Master in Chemical Engineering
Curriculum "Chemical engineering for innovative processes and products"

Syllabus 2023-24

Classes for the first year of the Master (2023-2024) will be given in two Semesters:
Semester 1: September 25 – December 22, 2023
Semester 2: February 26 – May 31st, 2024

All classes will be given in the headquarters of the Faculty of Civil & Industrial Engineering, in **Via Eudossiana 18 – 00184 Rome, RM**

Fundamental, mandatory courses, required

Course	ECTS	Year	Semester
Mathematical methods for chemical engineering	9	1	1
Non equilibrium thermodynamics with an application to the microscale	9	1	1
Separation processes with an application to lab-on-chips	9	1	1
Economics of technology and management	9	1	2
Water treatment processes and environmental technology	9	2	1
Computer aided process control	9	2	1
Theory and development of process design	9	2	2

Elective courses

Course	ECTS	Year	Semester
Applied metallurgy	6	1	1
Process and product safety in the chemical industry	6	1	1
Green and Sustainable Hydrogen Production	6	1	1
Corrosion engineering	6	1	2
Principles of biochemical engineering	6	1	2
Sustainable design of materials	6	2	1
Green chemistry and process engineering	6	2	1
Nanobiotechnology	6	2	1
Transport phenomena in microsystems and micro/nano reactive devices	6	2	1
Computational methods for chemical and biochemical reactor dynamics	6	2	2

To complete the Master curriculum, students must get a total of 120 ECTS, distributed as follows:

Course	**ECTS**
Common courses, required	63
Elective courses	24
Additional elective courses (may be chosen among Elective courses indicated above or among all the courses given in English by Sapienza University, provided their contents are compatible with a Chemical Engineering Master)	12
Seminars	1
Final thesis work	20

Time schedule of the courses: Year 1 - Semester 1
See attached file

The indication of the ClassRoom Number and the relative Building are given for each class.

The indication of the name of the Professor is given for each course. Any professor can be contacted by e-mail at the following type address: name.surname@uniroma1.it

Common courses - programs

Mathematical methods for chemical engineering

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1) Chapter 1: Review and basic tools. Review of basic concepts in vector-space algebra: Algebra of vectors and its representation, scalar product, vector product, projections, exponential of a matrix. Review of Vector Calculus: functions of several variables, integral theorems on curves, integral on surfaces, Gauss-Green Formula, Divergence and Stokes Theorems, Helmholtz decomposition. Review of Ordinary differential equations (ODE): Existence and uniqueness of solutions for general ODE's of first and second order, phase space and qualitative behavior of solutions, explicit solutions of first ODE's and of second order ODE's with constant coefficients. Banach and Hilbert Spaces: Dual Space, Lebesgue measure and Lebesgue spaces, weak derivatives and Sobolev spaces (H1), Motivation: Dirichlet Principle (Sketch). Review of Fourier Transform: Plancherel Theorem, Inverse Fourier Transform and applications to ODE's (Sketch). Review of Fourier series: Parseval Identity and convergence theorems.
2) Chapter 2: Partial Differential Equations. First order PDE's: method of characteristics, shocks, entropy solutions. Second order PDE's: Hyperbolic Equations: wave equations in dimension 1 and $N \geq 2$; Parabolic Equations: Fundamental solution, Maximum principle, Cauchy problem in dimension 1; Elliptic Equations: Harmonic functions, Green functions (space, disk, semispace...), minimization and weak formulation of elliptic problems, Lax–Milgram Theorem.
3) Chapter 3: Probability. Introduction to the elements of theory of probability: events, random variables, probability densities and distributions, joint densities and covariance matrices, correlation, conditional probabilities and Bayes Theorem, functions of random variables (one-to-one). Limit theorems and applications: convergence in law, convergence in probability, weak law of large numbers, Monte Carlo methods, central limit theorem, random walks (Gauss- ian). Markov processes: semigroups and generators (Brownian motion). Time-changed processes: Phillips' formula and subordinate semigroups (Stable processes).

