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

Syllabus 2024-25

Classes for the first year of the Master (2024-2025) will be given in two Semesters:
Semester 1: September 23 – December 20, 2024
Semester 2: February 24 – May 30, 2025

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

Common 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
Chemical reactors	9	1	2
Economics of technology and management	9	1	2
Theory and development of process design	9	2	2
Computer aided process control	9	2	1
Chemical & Biochemical Plants	9	2	1

Elective courses (4 courses to be selected)

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

To complete their 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

First year - first semester

Green & sustainable hydrogen production (6 CFU) – SSD ING-IND 24 & 25

Modulo I - Fundamentals (3 CFU):
Prof.ssa Martina Damizia (martina.damizia@uniroma1.it)
Modulo II – Processes (3 CFU):
Prof.ssa Maria Anna Murmura (mariaanna.murmura@uniroma1.it)

Objectives
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 both on processes that 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 aspects of hydrogen storage and transportation.

Program
Fundamentals
- 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

Processes
The course will cover the following areas
- Hydrogen properties
- Overview of traditional H2 production processes using either fossil or renewable feeds (steam reforming, partial oxidation, autothermal reforming)
- Carbon capture and storage in hydrogen production processes (steam reforming with CCS, sorption-enhanced reforming, methane cracking)
- Biomass gasification
- Chemical looping hydrogen processes and thermochemical cycles
- Electrolysis coupled with concentrating solar energy systems
- Hydrogen transportation and storage

Textbooks
Scientific articles and material supplied by the professor

Type of lectures
The lesson will be held in classroom

Final evaluation
Oral exam

Mathematical methods for chemical engineering (9 CFU) – SSD MAT/05 e MAT/08

(6 CFU) ***Roberto Conti (roberto.conti@uniroma1.it)***
(3 CFU) ***Prof. Mirko D'Ovidio (mirko.dovidio@uniroma1.it)***

MAT/05
Objectives
Provide an elementary treatment of the theory of partial differential equations (PDE), including important examples from mathematical physics. Some first-level mathematical analysis tools indispensable for the understanding of the program will be recalled, many examples will be presented and various exercises will be solved with the use of classical techniques such as the method of separation of variables, Fourier series, the heat kernel, the Green's function

Program
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 (H^1), 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.

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.

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 (Gaussian).
Markov processes: semigroups and generators (Brownian motion).
Time-changed processes: Phillips' formula and subordinate semigroups (Stable processes).
\end{document}

Textbooks
Salsa, Sandro: Partial differential equations in action. From modelling to theory.

Prerequisites
Contenuto dei corsi di Analisi Matematica I e Analisi Matematica II

Type of lectures
Chalk and talk

Attendance
Attendance is not mandatory

Final evaluation
Written examination consisting of exercises, and oral examination including a discussion of the written exam

MAT/06
Objectives
Provide an elementary treatment of the theory of probability and the PDEs connection with stochastic processes.

Program
Events. Operations on events. Probability of events. Random variables. Probability distributions. Expected value and moments. Stochastic independence. Cumulative distribution function and density function. Random vectors and marginal distributions. Transformations of random variables. Sum of random variables. Introduction to convergences and limit theorems. Introduction to stochastic processes (Brownian motion and boundary value problems).

Textbooks
Lecture notes + Probability Essentials, Jean Jacod, Philip Protter, Springer-Verlag, 2004

Prerequisites
Analysis, GeometryI

Type of lectures
Chalk and talk

Attendance
Attendance is not mandatory

Final evaluation
Oral and written exams aimed at verifying the achievement of the course objectives. In particular, the evaluation takes into account acquired skills (written exam, 50%) the acquired theoretical knowledge and the ability to process and communicate (oral exam, 50%). Please, consult the web page https://www.sbai.uniroma1.it/~mirko.dovidio/PGS/lectures
Examples:
Evaluate the probability of some events (example: number of success in n independent trials). Evaluate the density of a given transformation.

