TU DELFT MSC CHEMICAL ENGINEERING

Master electives guide 2026

INFORMATION ABOUT ALL THE ELECTIVES IN Q3 OF THE FIRST YEAR

Technologisch Gezelschap Sinds 1890

1 Introduction

Dear master students,

In Q3, you can choose from 22 electives, with no prescribed combinations. However, the electives are divided into four profiles: circularity, energy, health, and nuclear. Each elective is worth 3, 4, or 6 ECTS, and you should select a total of 12 ECTS. You are responsible for the scheduling of your electives and making sure that there is no overlap in exams, lectures etc.

In this guide all the electives are described, some descriptions have been written by teachers, while others have been adapted from the study guide. I hope this guide helps you with choosing your electives.
For more information, please join us for a Master Electives event during the lunch break on **January 6th** in the Beijerinck and Waterman halls. Teachers and TAs for most of the electives will be present to answer your questions and assist you in your choices.

Kind regards,

Kas Lemmers
Commissioner of Education 132nd Board Technologisch Gezelschap

Contents

2

Circularity

2.1. CH3102 Catalysis for Energy and Circularity

3ECTS

Course Contents
Unlock the enabling role of catalysis for the sustainability and energy transition. This course offers an in-depth exploration of catalysis, a cornerstone of modern chemical engineering, focusing on its critical role for the circular economy and advancing sustainable energy and chemical technologies.

Starting with a historical perspective, you'll delve into the relevance of catalysis today, exploring how it underpins the shift towards more sustainable practices. The course covers fundamental principles of catalysis chemistry and engineering, guiding you through the fundamentals and practice of catalyst preparation, performance testing, and mechanistic studies. Special focus will be on such topics as structure-activity relationships in catalysis, reaction kinetics, advanced characterization, and catalyst design.

We will discuss the principles of catalytic chemistry and engineering with the examples from the industrially-relevant chemical processes. We will demonstrate how an insight into the nature of catalytic sites and the reaction mechanism can help guide the design and optimization of new and improved catalysts. In this context, we will introduce and discuss application of such physical chemical characterization techniques as infrared spectroscopy, temperature programmed techniques, X-ray diffraction, electron microscope and X-ray photoelectron spectroscopy for understanding and optimizing the catalyst function and behavior. We will discuss the practical application of these methods and the scientific challenges facing the field, highlighting established and emerging catalytic applications that are crucial for the development of circular and sustainable energy technologies, preparing you to contribute to the next generation of chemical engineering solutions.

Study goals
Bring to life the black box that the catalyst often is to Chemical Engineers. This means gaining knowledge of:

- How catalysts work and what their role is in enabling circular economy and sustainable chemical technologies;
- How catalysts are prepared and what happens to them in the reactor;
- What the key characteristcs of catalysts and design principles are;
- Which techniques are used to characterize catalysts;
- How catalysts are evaluated.

Education method and assessment
Lectures, assignment, poster presentations (during plant visit or at TU Delft). Assessment is by a written examination (80%) + assignment (20%).

2.2. CH3543 Inorganic Materials Chemistry for Energy and Circularity

3ECTS

Course Contents

Explore the dynamic field of Inorganic Materials Chemistry, where cutting-edge research meets the pressing global challenges of energy sustainability and circularity. This course offers a comprehensive journey through the principles and concepts of contemporary inorganic chemistry, with a focus on the role of inorganic chemistry in the development of sustainable technologies and energy transition.

The course begins with a brief introduction to the role of inorganic chemistry in circularity, providing a solid foundation through a review of the periodic table, chemical bonding, and the fundamental relationships between structure, property, and function. From this base, we delve into the fascinating world of inorganic molecules, exploring coordination complexes, organometallic chemistry, and inorganic polymers. We will discuss what challenges and opportunities Earth-abundant elements present in creating functional materials, and how catalysis can be achieved with non-noble metals.

As we progress, the focus shifts to inorganic materials, where you will gain insight into the reactivity of solid-state materials and the unique chemistry of inorganic surfaces. We will explore the synthesis of these materials, the role of inorganic colloids, and the integration of coordination and organometallic chemistry at surfaces. The course also covers the development of hybrid organic-inorganic materials and their applications.

In the final part of the course, you will engage in the design of functional inorganic materials, learning how to combine the properties of composites to create advanced materials with specific functionalities, such as active materials and sensors. We will also explore nanostructured materials and their role in heterogeneous catalysis, a key area for advancing energy and circularity.

By the end of this course, you will not only have a broad understanding of the principles of inorganic materials chemistry but also the ability to apply these principles to solve real-world challenges in energy transition and material sustainability. This course prepares you to critically analyze and design innovative solutions that replace critical elements in functional materials with earth-abundant alternatives, driving forward the next generation of sustainable technologies.

Study goals

After this course, the student:

- Has a broad knowledge of the principles and concepts of contemporary inorganic chemistry of materials
- Can discuss and define challenges and opportunities in replacing critical elements in functional materials with earth-abundant counterparts
- Can discuss and define the chemical origin of specific functionality of the inorganic materials
- Can apply principles of contemporary inorganic chemistry to the topics of circularity and energy transitions (e.g. catalysis, functional materials, energy storage, etc)

Education method, Prerequisites and assessment

The course consist of lectures, self-studies, assignment.
Prerequisites: basic concepts of molecular structure; basic BSc level organic/inorganic chemistry.
Assessment: Written exam (70%) + Assignment (30%)

2.3. CH3921 Sustainable Polymer Materials

3ECTS

Course Contents

This course will focus on the question how the current oil-based polymer industry that produces non-degradable polymers that accumulate in our environment in massive quantities can be transformed in an industry that is green, sustainable and fits in a more circular economy. In this course we will provide background regarding(the 12 principles of) Green Chemistry. Various metrics that are used to quantify the greenness and sustainability of a process or a product will be introduced and discussed. We will make an inventory regarding the current practice in polymer manufacturing and polymer waste treatment. Subsequently we will introduce various scenarios towards (more) sustainable polymers, and discuss the pros and cons of these approaches.