Non equilibrium thermodynamics with an application to the microscale

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1) Introduction to the theory of transport phenomena: kinetic theory (Boltzmann equation, continuous approaches, stochastic methods). Theory of transport phenomena as the thermodynamics of out-of-equilibrium(irreversible) processes.
2) Structure of balance equations: concentration/fluxes formulation and constitutive equations. Continuous formulation of balance equations for mass, momentum and energy transport. Thermal balance equation. Lagrangian and Eulerian approaches to the analysis of transport phenomena. Entropy balance and its application in the assessment of the thermodynamic consistency of the constitutive equations. Classical constitutive equations: Fick, Newton and Fourier laws. Boundary conditions for the mass, momentum and thermal balance equations.
3) Mass transport. Diffusion in bounded and unbounded domains. Spectral properties of the Laplacian operator. Classical case studies of mass transport of chemical engineering interest. Chromatographic processes and moment analysis.
4) Momentum transport. Navier-Stokes equations. Hydrodynamic regimes: Stokes and Moffat regime and transition to turbulence. Inviscid flows and their properties. Incompressible flows: stream function (in two-dimensional problems) and its properties. Representation of incompressible flows in three dimensions. Stream function/vorticity
5) formulation of two-dimensional flow problems. Elementary flow problems: Poiseuille, Couette flow and other simple examples. Axial symmetric flows and solution of the Stokes problems for the motion around a solid sphere. Stokes law, friction factor and particle motion in a fluid phase. General solution of the Stokes problem: Oseen tensor and introduction to computational methods for Stokes flows.

6) Thermal transport: natural and forced convection. Examples. Blackbody radiation and radiative transfer.
7) Interaction between convection and diffusion: Taylor-Aris dispersion in straight tubes.
8) Survey of boundary layer theory.
9) Introduction to the stochastic theory of transport phenomena: random walk on a lattice, Langevin equation and connection with the Fickian nature of the constitutive equations.
8) Transport phenomena at microscales: examples and case studies.

Separation processes with an application to lab-on-chips

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Laminar flow and creeping flow of incompressible single-phase fluids. Stokes limit. Streamlines and stream surfaces. Stokes flow in spatially periodic systems. Convective transport in laminar flow and assessment of mixing efficiency. Optimization strategies in pure advection based on dynamical system theory. Poincaré sections and Lyapunov exponents. Application to optimal stirring conditions in a DNA microarray chamber. Dynamics of suspended mesoscopic objects in Stokes regime. Linearity principle and mobility tensor. Application to microfluics-assisted separation processes. Hydrodynamic chromatography. Size-based separation of particles in Deterministic Lateral Displacement devices: macrotransport model. Separation of chemical species: Gas Cromatography and Liquid Chromatography (HPLC).

Economics of technology and management

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1) Technology. Technological sets and production function. Total, average and marginal productivity. Isoquants and marginal rate of technical substitution. Elasticity of substitution and types of technology. Long run vs short run. Returns to scale and returns to varying proportions. Elasticity of scale. Technological Progress. High tech labour vs low tech labour.
2) Costs.The cost function and isocosts. Conditional input demands and Shephard's lemma. Price and output elasticity of input demands. Expansion path. Short run vs long run cost functions. Total costs. Variable, fixed and quasi-fixed costs. Sunk costs. Average and marginal costs. Economies of scale and the minimum efficient scale. Economies of scope and learning curves
3) Profits. Economic profits and opportunity costs. Profit maximization in the long run. Duality of production, cost and profit functions. Hotelling's lemma. Short run profit maximization. Profit maximization and return to scales. Supply curves and producer's surplus. Short run vs long run supply curves.
4) Competitive markets. Market demand. Individual supply and market supply. Perfect competition. Short run and long run market equilibrium. Meaning of 0-profits. Pareto efficiency
5) Monopoly. Demand elasticity. Elasticity and revenues. The monopolist maximization problem. Inefficiency of monopoly and deadweight loss. Causes of monopoly. Subadditivity of costs and economies of scale. Natural monopoly. Price discrimination (first degree, second degree, third degree).
6) Innovation. Product innovation vs process innovation. Drastic innovation. Willingness to pay for innovation. Innovation and market structure.
7) Value. Future Values and Present Values. Net Present Value. Risk and Present Value. Present Values and Rates of Return. Calculating Present Values When There Are Multiple Cash Flows. The Opportunity Cost of Capital. Perpetuities and Annuities. Continuous Compounding. Real and Nominal Rates of Interest. Calculating the Present Value of an Investment.
8) Financial accounting. The Balance Sheet and Account Categories: Assets, Liabilities, Owners 'Equity. The Income Statement: Revenues, Cost of Sales, Gross Margin, Expenses, Net Income. Relation between Balance Sheet and Income Statement. The Statement of Cash Flows. Misconceptions about Depreciation. Sources and Uses of Cash. Working capital flows. Analysis of the Cash Flow Statement.
9) Investment Decisions. Net Present Value and Other Investment Criteria. Discounted Payback. Internal Rate of Return. Pitfalls of IRR. Making Investment Decisions with the Net Present