Non equilibrium thermodynamics with an application to the microscale (9 CFU) – SSD ING-IND/24

Prof. Massimiliano Giona (massimiliano.giona@uniroma1.it)

Objectives
To provide the students with the basic physical (thermodynamical, statistical mechanical) tools and kinetic approaches for tackling the analysis of out-of-equilibrium and irreversible processes, and for expressing macroscopically the dynamics of thermodynamic variables in terms of transport equations. The goal of the course is also to foster the physical sensitivity for setting up the analysis and the design of processes at micro/mescoscale, which is the prerequisite for the subsequent more applied classes.

Program
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 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.

5) Thermal transport: natural and forced convection. Examples. Blackbody radiation and radiative transfer.

6) Interaction between convection and diffusion: Taylor-Aris dispersion in straight tubes. Survey of boundary layer theory.

7) 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.

Mathematical background: Review of vector analysis. Representation of differential operators in orthogonal curvilinear systems. Helmholtz decomposition.

Textbooks

1) De Groot, Sybren Ruurds and Mazur, Peter, Non-equilibrium thermodynamics, Dover Publ., 2013.
2) Balescu Radu, Statistical Dynamics: Matter Out of Equilibrium, Imperial College Press. 1997.
3) Bird, R Byron, Stewart, Warren E and Lightfoot, Edwin N, Transport Phenomena, John Wiley & Sons, New York, 2004.
4) Lecture notes edited by the instructor.

Final evaluation

Oral exam

Process and product safety in the chemical industry – SSD ING-IND/27

Prof.ssa Paola Russo (paola.russo@uniroma1.it)

Objectives

Il corso mira a fornire una comprensione più approfondita delle proprietà e della natura pericolosa delle sostanze chimiche, effettuando l’analisi dei processi chimici.
Il corso mira a raggiungere i seguenti tre Objectives:
- fornire agli studenti una panoramica delle statistiche sugli incidenti, gestire un incidente come processo dinamico e introdurre un approccio sistemico nei confronti degli incidenti

- essere in grado di valutare i pericoli che sono proprietà intrinseche dei prodotti e pericoli legati alle condizioni fisiche dei materiali o dei processi, per avere familiarità con la classificazione dei prodotti pericolosi
- essere in grado di valutare una strategia di prevenzione per l'uso di sostanze chimiche pericolose (in ambiente di laboratorio e industriale) e di adottare le misure di protezione adeguate contro gli incidenti

Program
Introduction to Safety in Chemical Industry. Definitions of safety, danger and risk. Accidents and statistical surveys. The types of process accidents. Some significant accidents (Flixborough, Seveso, Bhopal).
Substances that are hazardous to health and the environment
Classification, hazardous characteristics, safety data sheet. Regulation (EC) No 1272/2008 (GHS CLP), REACH; Atex; Seveso Directive.
Toxicity of substances. Effects of toxic substances on biological organisms. Dose-response curves and related models; threshold limits. Industrial Hygiene: identification, assessment and control of exposure to toxic substances. Remediation of contaminated soils.
Reactivity and stability of the substances. Runaway reactions. Identification of unstable structures. Incompatibility. CHETAH Criteria. Examples of exothermic reactions of decomposition, isomerization, polymerization.
Fires and Explosions. Combustion reaction. The fire triangle, flammability limits, limiting oxygen concentration, flammability diagram, ignition sources and energies, auto-ignition temperature. Fire: ignition sources, heat dispersion from the fumes. Types of fire in industrial processes. Effects of fires on structures and people. Detonations and explosions, confined explosions, flammable vapor cloud explosions, physical explosion, airborne dust explosions. Effects of the pressure wave on people and structures. Designs to prevent fire and explosions.

Textbooks
D. A. Crowl e J. F. Louvar, Chemical Process Safety, Fundamentals with Applications, 3rd ed., Prentice Hall, 2011
F. Stoessel, Thermal Safety of Chemical Processes: Risk Assessment and Process Design, Wiley 2008

Prerequisites
Conoscenze di Chimica e Chimica Organica, Termodinamica, Impianti e Processi Chimici

Type of lectures
Il corso prevede lezioni frontali e esercitazioni

Attendance
La frequenza è obbligatoria

Final evaluation
Prova orale

Transport phenomena in multiphase systems (6 CFU) – SSD ING-IND/24
Prof. Stefano Cerbelli (stefano.cerbelli@uniroma1.it)

Objectives
The course aims at providing the students with the basic theoretical and numerical tools to characterize transport of diluted solutions and solid particle suspensions entrained in laminar flows through confined geometries. These tools are then exploited for the optimal design of selected separation/fractionation operations, ranging from industrial scale adsorption units to lab-scale and

microfluidics-assisted chromatography of biologically and clinically relevant analytical targets. Practical design cases are developed through tailored projects that involve the use of commercial software as well as in-house developed code.

