MSc in Chemical Modelling Curriculum

Trimester 1	Trimester 2	Trimester 3
3 Aug 26 to 30 Oct 26	9 Nov 26 to 19 Feb 27	1 Mar 27 to 28 May 26

You may refer to this link for more information on the academic calendar.

Core			
Course Code	**Course title**	**Trimester**	**Academic Unit (AU)**
CH6250	Introduction to Numerical Methods & Machine Learning	1	3
CH6420	Advanced Statistics for Data Science Analytics for Chemical Engineering	1	3
CH6430	Data Mining in Chemical Engineering and Bioengineering	1	3
CH6440	Introduction to Optimization Using AI in Chemical Engineering	3	3

Unrestricted Electives			
Course Code	**Course title**	**Trimester**	**Academic Unit (AU)**
CH6310	Chemical Process Simulation and Technoeconomic Analysis	2	3
CH6470	Computational Design of Catalysts	3	3
CH6480	Large Language Model- Assisted Computational Material Science	2	3
CH6490	Process Design, Optimization and Supply Chain	1	3
CH6520	Applications of Modelling and Simulation in Pharmaceutical Processes	2	3
CH6530	Data-Driven Computational Fluid Dynamics for Chemical Engineering Applications	3	3
CH6540	Project Management in Digital World	2	3
CM6843	Computational Chemistry for Molecular Modelling	2	3
CM6844	Scientific Computing with Python	2	3
BG6820	Digital Twin of Human: Enabling Precision Health	1	3
BG6830	Quantitative Methods for	2	3

	Bioengineering		
BG6021	Academic Writing and Statistical Literacy	1	0
BG6022	Laboratory Attachment	1	0
BG6023	MSc Research I	2	3
BG6024	MSc Research II	3	3
BG6025	Professional Internship	1, 2, 3	3

Core Modules

CH6250 - Introduction to Numerical Methods & Machine Learning

This course introduces the fundamentals of data analytics for solving problems in both engineering and non-engineering contexts. Students will learn to apply numerical methods to understand, optimize, and make data-driven decisions. The course covers the development of algorithms for integration and differential equations, the use of data analytics tools, and the application of machine learning techniques such as regression, classification, and neural networks for modelling and analysis.

CH6420 - Advanced Statistics for Data Science Analytics for Chemical Engineering

This course develops students' proficiency in statistics and data science for analysing, interpreting, and modelling complex datasets. It integrates theory with practical application using Python and Jupyter notebooks, drawing on real-world datasets and chemical engineering case studies. Students will strengthen their analytical and problem-solving skills to design and evaluate data-driven solutions, while gaining awareness of ethical practices, data integrity, reproducibility, and responsible AI use. The course also prepares students for advanced research and industry roles requiring strong statistical and data analytics expertise.

CH6430 - Data Mining in Chemical Engineering and Bioengineering

This course aims to equip graduate students with the knowledge and practical skills required to extract meaningful insights from complex and noisy datasets commonly encountered in chemical production processes and biological systems. Designed for students in chemical engineering, bioengineering, and related disciplines,
the course provides a strong foundation in data mining concepts, algorithms, and their applications to real-world industrial and biological problems.
Through structured theoretical instruction and applied case studies, students will develop competencies in data pre-processing, regression analysis, dimensionality reduction, and machine learning techniques. Emphasis is placed on the effective interpretation and optimization of data-driven processes. The skills acquired in this course will enhance students' analytical and problem-solving capabilities, support advanced research activities, and prepare graduates for data-intensive roles in academia, industry, and emerging areas of big data analytics.

CH6440 - Introduction to Optimization Using AI in Chemical Engineering

This course introduces key concepts in optimisation and artificial intelligence, focusing on the use of AI models and algorithms to solve optimisation problems. Students will gain hands-on experience implementing AI-based optimisation techniques using Python, and learn how to integrate and interpret results effectively. The course also addresses important ethical, safety, and sustainability considerations in the application of AI-driven optimization.

Unrestricted Electives

CH6310 - Chemical Process Simulation and Technoeconomic Analysis

This course is intended for those of you who are new to process design or those who need to refresh and deepen your knowledge about process design and simulation. In this course, you will learn to effectively synthesize a process flow diagram by applying and integrating various chemical engineering principles and implementing techno-economic evaluation method with the aid of process simulation software, such as Aspen Plus and/or HYSYS.

CH6470 - Computational Design of Catalysts

This course aims to equip you with a rigorous, quantitative framework for designing and understanding catalysts using computational methods. This course is designed graduate students in chemistry, chemical engineering, materials science, physics, or a related field, especially if you are interested in modeling, simulation, or theory driven interpretation of catalytic phenomena. By taking this course, you will be able to critically analyze catalytic systems and to design new catalysts based on fundamental physical principles rather than trial and error. The insights and skills gained during the course are directly valuable for research careers in academia, national laboratories, and the chemical industry.

CH6480 - Large Language Model - Assisted Computational Material Science

This course aims to equip you with a rigorous, quantitative framework for designing and understanding catalysts using computational methods. This course is designed graduate students in chemistry, chemical engineering,materials science, physics, or a related field, especially if you are interested in modeling, simulation, or theory driven interpretation of catalytic phenomena. By taking this course, you will be able to critically analyze catalytic systems and to design new catalysts based on fundamental physical principles rather than trial and error. The insights and skills gained during the course are directly valuable for research careers in academia, national laboratories, and the chemical industry.