Value. Relevance of Cash Flow. Estimation of Cash Flows on an Incremental Basis. Treating of Inflation. Investment Timing. Equivalent Annual Cash Flows and Inflation. Equivalent Annual Cash Flow and Technological Change

Water treatment processes and environmental technology
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1) Waste characterization from industrial activities. Emissions and consumption: wastewater, solid wastes and air emission. Mass and energy balances. Quality control.
2) Source and nature of pollutants. Direct and indirect toxicity in natural systems. Pollutant dispersion modeling in water and soil. Clean technologies and wastes minimization: general principles and applications. Quality of process water and auxiliary water - Water resource optimization: water reuse and recycle.
3) Wastewater treatment processes. Physical and chemical processes. Thermodynamic and kinetic of biological aerobic and anaerobic processes. Suspended growth and biofilm processes. Stripping of volatile organic compounds. Case studies.
4) Organic sludge treatment by stabilization, thickening, dehydration. Final disposal. Process alternatives evaluation and design. Agro-industrial and manure wastes treatment. Energy generation from biomass – microbial fuel cell.
5) Soil and sediment remediation: in situ and ex situ technologies. Thermal, chemical and biological processes.
6) Nanotechnologies and nanostructured materials for innovative wastewater treatment and soil remediation.
7) Water and soil analysis and characterization. Overview of fundamental aspects of advanced oxidation processes (AOP's). Applications of AOPs based on Ozonation (O_3), UV light and hydrogen peroxide for disinfection and oxidation of toxic and refractory compounds. Fundamentals of electrochemical processes. Principles and mechanism of direct and mediated electrochemical oxidation. Electrochlorination. Novel electrode materials. Figure of merites of electrochemical processes.

Computer aided process control
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1. Introduction to control system
2. Brief description to units in chemical processes with insight to process control
   a. Heat exchangers and boilers
   b. Furnaces
   c. Chemical reactors
   d. L-L separation devices
   e. L-G contactors
   f. Distillation columns
   g. Evaporators
   h. Membranes
3. Measurement devices for different controlled variables
   a. Temperature
   b. Level in tanks
   c. Flow rate
   d. Pressure
4. Regulation valves
5. Introduction to dynamic modelling of chemical processes
6. Stability of controlled systems
7. P, PI and PID feedback controllers
8. Feedback controllers (FB)
   a. Introduction and general concepts

    b. Examples of controlled units by FB
9. Coupling of control systems and decouplers
10. Optimization of the controlled system
    a. Evaluation of the controlled system
    b. Optimization methods
11. Exercise: Optimization of controlled FB processes by use of a simulation software
12. Digital FB controllers: going from an analogue approach to a digital one
13. Digital feedforward controllers
14. Digital inferential controllers
15. Digital predictive controllers
16. Digital multivariable controllers
17. Distributed control systems
18. Exercise: Design of a predictive inferential control system on membrane processes by means of a simulation software

Theory and development of process design
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1. CHEMICAL PROCESS MODELING
Characterization and classification of mathematical models for chemical processes.
Process models in the presence of controls. Parameters and uncertainty.
2. NUMERICAL SIMULATION OF CHEMICAL PROCESSES:
Algorithms for integration of concentrated parameter systems.
Algorithms for stiff problems.
Algorithms for distributed parameter systems.
Application to transient analysis
of chemical reactor and process units..
3. NONLINEAR DYNAMICAL SYSTEMS
Continuous and discrete systems.
Transient behaviour and asymptotic regimes.
Floquet multipliers and Liapunov exponents.
Numerical methods for identification of limit cycles and attractors.
4. BIFURCATION THEORY
5. APPLICATION TO CHEMICAL PROCESSES
Phase diagrams for chemical reactor operating with and without automatic controls.
Multistability and basin of attraction.

Elective courses – Programs

Applied metallurgy

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1) DEFECTS IN CASTINGS: casting design, endogenous and exogenous inclusions, oxide films, expansion defects, preventive measures to avoid gas defects, shrinkage defects, contraction defects, hot tearing, distortions and residual stresses, stress relief, dimensional errors, segregations;
2) WELDING METALLURGY: WELDING PROCESSES; METALLURGY OF WELDING: welding joints, hydrogen in steel welds, functions of slags, weld metal solidification, gas porosity and cracks in the fusion zone, heat flow in welding; WELDABILITY; DISTORTIONS AND RESIDUAL STRESSES; WELDING DEFECTS;
3) NON DESTRUCTIVE TESTS: MAIN ASPECTS OF NON DESTRUCTIVE TESTS; LIQUID PENETRANT TESTING: physical principles, procedure for penetrant testing; MAGNETIC PARTICLE TESTING: principle of MPT, magnetizing techniques, dusting on magnetic particles, inspection, demagnetization, sensitivity; ULTRASONIC TESTING: piezoelectric transducers, transducers types, measurement techniques, defects measurement, welded joints inspection, AVG method; RADIOGRAPHIC TESTING: nature of radiation, wave nature of x-rays, absorption and scattering of X-rays in matter, unsharpness, penumbra, radiographic films, contrast, sensitometric curves, exposure diagrams.
4) LIMIT OF ACCEPTABILITY OF DEFECTS