Program

1. Basic fluid dynamics of low Reynolds number flows. Creeping flow. General properties and basic solutions of flows through simple geometries. Numerical approaches to laminar flows.
2. Separation in single-phase flows: Adsorption equilibria. Dispersion in laminar flows through capillaries and through packed columns with simultaneous adsorption. Macrotransport approach. Gas and liquid chromatography. Adsorption columns.
3. Separation of suspended nanoparticles: hydrodynamic chromatography and flow-based separations of suspensions and colloids. Current research trends in nanoparticle analysis and fractionation.

Textbooks

1. Panton, Ronald L. Incompressible flow. John Wiley & Sons, 2006.
2. Brenner, Howard. Macrotransport processes. Elsevier, 2013.
3. Articoli pubblicati su riviste scientifiche di riferimento

Prerequisites: Batchelor-level knowledge of equilibrium thermodynamics and transport phenomena.

Final evaluation
Oral exam. Access to oral examination is granted by the presentation of a computational project assigned by the instructor.

First year – second semester

Chemical Reactors (9 CFU) – SSD ING-IND/24
Prof. Antonio Brasiello (antonio.brasiello@uniroma1.it)

Objectives
Starting from the basic knowledge, already gained, in chemical thermodynamics, transport phenomena, and chemical plant design, the course seeks to lead the student toward a critical analysis of the phenomena that act in reacting systems. Additionally, students will acquire the skills required for the design and modeling of chemical reactors.
By the completion of the course, the student should be able to:
• Recognize the main variables that affect chemical reactor design and modeling
• Discuss problems related to the thermal effects occurring in chemical reactors and their implications on the design of heat exchange devices and the reactor stability
• Carry out the basic design of homogeneous and heterogeneous reactors (catalytic reactors, fluid-solid reactors, and gas-liquid reactors)
• Develop models for reactor simulations.

Program
Heat and mass balance in reacting systems; chemical equilibria
Kinetics of chemical reactions
Ideal reactors (BSTR,CSTR,PFR)
Heterogeneous reactors: general discussion; diffusion and chemical reaction
Heterogeneous catalysis: reaction mechanisms and kinetic models
Interaction between chemical kinetics and diffusional phenomena. Thermal effects.
Design of fixed bed reactors

Fluid-solid reactions: shrinking core and distributed conversion models
Fluid-solid reactor design
Gas-liquid reactions: slow reactions; fast reactions; instantaneous reactions.
Design of gas-liquid reactors and chemical absorption devices

Textbooks
O. Levenspiel - Chemica Reaction Engineering - J Wiley & Sons, 1999
H. S. Fogler - Elements of Chemical Reaction Engineering - Prentice Hall 2005
G. F. Froment - Chemical Reaction Analysis and design - J. Wiley & Son 1990
M. C. Annesini - Lezioni di Reattori Chimici - Edizioni Efesto 2023

Final evaluation
The students' preparation will be assessed through a written and an oral exam.
The written exam will last 3 hours. The students will be asked to solve problems on the topics discussed throughout the course. In some cases, the numerical solution may also be required. During the written exams, students will be allowed to consult their textbooks and notes. The aim of the exam is to determine the students' ability to independently apply the knowledge gained throughout the course to solve original problems.
Admittance to the oral exam is subjected to the achievement of a threshold result in the written exam, which may also be lower than 18/30.

The written test can be replaced by the presentation of a project assigned by the teacher during the lessons.

The oral exam may include both theoretical questions and the solution of problems regarding the design or simulation of chemical reactors. This examination is intended to verify the full grasp of the theoretical fundamentals introduced in the course, the ability of identifying the correct procedure for the solution of problems, and the capacity of critically analysing the procedures and the results obtained.