Study goals
After attending this course the student will:

- have detailed knowledge of the current industrial production of polymers
- know various scenarios to make polymers more green and sustainable
- be able to use the 12 Principles of Green Chemistry to assess the sustainability of a given polymer
- be able to critically assess the purport of green claims.

Education method and assessment
Frontal lectures, including guest lectures from external and internal experts, homework and discussions on selected papers in class. Lecture notes, and references for scientific articles and tutorials will be provided via Brightspace. The course will be tested via a written exam.

2.4. CH3085 Chemical Process Technology: Present and Future - Not available this year

4ECTS

Important notice
Unfortunately, due to certain circumstances, this course will not be available this year. On the bright side, the lecturers for this course are confident that it will be available again next academic year.

3

Energy

3.1. CH3061: Multiphase Reactor Engineering

4 ECTS

Prerequisites
The student is expected to:

- **Have followed a course on mass and energy balances (such as Molecular Transport Phenomena).**
- **Have followed a basic course in reactor engineering (such as Reactors and Kinetics).**
- **Is able to work with Python (or similar software; e.g., has followed a course on numerical techniques).**

Course Contents

- Multiphase reactor types: Fixed beds, trickle beds, fluidized beds, bubble columns, slurry reactors, microreactors, structured (monolith) reactors, electrocatalytic reactors.
- Engineering aspects: Flow regimes, mass transfer, conversion models. Hatta number, reaction enhancement. Residence time distribution. Catalytic reactors structured in time and space. Unifying concepts.
- Design aspects: reactor selection, decoupling of kinetics and transport phenomena, combination of reaction and separation, reaction coupling, separating catalytic steps, controlled energy input, circularity of materials.

Study Goals

- The student is able to describe for each of the archetypes of multiphase reactors, the various embodiments with practical relevance.
- The student is able to use the scientific literature to find relevant information for the various reactor types.
- The student is able to analyse a multiphase reactor and to describe the physical and chemical process steps in words.
- The student is able to explain the basic measurement techniques used in studying multiphase reactors.
- The student is able to write down the mass, energy, and momentum balances for the overall system and the steps identified under objective 3.
- The student is able to implement customary models in the balances mentioned under 5, such that a system of equations describing the reactor is obtained.
- The student is able to simplify the system of equations based on a quantitative analysis and identification of the rate-determining steps.

- The student is able to use Python to solve the systems of equations numerically for the basic types of reactors.
- The student is able to use the developed models to analyse defined cases.
- The student is able to present, both orally and in writing, the outcomes of modeling, calculations, and evaluation.

Education Method and Assessment
Each lecture will give a short overview of a specific multiphase reactor type (only 45 minutes). The slides available on Brightspace. You will get references to papers and/or chapters from textbooks that give more information about the reactor type. These will be made available via Brightspace.

After the lecture, an assignment (about 8 hours work) will be available via Brightspace for the specific reactor type treated. These assignments are made in teams of four students; this number may be changed depending on the number of participants. You are free to choose which software package you want to use for making the assignments, but Python is recommended.

After two weeks, each team hands in a detailed solution of the problem on paper the day before the discussion before the announced deadline. Moreover, each team prepares a summary of the solution for presentation in PowerPoint. Please bring this presentation on a memory stick. Each week, a few teams present their solution; the instructors choose the student that is presenting. The other teams challenge this solution.

The final grade consists of: * the solution to the assignments * an individual part; the nature of this part will depend on the number of participants

3.2. CH3065 Multiphase Reactor Engineering II - Design Project

2 ECTS

Prerequisites
The student is expected to:

- **Have followed a course on mass and energy balances (such as Molecular Transport Phenomena).**
- **Have followed a basic course in reactor engineering (such as Reactors and Kinetics).**
- **Is able to work with Python (or similar software; e.g., has followed a course on numerical techniques).**

This course is an extension of Multiphase Reactor Engineering (CH3061), and can only be followed when also taking CH3061.

Course Contents

- Multiphase reactor types: Fixed beds, trickle beds, fluidized beds, bubble columns, slurry reactors, microreactors, structured (monolith) reactors, electrocatalytic reactors.
- Engineering aspects: Flow regimes, mass transfer, conversion models. Hatta number, reaction enhancement. Residence time distribution. Catalytic reactors structured in time and space. Unifying concepts.
- Design aspects: reactor selection, decoupling of kinetics and transport phenomena, combination of reaction and separation, reaction coupling, separating catalytic steps, controlled energy input, circularity of materials.

Study Goals

- The student is able to use the scientific literature to find relevant information for the various reactor types.
- The student is able to analyse a multiphase reactor and to describe the physical and chemical process steps in words.

- The student is able to write down the mass, energy, and momentum balances for the overall system and the steps identified under objective 3.
- The student is able to implement customary models in the balances mentioned under 3, such that a system of equations describing the reactor is obtained.
- The student is able to simplify the system of equations based on a quantitative analysis and identification of the rate-determining steps.
- The student is able to use Python to solve the systems of equations numerically for the basic types of reactors.
- The student is able to use the developed models to analyse defined cases.
- The student is able to make a quantitative design of a multiphase reactor for a given application.
- The student is able to present, both orally and in writing, the outcomes of modeling, calculations, and evaluation.

Education Method and Assessment
The team, typically consisting of four students, will make a design project.The design project will be graded on a number aspects; more details will be given via Brightspace.