Green & Sustainable Hydrogen Production

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The course aims to introduce the main processes for the production of green and sustainable hydrogen. The course is dedicated to students who want to deepen their knowledge on renewable energy production, which in this historical period is becoming a fundamental aspect of chemical engineering. The course will be focused on the processes which are already developed at industrial scale and on those which are now under study and have a high industrial interest. The course will also take into consideration the critical aspect of the transportation and the storage of the hydrogen.

Program

- Hydrogen properties
- Traditional processes overview: possible feed fossil and renewable (Steam reforming, partial oxidation. authothermal reforming)
-Carbon capture and Storage in hydrogen production (Steam reforming with CCS, sorption enhanced reforming, methane cracking)
-Biomass gasification
-Chemical looping hydrogen processes and thermochemical cycles
-Electrolysis coupled with solar energy sources
-Transportation and storage

Corrosion engineering

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Effects and costs of corrosion. General principles of dry and aqueous corrosion: chemical and electrochemical reactions, definitions and expressions of corrosion rate and corrosion current, Faraday's law.
Thermodynamics of aqueous corrosion processes: electrode potential, electrochemical series, potential-pH Pourbaix diagrams.
Kinetics of aqueous corrosion processes: polarization. Evans diagrams. Concentration and activation polarization. Passivity.
Forms of corrosion: Uniform Corrosion in Acidic and Aerated Solutions; Galvanic corrosion; Differential aeration and Crevice corrosion; Pitting corrosion, Selective corrosion of alloys, Integranular corrosion and exfoliation; Mechano-chemical corrosion: Erosion, Cavitation, Fretting, Stress corrosion cracking, Fatigue corrosion, Hydrogen -induced corrosion; Stray current corrosion.
Corrosion environments: water, soil, atmosphere, concrete. Corrosion in petrochemical plants.
Corrosion Monitoring and Inspections. Non-destructive tests.
Prevention of corrosion by design.
Protection: Coatings, Inhibitors, Electrical protection (Cathodic and Anodic)
High temperature corrosion.

Principles of biochemical engineering

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Review of biochemistry of the macromolecules of biological interests (polypeptides and nucleic acids), stoichiometry and kinetics of biochemical reactions.
Enzyme kinetics. Elementary enzyme kinetics (Michaelis-Menten). Quasi-steady state approximation and its dynamic and perturbative interpretation based on the existence of slow-manifolds. Linearized representations. Enzymatic inhibition. Kinetics with multiple substrates. Allosteric enzymes.
Sequential and symmetric approach. Reaction rates for homotrope and eterotrope allosteric kinetics from the symmetric model. Examples: glycolytic oscillations. Reaction and regulation networks in the presence of allosteric enzymes.
Kinetics of immobilized enzymes: interaction between reaction kinetics and transport. Transport phenomenology in the presence of porous solid matrices: boundary layers and mass fluxes within a porous medium. mathematical modeling of enzyme kinetics at/in non-porous and porous solid supports. Porous matrices: efficiency factor. Instability effects (multiplicity of steady states) in the presence of substrate-inhibited kinetics. Shooting methods or solving the corresponding boundary-value problems.
Transcriptional regulation in procaryotes: the Monod operon model. Lac and Trp operons. Mathematical modeling of operon regulation.
Growth of procaryote and eucaryote (cell lines) population Structured and unstructured models. Descriptive models and models based on control parameters. Biomass growth in a batch reactor. Influence of substrate concentration: the Monod model (specific growth rates and yield factors).
Analysis of flow reactor for the growth of microorganisms. Predator-prey systems: the Volterra-Lotka descriptive model and the Monod approach for the interaction between bacteria and protozoa in a flow reactor. Aerobic growth.
Review of some concepts from dynamical system theory. Linear systems. Qualitative characterization of dynamical systems: equilibria, periodic orbits (central orbits, limit cycles) and more complex phenomena. Nonlinear system and linear stability analysis.