Corrosion Engineering (6 CFU) – SSD ING-IND/22

Prof.ssa Cecilia Bartuli (cecilia.bartuli@uniroma1.it)

Objectives
GENERAL PURPOSE: The course aims to provide the student with the necessary information to recognize the main forms of corrosion of metallic materials in contact with different aggressive environments, to understand the different mechanisms of degradation and to identify correctly the most suitable diagnostic tools and the potential preventative measures and protection systems, with special reference to the field of the chemical industries.

SPECIFIC PURPOSES: With specific reference to Dublin descriptors
Knowledge and understanding of the physico-chemical phenomena at the basis of the corrosion mechanisms of different metallic materials in different environments and in the presence of any additional stresses (either thermal or mechanical) (D.D. .A)
Ability to recognize the main forms of corrosion of metallic materials in contact with different aggressive environments and to identify the diagnostic tools suitable for the aforesaid recognition (D.D. B)
Ability to identify and plan the most suitable preventative and protective measures in the most general lines: choice of the most suitable materials and additional protection measures (protective coatings, environmental conditioning, electrical protection systems) (D.D. C)
The exam is sustained entirely in the form of an oral interview, and it is the teacher's special care to motivate students to pay careful attention to the correctness and amplitude of the technical vocabulary and to stimulate a good expressive capacity (D.D. D).

Program

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.

Textbooks

- P.Pedeferri, "Corrosion Science and Engineering", Springer 2018
ISBN 978-3-319-97624-2, ISBN 978-3-319-97625-9 (eBook)
- Teacher's notes from the lectures.

Prerequisites

No specific prerequisites are formally indicated for the course. However, the knowledge of fundamentals of metallic materials science and engineering represents a necessary basis for the acquisition of competences on corrosion and protection of materials: crystalline structure, defects, microstructure and mechanical properties of engineering alloys (steel, copper, titanium, nickel, aluminum-base alloys) and relative working, machining and thermal treatments. Physico-chemical knowledge of thermodynamics and kinetics of chemical and electrochemical reactions is also considered an important precondition. Useful can be the knowledge of extractive metallurgy and metallurgical processes.

Type of lectures

The activities are organized in: - face-to-face lectures (for the acquisition of knowledge) - discussion of case studies (for the acquisition of the capability of applying the knowledge and understanding for recognizing corrosion forma and identifying remedies and proposals for corrosion prevention/protection)

Attendance

The attendance to the lectures, though encouraged, is not mandatory. However, in case of autonomous preparation for the final interview, students are strongly recommended to seek for previous contact with the teacher, in order to be given important directions on the general sense of the course and on specific critical aspects.

Final evaluation

The assessment will be based on the results of an oral interview, aimed at verifying the acquisition of the following knowledge and skills:

- Knowledge of the physico-chemical mechanisms of corrosion.
- Ability of identify the main causes and forms of corrosion of metals in contact with various aggressive environments.
- Correct identification of the most suitable diagnostic tools and of the potential preventative measures and protection systems, with special reference to the field of chemical industry.
- Ability to communicate the acquired knowledge and to illustrate the proposed technical solutions with clear expression and convincing attitude.

During the course students are offered the opportunity to test their preparation by conducting self-assessment written tests (multi-choice questions, solution of numerical problems, essay questions), followed by common correction and, for those who request it, an evaluation of the test.

For the final vote the following aspects will be considered:

- the level of knowledge
- the ability to securely correlate different topics
- the ability of applying knowledge to the solution of problems of limited complexity in the field of materials engineering
- the ability to communicate the acquired knowledge and to illustrate the technical solutions proposed with clarity using a proper technical vocabulary.

To obtain the highest marks (30/30 cum laude), the student must demonstrate that he/she has acquired excellent knowledge of all the topics covered in the course, and that he/she can apply this knowledge to the solution of problems in the field of industrial engineering, proposing original solutions and showing the results of an autonomous extension of knowledge.

