | |

Course Requisites (if applicable)

| | |
|-----------------------|---|
| Pre-requisites | |
| Co-requisites | |
| Pre-requisite to | |
| Mutually exclusive to | MS7460 Polymer Recycling & Sustainable Polymeric Materials |
| Replacement course to | |
| Remarks (if any) | Coursework students who have previously completed MS7460 Polymer Recycling & Sustainable Polymeric Materials will not be allowed to read MS6015 Polymeric Materials Circularity & AI. |

Course Aims

1. This course is trying to achieve full awareness of the sustainability aspects of materials. This includes looking at existing materials and their ways of recycling as well as redesigning materials on the formulation and molecular level.
2. The course should be taken by course students that have a vested interest in sustainability of polymer materials, including the use of AI in this area.
3. Any professional in materials will be looking at sustainability aspects of materials, being it facilitating recycling or replacement by more sustainable alternatives. So for a future career in materials (being it in research or industry), this course is very useful.
4. Utilizing AI in this area is a rapidly evolving in this area. For students to connect to this trend in an early stage of their studies is of great importance.

Course's Intended Learning Outcomes (ILOs)

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

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| ILO 1 | Generate and pitch a presentation on applying new AI developments on sustainable materials and/or polymer recycling. |
| ILO 2 | Describe the different polymerization mechanisms, classify the main materials according to key materials properties and polymerization mechanism of formation. |
| ILO 3 | Identify the main environmental issues with polymer waste. |
| ILO 4 | Name the most important aspects of polymer waste collection and sorting. |
| ILO 5 | Name the main aspects and current industrial applications of the four polymer recycling routes. |
| ILO 6 | Name the main aspects of life cycle analysis and know the terminology used in LCA. |
| ILO 7 | Know the aspects of sustainable manufacturing of polymeric materials, in particular in copolymerization. |
| ILO 8 | Name examples of reformulation of materials to make them more sustainable. |
| ILO 9 | Know the main aspects of redesigning materials on a molecular level to make them more sustainable, in particular vitrimers and inserting weak bonds in polymers. |
| ILO 10 | To name the main biobased building blocks and biobased replacements of materials with their pro's and con's. |
| ILO 11 | In teamwork write and pitch a presentation (in ppt) on how new AI developments play a role in aspects of this course. |

Course Content

- Materials classification
- Key materials properties
- Step-growth polymerization
- Chain-growth polymerization
- Polymerization techniques
- Environmental issues
- Collecting and sorting of materials
- Primary recycling
- Secondary/mechanical recycling with deterioration of properties and remedies
- Tertiary/chemical recycling
- Quaternary recycling (energy recovery and/or compostable materials)
- Life Cycle Analysis
- Aspects of sustainable manufacturing of materials (e.g. emulsion polymerization)
- Reformulation of materials for increased sustainability
 - Monomaterials
 - Additives
- Redesign of materials on molecular level
 - Thermoplastic vs thermoharders;
 - Physical crosslinks (thermoplastic elastomers), reversible crosslinks (vitrimers)
 - Insertion of weak bonds
- Biobased building blocks
- Biobased materials replacements
- Applications of AI in polymer recycling and developing new sustainable materials
- Working in a team on a presentation on applications of AI in the topics of this course

Reading and References (if applicable)

Introductory readings:

1. *Nature* **2021**, 590, p423, Closed-loop recycling of polyethylene-like materials, S. Mecking et al.
2. *The Straits Times* Nov 2, **2019** Biodegradable disposables can harm environment too
3. *Resources, Conservation and Recycling* Vol 145, **2019**, p 67-77, LCA of plastic waste recovery into recycled materials, energy and fuels in Singapore, Hsien H. Khoo

