Master of Science in Chemical Modeling

Core Courses

1. CH6410 Numerical Methods for Chemical Modelling
2. CH6420 Advanced Statistics for Data Science Analytics for Chemical Engineering
3. CH6430 Data Mining in Chemical Engineering and Bioengineering
4. CH6440 Introduction to Optimization Using AI in Chemical Engineering

Elective Courses

1. CH6450 Molecular modelling
2. CH6460 AI for chemical
3. CH6470 Computational Design of
4. CH6480 Computational Material Sciences
5. CH6490 Process Design, Optimization and Supply Chain
6. CH6510 Physics-Informed Machine Learning in Engineering Applications
7. CH6520 Applications of Modelling and Simulation in Pharmaceutical Processes
8. CH6530 Data-Driven Computational Fluid Dynamics for Chemical Engineering Applications
9. BG6810 Bioimaging analysis
10. BG6820 Digital Twin of Human: Enabling Precision Health
11. BG6830 Quantitative Methods for Bioengineering
12. CH6540 Project Management in Digital World
13. CH6550 MSc Research on Chemical Modelling I (3AU)
14. CH6551 MSc Research on Chemical Modelling II (3AU)
15. CH6552 Professional Internship I (3AU)
16. CH6553 Professional Internship II (3AU)

Non-compulsory courses (Non-credit bearing)

1. CH6554 Lab Rotation (0 AU)
2. CH6555 Academic Communications (0 AU)

Core Courses

CH6410 Numerical Methods for Chemical Modelling

This course introduces key numerical techniques used to solve chemical engineering and modeling problems. Topics include optimization methods, numerical calculus, differential equations, and basic machine learning algorithms, with hands-on implementation for data analysis and decision-making in chemical systems.

CH6420 Advanced Statistics for Data Science Analytics for Chemical Engineering

This course equips students with advanced statistical tools for data analysis in chemical engineering. It covers regression, time-series, clustering models, and hands-on data analytics using Python, with applications in process optimization and decision-making.

CH6430 Data Mining in Chemical Engineering and Bioengineering

This course introduces data mining techniques for extracting meaningful insights from complex chemical and biological process data. Students will learn methods such as regression, dimensionality reduction, and machine learning algorithms, with a focus on real-world applications in chemical engineering and bioengineering systems.

CH6440 Introduction to Optimization Using AI in Chemical Engineering

This course introduces the application of artificial intelligence techniques to solve optimization problems in chemical engineering. Students will explore supervised, unsupervised, and reinforcement learning methods, and apply AI models using Python to optimize chemical processes and enhance decision-making.

Elective Courses

CH6450 Molecular Modelling

Learn core concepts in computational chemistry with a focus on ab initio methods. Explore how to model molecular structures, study reaction mechanisms, and analyze thermodynamic properties using simulation tools widely adopted in industry and academia.

CH6460 AI for Chemical Sciences

Discover how artificial intelligence can be applied to chemical data. This course teaches students to build machine learning models in Python for classification, regression, and visualization, using real-world chemical datasets and case studies.

CH6470 Computational Design of Catalysts

Understand how catalysts function at the molecular level and learn to design next-generation catalysts using computational tools and AI. Topics include surface reactions, microkinetic models, deactivation pathways, and AI-assisted prediction of catalytic behavior.

CH6480 Computational Material Sciences

Combine molecular dynamics simulations with the power of large language models (LLMs) to accelerate materials discovery. Students will use tools like LAMMPS and Python to analyze material structures and develop AI-enhanced research pipelines for solving complex material science problems.

CH6490 Process Design, Optimization and Supply Chain

This course provides foundational knowledge in designing chemical processes and optimizing them using engineering and operations research principles. It also covers supply chain logistics and decision-making strategies for sustainable and efficient process systems.

CH6510 Physics-Informed Machine Learning in Engineering Applications

Students will learn to integrate physical laws into machine learning models using Physics-Informed Neural Networks (PINNs). The course applies these hybrid models to solve real-world engineering problems in areas such as fluid dynamics and thermal systems.

CH6520 Applications of Modelling and Simulation in Pharmaceutical Processes

This course focuses on the use of simulation and modeling techniques to optimize pharmaceutical manufacturing processes. Topics include drug synthesis, crystallization, and product formulation with emphasis on process control and regulatory compliance.

CH6530 Data-Driven Computational Fluid Dynamics for Chemical Engineering Applications

Combines traditional CFD with machine learning methods to enhance simulation capabilities in chemical engineering. Students will develop reduced-order models and apply data assimilation techniques to improve the accuracy of fluid flow predictions.

BG6810 Bioimaging Analysis

Covers computational techniques for processing and analyzing biomedical and industrial images using Python. Students will gain hands-on experience in segmentation, classification, and AI-based image analysis for quantitative research.

BG6820 Digital Twin of Human: Enabling Precision Health

Introduces the concept of creating a digital replica of human health using data from wearables, health records, and sensors. Students will explore applications in predictive healthcare, smart cities, and space medicine.

BG6830 Quantitative Methods for Bioengineering

This course equips students with quantitative tools to analyze and model biological systems. Topics include stochastic modeling, control theory, and data analytics in genetic, cellular, and physiological processes.

CH6540 Project Management in Digital World

Provides a comprehensive overview of project management concepts with an emphasis on digital tools, AI, and sustainability. Students will learn to plan, execute, and manage complex engineering projects in a data-driven environment.

CH6550/CH6551 MSc Research on Chemical Modelling I & II

An independent research project spanning two trimesters where students apply chemical modeling or machine learning to a selected problem. Supervised by NTU faculty, the project culminates in a formal report and presentation.

CH6552/CH6553 - Professional Internship I & II

This course provides students with practical, hands-on experience in a professional setting within the chemical, pharmaceutical, or related industries. Through internship placements, students will apply their knowledge in real-world projects, develop industry-relevant skills, and gain insights into career pathways aligned with chemical modeling and engineering.s

Non-compulsory courses (Non-credit bearing)

CH6554 – Laboratory Rotation

This course provides students in the Master of Science in Chemical Modelling and Machine Learning (MSc-CMML) the opportunity to participate in research activities under the supervision of faculty members from the School of Chemistry, Chemical Engineering and Biotechnology (CCEB). Students will complete two 5-week laboratory rotations with different faculty members, each focusing on a distinct area within chemical modelling, computational chemistry, or machine learning applications. As an introductory research immersion, the course aims to expose students to various sub-disciplines, tools, and computational techniques relevant to their interests, while developing foundational skills in academic and industry-aligned research environments. This is a non-credit bearing core course and forms part of the programme's co-curricular learning component.

CH6555 - Academic Communications

The objective of this course is to help graduate students develop their written and oral communication skills in English in academic settings. The main goals of the course are to equip students with the necessary knowledge to write a publishable academic paper, as well as present their scientific knowledge and findings to both specialists and lay audiences. This course is a non-credit bearing core course and will be part of cocurricular learning course.