Economics of technology & management (9 CFU) – SSD ING-IND/35

Prof. to be defined

Objectives

Knowledge and understanding

The course deals with the decision making processes of firms. In particular, students are expected to learn the basic principles of

• microeconomic analysis of the firm,
• firm technology strategy,
• economic evaluation of investment projects,
• financial accounting

Applying knowledge and understanding

Students will be able to apply basic methods and models of microeconomics, organization theory and corporate finance in order to:

• identify the determinants of firms' strategic choices,
• analyze the relationship between technological change in the industry and firms' strategies
• evaluate the profitability of investment projects
• analyze the financial statement of a company

Making judgements

Lectures, practical exercises and problem-solving sessions will provide students with the ability to assess the main strengths and weaknesses of theoretical models when used to identify firms'strategies.

Communication

By the end of the course, students are able to discuss ideas, problems and solutions provided by the microeconomics of the firm and corporate finance both with a specialized and a non-specialized audience. These capabilities are tested and evaluated in the final written exam and possibly in the oral exam.

Lifelong learning skills

Students are expected to develop those learning skills necessary to undertake additional studies on relevant topics in microeconomics and corporate finance with a high degree of autonomy. During the course, students are encouraged to investigate further any topics of major interest, by consulting supplementary academic publications, specialized books, and internet sites. These capabilities are tested and evaluated in the final written exam and possibly in the oral exam, where students may have to discuss and solve some new problems based on the topics and material covered in class.

Program
PART I

1. Prerequisites: Analyzing Economic Problems; Demand and Supply Analysis
2. 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.

3. 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

4. Competitive markets

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.
Market demand. Individual supply and market supply. Perfect competition. Short run and long run market equilibrium. Meaning of 0-profits. Pareto efficiency; Applications (taxes, subsidies and quotas)

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.

PART II
1. 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.

Part III
1. 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.

2. 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

Textbooks

Microeconomics | 4th Edition, Ronald R Braeutigam, David Besanko (ISBN-13: 9780470563588, ISBN: 0470563583)

- Chapter 1
- Chapter 2 (only sections 2.1, 2.2 and 2.3)
- Chapter 6, including Appendix
- Chapter 7, including pag 283-284 of the Appendix
- Chapter 8 (excluding section 8.4 at pag 315,316 and 317), including Appendix
- Chapter 9, including Appendix
- Suggested reading: Chapter 10
- Chapter 11 (excluding section 11.7)
- Chapter 12 (excluding sections 12.5 and 12.6)

Robert N Anthony, David Hawkins and Kenneth A. Merchant, Accounting: Texts And Cases (13th Edition). Mc Graw Hill.

Chapter 2: Basic accounting concepts: the balance sheet
Chapter 3:Basic accounting concepts: the income statement
Chapter 5: Revenue and monetary assets
Chapter 6: Cost of sales and inventories
Chapter 7: Long-lived non monetary assets and their amortization
Chapter 8: Sources of capital: debt
Chapter 9: Sources of capital: equity
Chapter 11: The statement of cash flows
Chapter 13: Financial statements analysis
Brealey, R. A., Myers, S. C., Allen, F., Principles of corporate finance (12th Ed.). Mc Graw Hill.

Chapter 2: How to Calculate Present Values
Chapter 5: Net Present Value and Other Investment Criteria
Chapter 6: Making Investment Decisions with the Net Present Value Rule

Prerequisites

Analyzing Economic Problems; Demand and Supply Analysis

Final evaluation

Written exam (exercises and theoretical questions)

Principles of biochemical engineering (6 CFU) – SSD ING-IND/24

Prof. Massimiliao Giona (massimiliano.giona@uniroma1.it)

Objectives

The course provides the student with the qualitative and quantitative tools for understanding subcellular processes and / or involving microorganisms. Inoltrefornisce the biochemical basis and kinetics necessary for the characterization of enzymatic processes of genetic regulation and growth of microorganisms and cell lines and their quantitative description.

Program

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.

Textbooks
1) J. Bailey e D. F: Ollis, Biochemical engineering fundamentals
(McGraw-Hill, New York, 1976).
2) Course notes edited by the instructor.
3) Mark Ptashne and A. Gann, Genes and signals (Cold Spring Harbor, New York, 2002).

Prerequisites
No prerequisites.

Attendance
Participation to classes is not mandatory

Modalità divalutazione
Oral exam with the possibility of developing a study project to be discussed with the instructor.