3.3. CH3513 Electrochemistry for renewable energy

4 ECTS

Course Contents
Electrochemistry provides an important platform to convert (renewable) electricity into valuable products, chemicals, fuels and coatings. This course provides an overview of several electrochemical processes of societal importance, linking fundamental understanding with applied utilization. The scope of the course will cover processes from the nanoscale to the meter-scale, and methods to understand fundamental phenomena in practical systems. This course will include:

- Electrochemical potentials and definitions (electromotive force, formal potential, Donnan potential)
- Types of electrochemical reactions (reversibility, multi-step reactions)
- Electrochemistry at liquid-solid, liquid-liquid, solid-solid and gas-solid interfaces
- Electrode reaction kinetics in steady and unsteady state (Cottrell equation).
- Microscopic theories of charge transfer and (Marcus model, energy states, tunneling)
- Ion transport through diffusion and migration
- Electrochemical characterization techniques (cyclic voltammetry, chronopotentiometry, impedance, etc.)
- Electric double layers (Helmholtz model, Gouy-Chapman model)
- Examples of water electrolysis, CO2 reduction
- Industrial electrochemical systems (large scale electrolysers, batteries, etc.)
- Electrochemical equipment (potentiostats, reference electrodes, electrodes, electrolytes, membranes)
- Experimental setup (including practicum)

Study Goals
After this course, the student is able to:

- Explain electrochemical responses in complex electrochemical cells (steady and non-steady state, and mono- or multi-ionic systems) to peers;
- Demonstrate how theories for electrochemistry thermodynamics, kinetics (Marcus model, Tafel model) and electrolyte processes are applied to basic redox systems
- Break down limiting factors (overpotentials or limiting currents) in given practical electrochemical conversions
- Set up and perform suitable electrochemical tests for characterizing redox couples in practical electrochemical conversions

Education Method and Assessment
This course consists of: instruction videos, lectures and exercise sessions (combined), practicum, and guest lectures. Please be aware that attendance at the practicum is mandatory. The practicum will be scheduled 2x a timeslot of 2 hours in March. Grading is based on: homework assignments (0%, counting for 0.2 point bonus), a practicum report (30%) and an exam at the end of the course (70%).

3.4. CH3622 Process Intensification

3 ECTS

Course Contents
1. Introduction to Process Intensification(PI):

- sustainability-related issues in process industry
- definitions of Process Intensification
- fundamental principles and approaches of PI

2. How to design a sustainable, inherently safer processing plant:

- presentation of PI case study assignments

3. PI Approaches:

- STRUCTURE - PI approach in spatial domain (incl. "FOCUS ON" guest lecture)
- ENERGY - PI approach in thermodynamic domain (incl. "FOCUS ON" guest lecture)
- SYNERGY - PI approach in functional domain (incl. "FOCUS ON" guest lecture)
- TIME - PI approach in temporal domain (incl. "FOCUS ON" guest lecture)

Study Goals
After successfully completing this course, students will be able to:

- Understand the working principles and basic knowledge of process intensification
- Evaluate and analyze the current process intensification techniques in chemical processes
- Apply the principles of process intensification to suggest / propose advanced reaction and separation systems for chemical processes
- Develop further chemical processes to enhance energy efficiency, reduce the capital and operating expenses, while making less wastes and improving process safety

Education Method and Assessment
Lecture notes via Brightspace and the book "Fundamentals of Process Intensification" by A. Stankiewicz, T. van Gerven and G. Stefanidis, Wiley-VCH . The course will be assested via a written exam.

3.5. AP3362 From Semiconductors to Solar Cells

4 ECTS

Course Contents

The energy transition is to a large extent possible due to massive production of cheap solar cells. While Si devices become cheaper, limits to the power conversion efficiency are almost reached. For the progression of the energy transition substantially more photovoltaic modules have to be installed on limited available land. Therefore, cost effective improvement of the power conversion efficiency is one of the central current challenges. The present course deals with the mechanism of various solar cell technologies, including traditional crystalline silicon solar cells and cells based on poly crystalline thin layers. Corresponding material property requirements, and the chemical processing is included. Fundamental efficiency limits for different technologies are analysed and new technologies offering the prospect of increased efficiency are discussed extensively.

In this course we will discuss the operation of solar cells in general and will pay particular attention to the chemistry of recent solar cell technologies and the related challenges and opportunities. Understanding the operation of solar cells requires knowledge about the physics of semiconductors. Therefore the main part of the course will focus on the properties of semiconductors, following the book " Principles of Solar Cells, LEDs and related devices; The role of the PN junction" by Adrian Kitai.

Study Goals

After this course the student:

- Has a good understanding of the structure of semiconductor materials
- Can explain the origin of electronic bands in semiconductors and the occupation of those bands by charge carriers
- Can discuss the factors that govern charge transport in semiconductors
- Can discuss electronic doping the the formation of junctions
- Can interpret the effect of specific junctions on the behavior of charge carriers
- Can explain the operation of pn junction solar cells
- Knows various types of solar cell technologies, is able to discuss their respective promises and challenges

Education Method and Assessment

The course will take place as a traditional on campus course. There are three blocks of 2 hours per week scheduled. The first two blocks (roughly) will be used for on campus lectures. After the lectures quizzes will be used to test if the students have understood the course material.
The third block is reserved for an exercise class. A TA and a lecturer will be present to help with the exercises. Some relevant problems will be treated classically. For this course it is very important to make the exercises! This will allow you to put the course material to use and will prepare you for the exam. It will also make you realize what you understand and what you do not yet understand.