Concepts of bifurcation theory. Elementary bifurcations of equilibria: saddle-node, transcritical and pitchfork. Hopf bifurcation and birth of limit cycles.

Sustainable design of materials

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In this course a basic analysis will be carried out on the general characteristics of the various classes of materials: polymers, ceramic metals and composites highlighting the peculiarities, the weakness and the link to microstructure and properties of the various classes of materials.
Subsequently, the production processes will be analyzed, and above all the transformation of the different materials that will be used in the second phase, relative to the assessments of the LCA.
The philosophy that guides the development and use of synoptic charts and graphs comparing the specific characteristics of the materials in the major fields of engineering application will be introduced, such as: Chemical, Mechanical, Aerospace, Civil, Energy, Bioengineering Engineering and Ecodesign.
Finally we will try to outline methods for the "strategic" design of components and systems considering the materials both from the point of view of the optimization of the functional and mechanical characteristics as well as the processes and impacts that they have on the overall costs of the processes and products; looking in particular at the entire cycle of components and potential economic and industrial consequences in terms of environmental costs.
This last part will be addressed with the approach and philosophy of the life Cycle Assessment.

Green chemistry and process engineering

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Principles of Green Chemistry

- Introduction to Green Chemistry
- Control of Environmental Impact
- Alternative Reaction Media
- Catalysis for Green Chemistry

Objectives

- To learn the fundamental philosophy and tools of green chemistry
- To develop an awareness of the legislative, financial and social factors connected with reducing environmental impact
- To understand the importance and role of solvents in chemical and related processes
- To understand why solvent replacements are being sought
- To understand the importance of heterogeneous catalysis to green chemistry
- To recognise the key difference between homogeneous and heterogeneous catalysis in chemical processes

Application of Green Chemistry to Process Engineering

- Clean Synthesis
- Renewable Resources
- Energy Efficiency & Emerging Technologies
- Chemical Engineering & Clean Technology

Objectives

- To use real examples to illustrate how the principles of green chemistry can be applied to chemical process engineering.
- To study the changing trends in raw material utilisation and to understand the potential of alternative feedstocks.
- To study engineering methods for improving process efficiencies and sustainability.
- To calculate the mass and energy balance in a chemical production process
- To learn about the importance of energy efficiency and the range of energy sources

- To understand the role between energy pollution and climate change
- To understand how biomass can be used as a feedstock for future production industries

Commercialisation of Green Chemistry

- Greener Products
- Objectives
- To understand the potential for and difficulties in achieving the use of greener chemical products.

Nanobiotechnology
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Biological substances and microorganisms as biocatalysts and raw materials feedstock for the formation of nanoparticles (fundamentals, biological fractions of nanotechnology relevance, production of biological fractions of nanotechnology relevance). Nucleation and crystallisation of proteins (fundamentals, characterisation, process screening and identification, production). Formation and deployment of nanoparticles by biological techniques (microorganisms, culture media, extracts, switchable solvents). Applications of nanoparticles in the bio-related fields (food, pharma, cosmetic, agriculture).

Transport phenomena in microsystems and micro/nano reactive devices
stefano.cerbelli@uniroma1.it

Review of transport phenomena fundamentals and of the thermodynamic of irreversible processes: continuum approach, kinetic theory (Boltzmann equation).
Stochastic theory of transport phenomena. Review of probability theory. Stochastic processes: Markovian and non-Markovian.
Chapman-Kolmogorov equation. Wiener processes. Stochastic integrals: Ito and Stratonovich formulation and their properties.
Ornstein-Uhlenbeck processes: fluctuation-dissipation relation (Stokes_Einstein) and thermodynamic analysis.
Fokker-Planck equations and their properties. Stochastic processes possessing finite propagation velocity. Analogy with the Dirac equation.
Fluid mixing in microdevices. Kinematic approach. Chaotic mixing and its characterization. Influence of diffusion. Spectral analysis. Applications and numerical simulation of fluid mixing processes. Physical analogies: interaction between deterministic vector fields and fluctuations. Quantum analogies (with the Schrodinger equation). Reactive flows in microdevices.
Dispersion in microchannels. Taylor-Aris theory: moment analysis and determination of the effective dispersion coefficient.
Numerical simulation of dispersion in microchannel using the stochastic Lagrangian approach.
Microdevices for particle separations based on their sizes. Deterministic lateral displacement devices. Particle transport in periodic arrays of obstacles and potential and determination of their long-term/large-distance properties:effective velocy and effective dispersion tensor. Lumped description using space-time diffusion models with a finite number of states. Relativistic analogies.