Second year - first semester

Computer aided process control (9 CFU) - SSD ING-IND/25

Prof. Marco Stoller (marco.stoller@uniroma1.it)

Objectives

The course introduces advanced digital control strategies in process industry.

Typical chemical engineering concepts are recalled, such as instrumental technical drawing and details on chemical units. This part of the course includes exercises. In addition, typical elements of controlled systems, such as measuring elements and control valves, will be introduced.

Successively, the controller was introduced, starting from the basic one (feedback controller) up to more advanced ones. At the same time, the concepts of digital control, applied in different operations, will be presented. Finally, the control will be discussed not only with insight to its basic function of monitoring elements of production processes, but as an element capable of achieving technical, technical-economic and safety optimization.

At the end of the course, the student should acquire a basic knowledge of P&I and of typical chemical units characterizing the framework of process engineering; moreover, the ability of a correct application of measuring elements and controls to ensure best operation should result as established.

Program

Introduction to the course, control systems, block schemes and understanding the P&I
Measurement devices and Regulation valves
Introduction to analogue feedback controllers, Laplace transform, open loop and closed loop feedback control schemes
Brief description of process units and their control
Going from analogue to digital controllers: Z-transform and digital feedback controllers
Quality and stability of control loops, coupling and digital decouplers
Digital feedforward controllers and digital feedback-feedforward controllers
Digital inferential, adaptive, predictive and neural controllers
Digital multivariable controllers
Safety devices in controlled processes
Distributed control systems

Textbooks

Process Control, Designing Processes and Control Systems for Dynamic Performance, 2nd Edition by Thomas Marlin

Final evaluation

The written exam will last 100 minutes and will cover the topics of drawing a P&I and optionally perform some design calculations.

At the same day, after 30 min from the end of the written exam, or in a different day depending on the number of candidates, oral exams will start according to the order of booking of admitted candidates (not by alphabetical order). The test consists of three questions, which focus on knowledge and problem solving.

The students should send by e-mail the solved exercise on controller tuning as reported at the end of the lesson CAPC E04, at least 2 days before sitting the written exam. The exercise can be solved in group with other colleagues (max 3 people) or alone.

Chemical & biochemical plants (9 CFU) - SSD ING-IND/25

Prof. Marco Bravi (marco.bravi@uniroma1.it)

Objectives

Momentum and Heat Transfer analysis for Consolidated and Biorefinery applications (1 CFU): Momentum and heat transfer analysis (Newtonian and non-Newtonian fluids); special pumping and heat transfer equipment (for biomass and food applications).

Distillation for Consolidated and Biorefinery applications: Fundamentals of Distillation (Vapor-liquid equilibrium theory; Separation principles and relative volatility; Types of distillation: simple, fractional, batch, continuous; Staged distillation, theoretical stages and stage efficiency), Mass and Energy Balances (Applying balances to distillation processes; Reflux and reflux ratio), Equipment and Instrumentation (Distillation column components, Instrumentation for control, Troubleshooting common distillation problems), Safety considerations, Economics (Cost factors in choosing a distillation process). Special Distillation Techniques: Steam Distillation (Theory and principles for separating heat-sensitive materials, Design and operation of steam distillation equipment, Applications) (essential oils, pharmaceuticals), Hydrodistillation (Comparison with steam distillation, Advantages and limitations, Applications), Vacuum and Molecular Distillation (Principles of high vacuum distillation for separating high-boiling and/or high-sensitive components, Equipment design and operation, Applications), Azeotropic Distillation (Challenges in separating azeotropic mixtures, Entrainer selection and application, Extractive distillation techniques).
Liquid-Liquid Extraction for Consolidated and Biorefinery Applications : Fundamentals (Partitioning, Distribution Coefficient, Selectivity; Thermodynamics of LLE; Mass Transfer in LLE and Stage Efficiency); Solvent Selection and Design (Solvent Properties for LLE: Selectivity, Solubility, Toxicity, Biodegradability; Designing Sustainable Extraction Processes: Novel biomass-derived solvents, Ionic Liquids, Deep Eutectic Solvents; Switchable solvents; Aqueous Biphasic Systems); Process Design and Optimization (Multistage Extraction, Process Modelling and Simulation, Equipment Selection and Design), Safety, Economics. (1 Credit)
Solid-Liquid Extraction for Consolidated and Biorefinery Applications: Principles of Solid-Liquid Extraction (SLE) (Mechanisms involved in SLE, including diffusion, mass transfer, and solubility. Factors affecting extraction efficiency, including particle size, solvent properties, temperature, liquid-solid contact dynamics, dissociation extraction, association extraction). Solvents for Biorefinery SLE (Selection criteria for solvents in biorefineries, solvent properties: polarity, hydrophilicity, selectivity, biodegradability; green solvents; potential health and safety concerns). Novel extraction processes (Consolidated batch and continuous extraction systems; Supercritical Fluid Extraction, SFE; Microwave-Assisted Extraction, MAE; Ultrasound-Assisted Extraction, UAE; Surfactant-Assisted Extraction; Three-Phase Partitioning); Process design and equipment choice. Safety considerations. Economics.