Halfway through the course a formative test will be held about the first chapters. This will not count for your grade. The final grade of this course consists of a written exam (100% of the final grade)

3.6. SET3110 Energy Storage in Batteries

4 ECTS

Course Contents

Efficient energy storage in batteries is of major importance for electronic equipment, electrification of cars and buses, grid stability and for the introduction of fluctuating renewable energy sources including wind and solar. In this course we will learn about the thermodynamics and charge kinetics in batteries including the electrochemical driving force, thermochemistry, phase transitions and charge transport kinetics. The principles of state of the art and future rechargeable batteries, also touching super capacitors, will be discussed. The aim is to develop understanding of the battery performance parameters and to relate these with the underlying atomic scale material properties. Along these topics, current battery developments and research directions will be discussed. After seven lectures on the fundamental properties of batteries, six dedicated working lectures will focus on important battery technologies including:

- Redox Flow
- Na-ion
- next generation Li-ion batteries
- Solid State batteries
- Supercapacitors

Study Goals
At the end of the battery lectures, students should be able to:

- List the major types of Li and other batteries and their characteristics.
- Reproduce the major challenges in batteries.
- Explain how a battery works and the functioning of each component.
- List and explain the different reaction types in batteries.
- Explain the different charge transfer processes in batteries.
- List and explain the different mechanisms that limit the cycle life of batteries.
- Apply Nernst Law describing redox reactions.
- Calculate conductivities and overpotentials.
- Apply the Tafel equation describing the charge transfer between electrode and electrolyte.
- Calculate energy densities and power densities from observed properties.
- Derive from a phase diagram the different phases that will occur upon lithiation.
- Apply the Gibbs Phase rule to predict constant or variable output voltage.
- Derive the voltage curve from the shape of the Gibbs Free energy.
- Predict the basic redox reaction of two electrodes given the formation energy or the standard potentials.
- Compare different battery systems and differentiate.
- Discuss scientific results observed in battery performance and relate this to material properties.

Education Method and Assessment
The course contains fourteen 2-hour lectures. The first seven 2-hour lectures focusses on building the underlying thermodynamics, material science and electrochemistry chemistry and the principles of energy storage in batteries. This knowledge will be used to develop understanding of the material properties that determine performance of current and next generation battery. In the second seven lectures will be working lectures with focus on six important battery technologies. The first half hour will be a lecture on the specific battery technology followed by half an hour assignment. In the final half hour of the working lecture the assignment will be discussed. In the final lecture example exams will be discussed.
The final grade of the course consists of the following components: Written exam (100% of the final grade).

4
Health

4.1. CH3382 Molecular Engineering of Soft Materials in Health Care

4 ECTS

Course Contents

This course provides an overview of the design, analysis and engineering principles for soft materials in health applications on a molecular scale. Such soft materials cover a wide range of health applications, including drug delivery, imaging, tissue engineering, and implants. We will cover practical knowledge in the engineering and advancement of these biomaterials that enables their use in biological tissues, including the properties of materials (e.g., biocompatibility and biodegradability), the biological response associated to them (e.g., inflammation and clearance), and the practical concerns during development and commercialization (e.g., safety and quality control).

Case studies of health applications (e.g., biomaterials for COVID vaccination, artificial organs, tumor imaging and diagnosis) will be covered in this course to further integrate your knowledge into real-world applications.

Study goals

After successful completion of this course, the student should be able to:

- Understand the general properties required for healthcare materials.
- Understand the interaction between living systems and soft materials.
- Explain the process of biodegradation.
- Explain the lab-to-commercialization process of biomaterials.
- Identify the applications of biomaterials (e.g., drug delivery, tissue engineering, imaging, implants).
- Evaluate the safety of biomaterials.
- Design biomaterials based on their application in health.

Education method and Assessment

Standard 2-hour lectures Practical Guide Assessment Case study (100%): Composed of a Mid-term presentation (0%, mandatory to be eligible for final presentation), and a Final presentation (100%)

Recommended knowledge: Interfaces & Particles, Soft Materials Engineering

4.2. CH3412 Biological Transport Phenomena

4 ECTS

Course Contents
Expected prior knowledge

- **Concepts from a B.Sc. Transport Phenomena course**
- **Bulk Transport: mass, energy and momentum transport**
- **Micro-scale transport: Diffusion, Conduction, Laminar Flow**
- **Fick's Law, Fourier's Law, Newton's Law of Viscosity**
- **Concepts of Velocity profiles and Shear Stress profiles in Momentum Transport**
- **Derivation of Navier Stokes Equation**

In this course, we will deal with:

- Mass Transport in Biological Systems
- Momentum Transport in Biological Systems
- Energy Transport in Biological Systems
- Micro-scale Flows in Biological Systems
- Transport at/across Interfaces in Biological Systems

Study goals
After completing this course, you will be able to:

- Demonstrate understanding of the relevance of transport phenomena in various biological systems.
- Apply the concepts of mass, energy and momentum transport for various examples related to plants and human body.
- Analyse the features of transport in human body.
- Apply the concepts of micro-scale transport to relevant biological systems, both natural (blood-stream to cell) and artificial (drug delivery).

Education method and Assessment
Lectures & tutorials, and familiarity to contemporary relevant literature through group project. No programming is involved.
There are two parts in the assessment: a literature review (in group) and a final written exam. 40% of the Final Grade will be from the group project literature review, and 60% of the final grade will be from the written exam.

4.3. CH3564 Particle Technology for Health and Energy

3 ECTS

Course Contents

The course starts with the basics of general particle technology / solids processing. After the introduction, we will treat special topics focusing more on health/pharma and energy applications of particle technology. The exact course structure may vary depending on the number of students.

Topics:

- Basic properties & characterization of particles
- Particles in a fluid, particle-particle interaction
- Motivation of applying (nano)particles; difference in behavior between small particles and large particles
- Particle production & functionalization
- Pharmaceutical processing
- Nanoparticle formulation & controlled release
- Safety, Health & Environment aspects of particles
- Battery applications of particles
- Catalysis, critical materials & circularity
- Large-scale energy processes involving particles

Study goals

- The student is able to describe the synthesis, characterization and application of particles.
- The student is able to use the scientific literature to find relevant information on particles.
- The student is able to develop and apply model descriptions for particle synthesis, characterization and applications (i.e., both qualitative and quantitative).
- The student is able to apply the obtained knowledge and skills to analyse defined cases.
- The student knows and understands the main applications of particles in the area of health and energy.