CH6490 - Process Design, Optimization and Supply Chain

This course aims to develop simulation skills to consider complex process design in the context of cost, and sustainable process plant development. It equips with a systematic design methodology to design key unit operations (i.e. reactor, separator, and heat exchanger) in a chemical plant, with an emphasis on the conceptual issues that are fundamental to the process creation. Linear, Mixed-Integer Linear and nonlinear programming is studied. Process simulation and modelling tools (e.g. MATLAB/GAMS) are explored and several Case studies on process optimization are discussed. One part of this course will also introduce Supply Chain Management and supply chain networks will be studied and Strategic, tactical and Operational decisions that optimizes supply chain performance will be explored.

CH6520 - Application of Modelling and Simulation in Pharmaceutical Processes

This course aims to provide the students with knowledge and understanding of pharmaceutical manufacturing processes and how modelling and simulation aid in the development and validation of such processes. This course covers the engineering basics of important processes in the manufacturing of active pharmaceutical ingredients (API), including crystallization, granulation, drying, and tableting. This course also covers key pharmaceutical formulation processes to enhance the solubility of poorly soluble pharmaceuticals, and how modelling and simulation can be used to predict the performance of such pharmaceutical formulations. This course also discusses the roles of life cycle assessment in simulating the effects of pharmaceutical processes on the environmental footprints of pharmaceutical manufacturing from the drug inception stage to the drug disposal stage. This course will enable the students to apply modelling, simulation, and life cycle assessment approaches to improve the performance and sustainability of pharmaceutically relevant processes.

CH6540 - Project Management in Digital World

This course aims to introduce basic concepts in project management with coverage of evolving trends and application of sustainability, artificial intelligence, managing large datasets, and machine learning. It helps to apply the concepts while executing modelling as well as product development projects. This equips the participants to enhance their skill set, improve employability, and career growth, key concepts such as project integration, scope management, project planning, project budget & cost management, project risks and opportunities, communication and conflict management shall be covered.

CM6843 - Computational Chemistry for Molecular Modelling

Having successfully completed this course, you will develop the necessary knowledge and skills for a career that involves computational chemistry and molecular modelling for research and applications in chemical industry. This course will introduce students to learn basic computational chemistry and its applications with ab initio software. Students will learn how to start collaborations on performing a research project based on ab initio software in this course and they will also present their results in a scientific manner.

CM6844 - Computational Chemistry for Molecular Modelling

Having successfully completed this course, you will develop the necessary knowledge and skills for a career that involves scientific data processing and automation for research and applications in chemical industry. This course will introduce students to learn Python programming and its applications in numerical simulations in the chemical sciences. Students will learn how to develop home-made computational programme to solve routine chemical problems to achieve automation. They will also learn how to present their results in a scientific manner.

BG6820 - Digital Twin of Human: Enabling Precision Health

This course aims to equip Master's students with a systems-level understanding of Digital Twin technologies and precision health, with a particular emphasis on how these approaches can be harnessed to enhance population health in Singapore and Asia.Building on the distinctive strengths of Singapore's biomedical sciences ecosystem— including Asian biology, precision health, population health, and biomedical technology innovation—the course introduces students to the conceptual, computational, and ethical foundations required to design and evaluate next-generation healthcare systems.

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BG6830 - Quantitative Methods for Bioengineering

At the interface of chemistry, physics, and computation lies a frontier waiting to be explored. In recent years, researchers with chemical and bioengineering backgrounds have increasingly turned to modelling and simulation as chemical and biological sciences become more quantitative and data-driven. The world now needs chemists and bioengineers who can translate molecules and processes into predictive models, run simulations, and interpret complex data with confi dence. This course aims to introduce quantitative modelling through a diverse set of problems spanning genetics, sensing, and control. You will learn essential mathematical and computational techniques and see how these tools deepen understanding and guide design in chemical and bioengineering. If you are trained in chemistry, chemical engineering, or bioengineering with basic knowledge in calculus, linear algebra, and statistics, this course is ideal for you. Join us to position yourself for advanced study and careers in pharmaceuticals, medicine, data science, consulting, etc.

BG6021 - Academic Writing and Statistical Literacy

Academic Writing and Statistical Literacy is a pass/fail course comprising thirteen two-hour lessons. The course develops students' ability to produce clear, coherent, and well-structured academic writing while building a foundational understanding of statistical concepts and their application in academic contexts. Students will learn to interpret, analyze, and present quantitative data effectively, and to integrate statistical evidence into logical and persuasive written arguments. Emphasis is also placed on strengthening critical thinking in evaluating research findings and data sources, as well as cultivating academic integrity through proper citation, referencing, and ethical use of data. The course prepares students to conduct and communicate research effectively across academic disciplines.

BG6022 - Laboratory Attachment

This course offers students the opportunity to engage in research activities under the guidance of faculty members within the School of Chemistry, Chemical Engineering and Biotechnology. Students are expected to undertake a 10-week laboratory attachment with a faculty member of the school. Designed as an introductory research immersion experience, its primary aim is to familiarize students with different sub-disciplines and techniques related to their main interest, as well as fundamental protocols and techniques employed in academic research laboratories. The student is expected to immerse him/herself in the laboratory chosen to gain direct exposure working in the laboratory, interact with members of the laboratory that are at various stages of training and career development, and obtain a basic

understanding of the research interests and the key research approaches of the laboratory.

BG6023 - MSc Research I / BG6024 - MSc Research II

MSc research project is specifically crafted for students to work on technology development in a research setting under the guidance of a faculty member. The project is required to involve some degree of new and original research, not just a review of previous work. Conducting relevant research provides students with opportunities to further apply the theoretical knowledge and analytical skills developed in the courses taken.
*Prerequisite: BG6022

BG6025 - Professional Internship

This Graduate Internship programme is offered as an optional course for all cceb coursework students. The purpose of this Internship is to enable the application of knowledge and skills you have learned in the university in an authentic work environment. You can gain exposure and develop practical industry experience that will enhance your employability and lifelong learning capabilities. Moreover, you may be able to get a head start in your career if you apply to the same company later.