Membrane Separations for Consolidated and Biorefinery Applications: Fundamentals (Different types of membranes: microfiltration, ultrafiltration, nanofiltration, reverse osmosis; dialysis; transport mechanisms: diffusion, convection; Principles of Membrane Separation: Dead-End and Cross-Flow Separation, Driving forces, membrane fouling and cleaning). Membrane Separations in Consolidated Bioprocessing (Pretreatment: Microfiltration and ultrafiltration for biomass fractionation, removal of enzymes inhibitors; Fermentation Broth Clarification; Downstream Processing: Nanofiltration and reverse osmosis for product concentration, purification, solvent recovery). Membrane Separations in Biorefinery Applications (Pervaporation for Alcohol Recovery; ultrafiltration for enzyme recovery). Membrane Selection for Biorefinery Applications (Factors to consider: material, pore size, fouling resistance, economic aspects).

Industrial Chromatography: Fundamentals of chromatography (Principles of Adsorption Chromatography, Chromatograms and their Parameters; Influence of Adsorption Isotherms and fluid dynamics on the Chromatogram; Efficiency of Chromatographic Separations; Thermodynamic Effects on Mass Separation; Elution Modes: isocratic and gradient; Normal-Phase and Reversed-Phase Chromatography). Industrial chromatographic systems (Column Design; Criteria for Choice of Chromatographic Systems; Design and Operation of Equipment; Discontinuous Processes: Isocratic, Flip-Flop, Closed-Loop Recycling, Gradient; Continuous processes: Column Switching; Simulated Moving-Bed). Application examples.

Industrial Bioreactors and Photobioreactors: Principles of Microbial Biotechnology and Photobiotechnology (cellular growth and metabolism, enzyme processes; Light and photosynthesis in microalgae and cyanobacteria; Different types of hetero and phototrophic organisms used in bioprocesses); Bioreactors (Mechanically, hydraulically and pneumatically stirred types; Design and debottlenecking; Mixing; Mass transfer; Scale-up and scale-down); Photobioreactors (Open and Closed Photobioreactors; Scale-up; Light source selection and optimization; Mass transfer considerations for CO_2 and oxygen in photobioreactors; Mixing strategies for efficient light utilization). Bioprocess Management (Upstream and media, Bioprocess Monitoring and Control, Downstream processing). Special bioreactors (Single-Use Bioreactors). Regulatory issues (Biosafety and GMP; Axenicity and Containment).

Operation Synthesis in the Biorefinery: Biorefinery overview (Concept of biorefineries, their role in the bioeconomy, and types of products they can generate: biofuels, biomaterials, biochemicals, food, feed). Process integration principles (Principles of process integration, Benefits of process integration: reduced energy consumption, waste minimization, cost optimization; process integration approaches: heat integration, mass integration, equipment integration). Conception and analysis of alternative process routes. Variability. Sustainability.