Education method and Assessment

Lectures and assignments. The assessment will be via Essay (50%) + multiple choice test (50%).

5
Nuclear

5.1. CH3764 Nuclear medicine

4 ECTS

Course Contents

Nuclear Medicine is responsible for the diagnosis of more than 30 million patients yearly as well as for the treatment of cancer, especially when tumours have spread all over the body. In this course we will cover the basics of NM including production of radioisotopes, preparation of radiopharmaceuticals, imaging modalities and radionuclide therapy. As part of this course several guest lectures are incorporated given by researchers working in Nuclear Medicine departments who can provide insight into real practice in the clinic.

Study goals

At the end of this course, the student should be able to:

- Evaluate which properties of radionuclides are relevant for imaging and therapy
- Understand the working principles of nuclear imaging techniques
- Distinguish different radiolabelling approaches for radiopharmaceuticals
- Describe different production routes for radionuclides and calculate production yields
- Explain the working mechanism of radionuclide therapy and distinguish between the different radionuclide therapies
- Understand the damage of radiation induced to cells
- Understand the role of a nuclear medicine practicioner in the hospital
- Analyse advanced literature within the field of nuclear medicine, critically discuss the findings, present these to an educated audience, and write a comprehensive report on these findings.

Education method and Assessment

Lectures + case study. The final grade consists of 70 % of the case study and 30 % of the exam. At least a 5 needs to be obtained for the exam to pass the course. The exam will be a written, closed-book exam on campus.

5.2. CH3765 Advanced Materials Characterisation

3 ECTS

Course contents

Prerequisites: BSc in Chemical Engineering, Chemistry, Materials Science or Physics

This course focuses on the characterisation of materials using X-ray and neutron scattering, nuclear magnetic resonance (NMR) and X-ray absorption techniques. During the course, a wide range of experimental techniques will be presented that are relevant for chemists and chemical engineers, such as X-ray/neutron diffraction, reflectometry and small-angle scattering to determine the structure of materials at length scales from the Angstrom (atoms) to the micrometer length scales (aggregates, colloids, etc.) as well as nuclear magnetic resonance and X-ray photoelectron spectroscopy to determine, amongst others, the presence and chemical environment of atoms in a material. The measurement techniques will be presented from an application point of view, focusing on the basic principle behind the measurement technique, the information that can be derived from the measurement technique, and how a typical experiment would look like and can be performed. All measurement techniques will be illustrated with a broad range of examples applicable to chemical engineers and chemists (e.g. applications in soft matter, battery materials, solar cell materials, perovskites, thin films, etc.).

An experimental project in which students can apply one technique and a tour along the facilities of the Reactor Institute Delft will be part of the course.

Study goals

By the end of this course, the student should be able to:

- Explain the principles of several X-ray and neutron scattering techniques (diffraction, reflectometry, small-angle scattering etc.) used to obtain structural information about materials at various length scales.
- Explain the principles of Nuclear Magnetic Resonance spectroscopy.
- Explain the principles of X-ray spectroscopy techniques such as X-ray Photoelectron Spectroscopy.
- Argue based on the interaction of X-rays and neutrons with matter whether X-rays or neutron radiation is the preferred option to answer a specific science question.
- Argue which material characterisation technique is most suitable to answer a specific science question.
- Perform a basic material characterisation experiment using X-ray or neutron radiation.
- Interpret data obtained from a material characterisation experiment.

Education method and Assessment

Plenary lectures (2h). Problem sets are provided by the instructors after each lecture and that can be solved by the student. Solutions to the problem sets will be provided and questions can be asked about the problem sets during the next lecture. A mandatory experimental project where students perform an experiment in groups is part of the course. Excursions to the facilities of the Reactor Institute Delft are also organized.

The final grade of the course will be based on the group experimental project (small report + presentation) that will count for 30% and a written final exam with a weight of 70%. The grade for the group project will also be valid for the resit, but not for next years edition of the course. Depending on the number of students, the resit may be an oral exam.

5.3. CH3771 Nuclear chemistry

6 ECTS

Course Contents

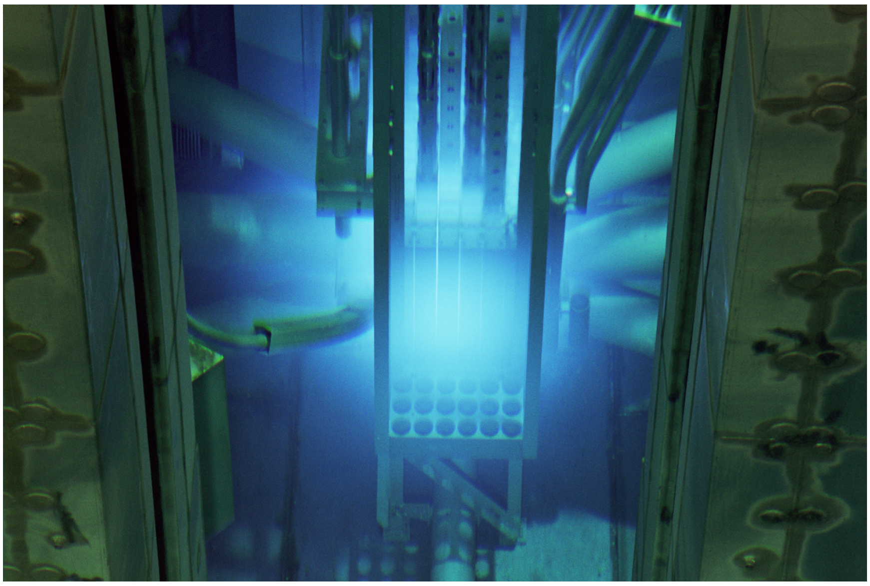
This course is designed for students having either chemistry or physics background who are interested in learning more about nuclear chemistry and applied radiochemistry. This course covers topics from the Bing Bang to the production of radionuclides for medical and industrial applications. This course also provides hands-on-experience through practicals where you get to work with radioactive materials. Students should complete this course with an in depth knowledge of nuclear and radiochemistry.