Further references for the papers to support the slides

4. *Science* **2021**, 373, 51, Plastics in the earth system, Stubbins et al.
5. *J. Industr. Ecology* **2021**, 25, 1318, recycling pathways, Volk et al.
6. *Recycling*, **2024**, 9, 59, AI in sorting, Lubongo et al.
7. *Recycling*, **2022**, 7, 11, Assessment of performance and challenges in use of commercial automated sorting technology for plastic waste. C. Lubongo and P. Alexandridis
8. *Macro Chem Phys* **2022**, 223, 2100488 Plastic as a resource, Mangold et al.
9. *Environm. Sci. Tech.* **2010**, 44, 8264 Sust Metrics LCA, Tabone et al.
10. *www.Intechopen.com* **2012** Recent Advances in the Chemical Recycling of Polymers, D.S. Achilias et al.
11. *Sci. Adv.* **2020**; 6 : eaba7599, Recycling of multilayer plastic packaging materials by solvent-targeted recovery and precipitation, Walker et al.,
12. *Polym. Chem.* **2023**, 14, 2779, An artificial neural network to predict reactivity ratios in radical copolymerization Farajzadehahary et al..
13. *Macromolecules* **2020**, 53, 3994-4011 .Degradable Poly(alkyl acrylates) with Uniform Insertion of Ester Bonds, Comparing Batch and Semibatch Copolymerizations, Lena et al.
14. *J. Am. Chem. Soc.* **2020**, 142, 2100–2104 A Polymer with “Locked” Degradability, Hsu et al.
15. *www.bio-based.eu/markets* Bio-based Building Blocks and Polymers in the World, Pia Skoczinski, et al. Edition **2020**
16. *Macromol. React. Eng.* **2025**, 2400055 W. Rusli, A.M. van Herk, “An improved iterative method to obtain optimal monomer addition profiles in copolymerizations”
17. *Canadian Journal of Chemical Engineering*, **2021**, vol 99, p 31–60. Sustainable polymer reaction engineering: Are we there yet?, M. Dube et al.
18. *Macromol. Rapid Commun.* **2021**, 42, 2000415, Mechanical Recycling of Packaging Plastics, A Review, Z.O.G. Schijns, M.P. Shaver
19. *Nature Reviews Materials* **2020**, 5, 501–516 Chemical Recycling to monomer for an ideal, circular polymer economy, G.W. Coates and Y.D.Y.L. Getzler.
20. *Resources, Conservation & Recycling* **2022**, 179, 106126 Monomaterials, Guerriere et al.
21. *J. Chem. Educ.* **1995**, 72, 138 Visualization of sum of squares space, v Herk
22. *Science* **2011**, 334, 965 Silica-like malleable materials from permanent organic networks. L. Leibler et al.
23. *Angew. Chem.* **2024**, 136, e202402436, Photocatalysis, Anastasaki et al.
24. *Procedia*, **2023**, 116, 522, LCA for Singapore, Low et al.
25. *Macromolecular Symposia* **2025**, 414, 2400185 Advancements in Machine Learning and Artificial Intelligence in Polymer Science, Mavi et al.
26. *ACSAMI* **2022**, 14, 42771 -machine-learning-based-predictions-of-polymer-and-postconsumer waste andraju-et-al
27. *Chemistry A European J* **2025**, 31, e202500718 Machine Learning for Developing Sustainable Polymers, Huo et al.
28. *PNAS* **2023** 120, 23 e2220021120 High-throughput experimentation for discovery of biodegradable polyesters, Fransen et al.

29. *Journal of Material Cycles and Waste Management* **2021** DOI: 10.1007/s10163-021-01182-y, Applying machine learning approach in recycling, Ozedemir et al.

30. *J. Chem. Inf. Comput. Sci.* **1988**, 28, 31-36 SMILES, Weininger

Note: The above listing comprises the foundational readings for the course and more up-to-date relevant readings will be provided when they become available.

Planned Schedule

| Week | Topics/Themes | ILO | Readings | Delivery Mode | Activities |
|------|--|---------------|-----------------|---------------|--|
| 1 | Materials classification Key materials properties Step-growth polymerization Refresh on AI | 1, 2 | 21, 25 | Online | Watch pre-recorded lecture (M1L1, M1L2) Live session 1: Brief introduction on AI |
| 2 | Chain-growth polymer (radical polymerization) | 1, 2 | 30 | Online | Pre-recorded lecture (M1L3) Live session 2 |
| 3 | Chain-growth polymer (Ionic, Coordination) Environmental issues, Collecting and sorting of materials | 1, 2, 3, 4, 5 | 7, 6 | Online | Pre-recorded lecture (M1L3, M2L1, M2L2) Live session 3: Examples of AI in sorting |
| 4 | Primary recycling Secondary/mechanical recycling with deterioration of properties and remedies | 1, 3, 4, 5 | 4, 11, 18 | Online | Pre-recorded lecture (M2L3) Live session 4 |
| 5 | Tertiary/chemical recycling | 1, 5 | 10, 23 | Online | Pre-recorded lecture (M2L4) Live session 5: Examples of AI in recycling |
| 6 | Quaternary recycling (energy recovery and/or compostable materials) Continual Assessment 1 (CA1): Individual Quiz (Module 1 and Module 2) | 1, 5 | 2 | Online | Pre-recorded lecture (M2L5) Live session 6 Continual Assessment 1 (CA1): Individual Quiz (Module 1 and Module 2) |
| 7 | Life Cycle Analysis | 1, 6 | 3, 8, 9, 24, 30 | Online | Pre-recorded lectures (M3L1-L2-L3) Live session 7: AI, in depth, methodologies, use of SMILES |