Study goals

- Identify the factors that affect nuclear stability and apply to predict decay.
- Explain the different kinds of radioactive decay.
- Interpret a radioactive decay series.
- Understand the interaction of radiation with matter.
- Be able to calculate ranges of different ionising particles.
- Analyse and design different radionuclide production routes.
- Identify the best separation techniques for a specific radionuclide.
- Evaluate the quality of produced radionuclides with respect to specific activity, radionuclidic purity and os on.
- Describe the different nuclear analytical techniques and select the suitable techniques for certain application.
- To apply radiotracer principles
- Understand the basic principles of radiodating and perform associated calculations
- Discuss various techniques commonly used to enrich stable isotopes
- Describe the production and chemistry of the superheavy elements

Education method and Assessment

Oral lectures and practicals. A midterm exam counts for 20% and a final exam for 80% of the grade. The midterm exam will be 'a closed book' written exam on campus. The duration will be 1 hour. The final exam will be a 3 hour written, closed book exam on campus. Attending the practicals and writing corresponding measurement reports is obligatory to pass the course. Mid-term grade is only valid for the final exam but not for the retake.



5.4. CH3783 Materials chemistry for the nuclear fuel cycle

3 ECTS

Course Contents

This is a 3 ECTS course composed of 28 total lecture hours, 56 self-study and a final examination. This course is designed for Chemical Engineering, Applied Physics, Materials Science & Engineering, and Sustainable Energy Technology students that are interested in developing a working knowledge of nuclear materials chemistry and the nuclear fuel cycle.

The course will cover various aspects of solution and solid state chemistry as well as materials science that play a key role at each step of the nuclear fuel cycle, from the metallurgy of uranium to the disposal of spent reactor fuel or high level waste. While the physics and engineering of controlled fission are central to the generation of electricity by nuclear reactors, chemistry in general and especially materials chemistry dominate all other aspects of the nuclear fuel cycle. This course will give students a comprehensive knowledge of the traditional fuel cycle (the uranium once-through cycle) in Light Water Reactors (LWRs). It will also cover some of the proposed nuclear fuel cycles that may well carry nuclear power through the coming decades. As an outcome of the course, the students will be able to compare and contrast existing and innovative fuel cycles, and discuss the pros and cons of each.

In addition, the course will cover some of the unique properties of the actinide 5f-elements. The first three of the actinide series - Th, Pa and U - occur naturally, while the elements following uranium in the Periodic Table (transuranium elements) are man-made. The actinides are essential to nuclear power generation, but also find applications in many other areas of industry, medicine and research. The course will address 5f-electronic configurations, oxidation states, redox potentials, inorganic and structural chemistry, as well thermodynamic properties of actinide compounds. The actinides behaviour in the environment and in the geosphere will be discussed, together with analytical tools for their identification. The biological and environmental hazards associated with these elements pose certain risks which must be controlled and minimized. Due to their significant role and because the final destination of transuranic elements originating from the nuclear fuel cycle is still an open issue, the actinides chemistry and physics continue to be one of the major areas of nuclear research.

The materials science part of the course will cover the main features of materials microstructures and behaviour in conditions that are relevant for nuclear reactors. The various types of defects at the atomic or micrometre scale will be explained as well as their consequences in terms of energy. This forms the basis of understanding the changes that materials undergo when subjected to elevated temperature and high-energy radiation. Changes in the microstructure and the defect configurations lead to changes in properties and behaviour and can thus jeopardise the material performance, forming a threat to safety.

Study goals

- Students can demonstrate how chemistry and materials science influence almost all aspects of the fuel cycle.
- Students can describe the key steps involved in the traditional nuclear fuel cycle and explain the involved chemical processes.
- Students can apply the concepts addressed in the course to discuss alternative fuel cycles, not covered in the class, and explain the fundamental differences with the presented traditional fuel cycle.
- Students can justify, at each step of the fuel cycle, the behaviour of the different actinide elements in view of their chemical and physical properties (electronic structure, redox potentials, solubility, complexation, speciation, thermodynamics, etc.).
- Students can predict and explain the behaviour of fission products in the irradiated fuel, during the reprocessing and in geological environment.
- Students are able to predict the environmental behaviour of various actinide species.
- Students can discuss major analytical techniques for actinide studies.

- Students can perform numerical evaluations to predict the behaviour of the actinide elements and fission products at each step of the fuel cycle.
- Students are able to discuss the major features of materials microstructures and behaviour when subjected to the conditions in a nuclear reactor.
- Students write an essay and make a presentation on a supplemental topic related to the course material, but not covered in class, in which they apply the key concepts presented during the lectures and perform critical analysis of the information.

Education method and Assessment
This is a 3 ECTS course composed of 28 total lecture hours, 56 (supported) self-study and a final examination.The final grade is composed of the weighted average of the final exam (60%), presentation (40%).

6
Other

6.1. CH3112 Artificial Intelligence in (Bio)-Chemical Engineering
3 ECTS

Prerequisites

- **Master-level numerical methods or computational practical.**
- **Fundamental computer programming in Python: elementary instructions, conditional statements and loops, functions, and main program.**

Course Content

The digital transition of the (bio)-chemical industry and research requires new intelligent knowledge and decision-making tools. The increasing availability of data and computational resources over the past decade has led to a resurgence of machine learning-based research. Artificial intelligence has significant advantages over traditional modeling techniques, including flexibility, accuracy, and speed of execution. Therefore, artificial intelligence holds great potential in the digital transformation and full automation in the (bio)-chemical industry.
This course aims to introduce the concepts of artificial intelligence and machine learning and discuss the potential and limitations of different machine learning methods for given (bio)-chemical engineering applications. Moreover, a machine learning and deep learning framework will be introduced during the course, including hands-on practice.

Study goals

- Explain the concepts of artificial intelligence and data analysis, and the potential and limitations thereof on (bio-)chemical engineering applications (Cognitive level: understand).
- Develop an artificial intelligence system to solve a given (bio-)chemical engineering problem using existing artificial intelligence methods. (Cognitive level: create).
- Implement a given or developed artificial intelligence system using Python. (Cognitive level: Apply).
- Evaluate the results obtained with an artificial intelligence system in the context of (bio-)chemical engineering applications. (Cognitive level: Evaluate).

Education method and Assessment

This course is based on lectures and practical assignments, which include programming in Python. Python is the programming language for this course. Also, Jupyter notebooks are used. Assessment is a final exam (100% weighting)

6.2. CH3673 Computational Approaches for Chemistry and Materials

4 ECTS

Course Contents

Expected prior knowledge: Basic knowledge on quantum chemistry (BSc level) and electronic properties of materials (for instance the course Solid State Materials (CH3175)).

In the course, the background of modern methods for electronic structure calculations are discussed from an application centered approach. The first part of the course treats the background of electronic structure methods, including the basics of Hartree-Fock and Density Functional Theory, basis sets and DFT functionals. This forms a basis for applications of electronic structure methods to study different properties and processes in molecules and materials. These applications include:

- Potential energy surfaces, geometry optimizations (vibrations, transition states, and chemical reactions) and electrostatic properties of molecules (dipole moment, charge distribution, polarisability).
- Excited state properties of molecules: Absorption, fluorescence.
- Intermolecular interactions between molecules, related to self-assembly: Van der Waals, electrostatic interactions, hydrogen bonds.
- Electronic band structure and optical properties of periodic systems including 1D molecular wires, 2D sheets, and 3D bulk solids.
- Multiscale modeling of chemical reactions, transition states, catalytic processes, and connection with experimental reaction rates.

Study goals

- Student has an overview of the existing molecular simulation techniques.
- Student has basic knowledge of quantum chemical methods.
- Student is able to choose a suitable simulation technique for a specific problem.
- Student is able to evaluate and interpret the result of calculations performed by themselves or in literature.

Education method and Assessment

The classes will be taught in a block-approach, starting with a short (60 minute) lecture on the theoretical background of electronic structure methods, followed by hands-on exercises using state-of-the art software for DFT calculations. Students use their own laptop for the calculations.The assessment of the course is in the form of a computational "mini-project" in combination with a written report on this project. Projects can be provided by the lecturers but ideally students supply their own ideas, for instance a subject that fits with their MSc thesis project.

6.3. CH3421 Computational Transport Phenomena

6 ECTS

Course Summary

Prior knowledge: MSc level Transport Phenomena: Applied Transport Phenomena for Chemical Engineering students, or Advanced Transport Phenomena for Applied Physics students.

This elective course Computational Transport Phenomena is complementary to Molecular Transport Phenomena (about the fundamental processes at molecular level) and Applied Transport Phenomena (how to scale and reduce the model equations and introduce techniques to get approximate solutions which still reflect the relevant mechanisms and processes), all of the MSc program Chemical Engineering. For Applied Physics MSc students of the Physics for Fluids Engineering track, this course builds on the modules Advanced Fluid Dynamics and Advanced Physical Transport Phenomena. Computational Transport Phenomena is about numerical techniques for solving the Navier-Stokes and other transport equations - all being partial differential equations which do not have an exact analytical solution. The course is intended to provide some guidance as to a number of numerical issues and on simulation strategies such as size and type of the computational grid (including 2D vs 3D). The course, however, is not just a tutorial as to how to run Fluent for a variety of applications. Most of the course is devoted to the wide variety of models available for simulating turbulent flows, multi-phase flows (including free-surface flows) and micro-fluidics. If time permits, simulating chemical reactions will also be discussed. While most of the course will deal with finite volume techniques, as used in the common commercial solvers and OpenFoam, attention will also be paid to Lattice Boltzmann techniques.

6.3.0.1. Course Contents

An introductory course on Computational Fluid Dynamics (CFD) and Computational Transport Phenomena (CTP): elementary fluid mechanics; numerical and computational aspects; turbulence en turbulence modelling; RANS vs Large-Eddy Simulations; operations and mixing en transport processes in process equipment among which stirred vessels and cyclones; fluid-particle interaction; two-phase flows (Euler-Lagrangian vs Euler-Euler)

Study goals

Building an understanding of CFD, its promises and its limitations; acquire some experience in numerical and computational exercises; understanding turbulence and multiphase flows and their modelling; getting a good idea about the effects of all types of models on the CFD outcomes; becoming capable of interpreting and assessing CFD results.

Education method and Assessment

The course comprises regular classes (where new material is presented by the Professor) as well as hands-on workshops for exploring ANSYS/Fluent CFD software in a Studio classroom type of environment, with the help of Fluent tutorials, a TA being present for assistance. In these workshops and also in the final assignment, students work in teams of two.
The emphasis in the course is on the physics and the models underpinning a software code such as Fluent as well as on the the impact of boundary conditions, input parameters and numerics.
Make sure you will have sufficient time during the semester to be an active participant in the course and to stay on board till the very end. You are also obliged this towards your fellow team member.
Attending CLASS AND WORKSHOP is therefore COMPULSORY.
The grading is based on two elements: (a) the active participation in the mandatory weekly tutorials (counts for maximum 10The latter report should make clear that the student has understood the course material, at least as far as relevant to the final assignment. This report should be a critical assessment (using literature data) of the simulation results carried out for the final assignment. A more detailed scheme of aspects contributing to the eventual grading of the final report is to be found on Brightspace. The effort in writing such a report is not to be underestimated!
Students are allowed to improve their grades on the basis of the review by the teacher but cannot improve their grade by more than 1.5 on the scale 1-10. The lecturer may invite students for an oral assessment of their final assignment report.