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|----|---|-----------|-------------------|--------|--|
| 8 | Aspects of sustainable manufacturing of materials, polymerization techniques | 1, 7 | 17 | Online | Pre-recorded lecture (M4L1) Live session 8 |
| 9 | Aspects of sustainable manufacturing of materials (e.g. emulsion polymerization, copolymerization) Reformulation of materials for increased sustainability - Monomaterials - Additives | 1, 7, 8 | 12, 16 | Online | Pre-recorded lecture (M4L2-L3, M5L1-L2-L3) Live session 9: AI in sustainable manufacturing; copolymerization |
| 10 | Redesign of materials on molecular level; physical crosslinks, reversible crosslinks (vitrimers) -Selection of presentation topic for CA3: Team Presentations | 1, 9 | 20, 26 | Online | Pre-recorded lecture (M6L1-L2) Topic Selection (CA3) Live session 10 |
| 11 | Redesign of materials on molecular level - Insertion of weak bonds | 1, 9, 11 | 1, 13, 14, 22, 28 | Online | Pre-recorded lecture (M6L3) Live session 11: AI in predicting (bio)degradability; -Work on team presentation |
| 12 | Biobased building blocks Biobased materials replacements Submit presentation Peer review. Continual Assessment 2 (CA2): Individual Quiz (Module 3 to Module 7) | 1, 10, 11 | 15 | Online | Pre-recorded lecture (M7L1-L2-L3) Live session 12 Continual Assessment 2 (CA2): Individual Quiz (Module 3 to Module 7) |
| 13 | Continuous Assessment 3 (CA3): Team Presentations | 1, 11 | N/A | Online | Live session 13: Continuous Assessment 3 (CA3): Team Presentations |

Learning and Teaching Approach

| Approach | How does this approach support you in achieving the learning outcomes? |
|------------------------|--|
| Prerecorded lectures | The lecture materials are accompanied by self-practice questions, not only help to build the fundamental technical knowledge required for this course, but also help to develop your individual learning abilities and attitudes toward active learning. |
| Live sessions (online) | These sessions will allow you to ask specific questions and for the teacher to assess your understanding of the course materials. We will give live lectures on applications of AI in the area. Each second live session is followed by a quiz about the preceding videos and live lectures. |
| Practice tests | For each module there are self-practice questions that you can go through anytime, anywhere. They are not part of the assessment but simply give you the opportunity to see where you stand in your learning process and anticipate the kind of question that are asked during the quizzes. |

Assessment Structure

Assessment Components (includes both continuous and summative assessment)

| No. | Component | ILO | Related PLO or Accreditation | Weightage | Description of Assessment Component | Team/Individual | Rubrics | Level of Understanding |
|-----|---|------|------------------------------------|-----------------|--|-----------------|----------|---------------------------|
| 1 | Continuous Assessment (CA): Test/Quiz(Continuous Assessments 1 & 2 | 1-10 | N/A | 60 (30 each) | There are 2 quizzes conducted in person at NTU. Each quiz contains between 15 and 20 multiple-choice questions. The students are given 60 minutes to complete each quiz. | Individual | Analytic | Multistructural |
| 2 | Continuous Assessment (CA): Class Participation(In-class participation and discussions on applications of AI (live sessions)) | 1-10 | N/A | 20 | The live sessions themselves contain continuous assessment through interaction with the instructor. The students can ask questions beforehand by email and during the session, also the instructor will also ask questions to the students. The teacher will present new slides on AI in the live session. | Individual | Holistic | Multistructural |

| No. | Component | ILO | Related PLO or Accreditation | Weightage | Description of Assessment Component | Team/Individual | Rubrics | Level of Understanding |
|-----|---|-----|------------------------------|-----------|---|-----------------|----------|------------------------|
| 3 | Continuous Assessment (CA): Presentation(Continuou s Assessment 3 (CA3): Team Presentations) | 11 | N/A | 20 | The presentation is collated on a topic of choice on applications of AI in sustainable materials by the team of students but with a clear relation to the course and AI. The students should be able to show that they can comprehensively summarize the recent literature on the topic and apply the concepts of the course in what is written and presented (for example applications of AI in redesign of products/molecules). | Team | Holistic | Multistructural |

Description of Assessment Components (if applicable)

Formative Feedback

Feedback is an important aspect to this course. You will receive the scores per question in the quiz right after the quiz. In the next live session, the quiz questions and answers will be explained. Email feedback can be expected from me about your performance during the live sessions if needed.

NTU Graduate Attributes/Competency Mapping

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

| Attributes/Competency | Level |
|-----------------------|--------------|
| Care for Environment | Intermediate |
| Care for Society | Intermediate |
| Ethical Reasoning | Intermediate |
| Global Perspective | Intermediate |
| Design Thinking | Intermediate |

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 complete all assigned video viewings and readings, attend all classes punctually and complete all scheduled quizzes and submit the powerpoint presentation within the allocated times. You are expected to take responsibility to follow up with assignments and course related announcements. You are expected to participate in all class discussions and activities.

Policy (Absenteeism)

In-class activities make up a portion of your course grade. Absence from class without a valid reason will affect your participation 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 no make-up opportunities for in-class activities.

Policy (Others, if applicable)

Use of AI in preparing the team presentation is allowed, however the students should "own" the contents of their presentation.

Last Updated Date: 24-10-2025 13:20:13

Last Updated By: Tan Yong Lay Hayden