6.4. AP3171 Advanced Physical Transport Phenomena

6 ECTS

Course Contents

Analytical/Numerical/Modelling Aspects of Advanced Physical Transport Phenomena

(The unifying approach: Fluid Flow Heat and Mass Transfer Turbulence):

(1) Basic Equations of Transport Phenomena - Field Description;

(2) Mathematical Methods for Solving Transport Equations (PDE, separation of variables, eigenfunctions and eigenvalues, Bessel functions, Laplace transformation, Error-Gamma functions, integral methods);

(3) Transport in Stagnant Media (diffusion, moving front problems, diffusion with source terms);

(4) Momentum Transport (potential flows, creeping flows, boundary layers);

(5) Transport in Flowing Media (stationary transport in flows with uniform velocity, heat transfer in laminar pipe flow, natural convection);

(6) Numerical Heat and Fluid Flow (discretization methods for heat conduction, convection, and diffusion; differencing schemes, numerical diffusion; steady and time-dependent convection and diffusion; calculation of flow field/velocity-pressure coupling, SIMPLE algorithm);

(7) Turbulence:

- Some Features and Rationale for Modelling (instantaneous features through Direct Numerical Simulations (DNS), Large-Eddy Simulations (LES));
- Some generic types of turbulent flows and convective processes;
- The wall-bounded turbulent flows: velocity and temperature distributions/wall functions;
- Reynolds decomposition, Reynolds-Averaged Navier-Stokes (RANS) turbulence models;

(8) Turbulence Modelling (closure problem, eddy viscosity/diffusivity models, k-e model, other two-equation eddy-viscosity models).

Study Goals

- To be able to identify and define particular physical mechanisms of the complex transport phenomena mathematically;
- To be able to specify and solve characteristic PDEs describing simplified transport phenomena analytically;
- To be able to discretize the system of governing transport equations by using a finite volume method by performing the term-by-term analysis (time-dependent, diffusive, convective, source/sink terms) for one-, two- and three-dimensional generic cases;
- To be able to understand the basic mechanisms of turbulence and to derive the transport equations for fluctuating field variables (Reynolds-decomposition);
- To learn characteristic classes of the turbulence models (zero-, one-, two-equations, full-stress models);
- To be able to computationally perform some primary generic cases of flow, heat, and mass transfer (CFD) (channel flow, back-step flow, differentially heated enclosure, in both laminar- and turbulent-regimes).

Education method and Assessment

Combination of Lectures (4 Lectures per week, covering theoretical aspects) and practical exercises (both analytical and computational/computer exercises, 2-3 hours per week). Computational exercises covering step-by-step solving some of basic generic cases of flow, heat and mass transfer on Linux computers (mesh-definition, specification of the boundary and initial conditions, solving, postprocessing, analysis and critical assessment of results).

Written Exam (two times per year). The exam contains three distinct parts: (1) analytical; (2) numerical discretization; (3) turbulence modeling. At least 50% of each part needs to be completed correctly to successfully pass this course.

6.5. MS43040 Machine Learning for Materials Design

4 ECTS

Course Contents

The graduate-level introductory course on “Machine Learning for Materials Design” will explore the principles, methodologies, and applications of machine learning (ML) in the domain of materials science and engineering. By bridging the gap between traditional materials design approaches and the cutting-edge field of machine learning, we will learn the tools and knowledge necessary for data-driven discovery and development of materials.

The following ML aspects are first covered through lectures and live coding:

- Introduction to PyTorch
- Automatic differentiation

- Gradient-based optimization
- Best practices in machine learning
- Feed-forward neural networks
- Convolutional neural networks
- Recurrent neural networks
- Autoencoding neural networks
- Inductive biases

Next, a wide range of materials science and engineering applications of the above ML topics will be explored via hands-on and latest research-oriented group projects. Some representative examples include (may vary during the course):

- Predicting mechanical behavior of composites and polymers
- Identifying molecules with unique properties
- Designing metamaterials with tailored mechanical behavior
- Characterizing imperfections and defects in additive manufacturing through data and physics

IMPORTANT: Good knowledge of linear algebra and familiarity with Python are required. Following are the representative topics that are recommended pre-requisites.

Mathematics topics:

- Vectors and matrices
- Tensors
- Coordinate transformations
- Differentiation (including of matrices)
- Eigenvalues and eigenvectors of matrices
- Basic knowledge of probability

Python Topics

- Creating a Function
- Creating a Class and Objects
- Plotting and visualization of data
- Using Numpy for matrix manipulations
- Familiarity with Jupyter notebooks

Study goals
After successfully completing this course, you will be able to:

- Understand the fundamentals of machine learning and its application in material science.
- Develop basic machine learning algorithms based on neural networks.
- Identify appropriate machine learning algorithms based on the data and application in material science context.
- Develop data-driven strategies based on machine learning for new problems.

Education method and Assessment
Lectures, exercises, and project. Lectures will involve live coding. Students are asked to bring their own laptops. Summative assessment: The assessment will be done based on a project, which will have two components: a final presentation and a report. Both final presentation and report will carry 50% of the final grades each.

Formative assessment: During the course, there will be several office hours to provide feedback on the project progress. There will also be a mid-term presentation to discuss the project progress. Additional details will be provided at the beginning of the course.