Conventional and Novel Sterilisation Processes. Introduction to Sterilization (Definition and principles of sterilization; Importance of sterilization in different sectors: biotechnological, pharmaceutical, food; Factors affecting the effectiveness of sterilization: microbial resistance, process parameters; Regulatory considerations for sterilization processes). Heat Sterilization (Dry heat sterilization; Moist heat sterilization: autoclaving, steam sterilization; Factors influencing effectiveness: time, temperature, moisture; design techniques and optimisation criteria; Applications in various industries). Filtration Sterilization (Types of filters; Principles of filtration and selection criteria; Applications for sterilizing liquids and gases). Radiation Sterilization (Types of radiation; Applications in food; Safety considerations). Chemical Sterilization (Types of chemical sterilants; Safety concerns). Pressure Sterilization (Mechanism of action, factors affecting effectiveness; applications in food preservation and potential for other industries, potential impact on sensory qualities). High CO_2 Pressure Sterilization (HPCD). Aseptic Processing (Food industry, pharmaceutical industry).

Green chemistry and process engineering – SSD ING-IND/27

Prof. Marco Scarsella (marco.scarsella@uniroma1.it)

Objectives

Principles of 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

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

Program
Principles of Green Chemistry
• Introduction to Green Chemistry
• Control of Environmental Impact
• Alternative Reaction Media
• Catalysis for Green Chemistry

Application of Green Chemistry to Process Engineering
• Clean Synthesis
• Renewable Resources
• Energy Efficiency & Emerging Technologies
• Chemical Engineering & Clean Technology

Commercialisation of Green Chemistry
• Greener Products

Textbooks
Green Chemistry and Engineering: A Pathway to Sustainability. (2014) John Wiley & Sons, Inc., Hoboken, New Jersey. Online ISBN: 9781118720011; Print ISBN: 9780470413265

Prerequisites
Basic knowledge of physical chemistry and chemical engineering gained during the Bachelor's degree

Final evaluation
oral exam

Nanobiotechnology (6 CFU) – SSD ING-IND/25

Prof. Marco Bravi (marco.bravi@uniroma1.it)

Objectives
Aim of this course is getting to know the technologies to produce biocompatible nanomentric particles by using highly sustainable and maximally green processes which mainly resort to using naturally-sourced biological matrices.
The student will learn: 1. The main classes of biological substances, 2. The methodologies for obtaining these substances from natural biomass, 3. the methodologies for producing functional nanoparticulate from each of these classes of substances, 5. The main processes and equipment that implement these production processes. The student will also learn the main problems of biomedical and cosmetic use of nanotechnologies.

The student who will exhibit a regular attendance of the course will be able to participate in group work intended to develop and strengthen soft skills such as: the ability to work in a group, the ability to dialogue with colleagues from different backgrounds, the ability to write a scientific/technical report and the ability to present one's work.

Program
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 use of nanoparticles by biotechnological techniques (microorganisms, culture media, extracts, switchable solvents). Applications of nanoparticles in the bio-related fields (food, pharma, cosmetic, agriculture).

Textbooks
ALL information relating to the teaching activity of prof. Marco Bravi (lesson times and any exceptions; methods of conducting lessons and tools used; student reception hours; exams; available project works), updated in real time, can be found by consulting the URL:
https://sites.google.com/site/marcobravi/

Study materials (generally scientific review articles) will be shared to the attending students during the semester the course is being taught. Students will receive a Google Drive share by being included in the Google Classroom of the course itself.

Attendance
Attendance is facultative. However, only regularly attending students will have their "small groupwork projects" evaluated for the final mark (together with the compulsory written test).

Final evaluation
The written exam includes 10 multiple choice questions, plus an open-ended question (to be provided by the student).
The oral exam is optional. If it is not carried out, it will be counted as passed with the vote of 18/30.
The final mark will be assigned as the average of the marks obtained in the two tests.

Only those admitted to the "evaluated groupwork" can replace the oral test with the presentation of their groupwork.

Environmental chemical engineering (6 CFU) - SSD ING-IND/25
Prof.Luca Di Palma (luca.dipalma@uniroma1.it)

Objectives
The course aims to provide students with:
- The principles of sustainability and circular economy applied to Environmental Protection
- the theoretical aspects and design criteria of innovative tertiary processes for the treatment of industrial wastewater
- Basic and advanced knowledge on the characterization and treatment of contaminated sites (land reclamation and groundwater treatment)
- The chemical-physical fundamentals of the design of units for the treatment of industrial and hazardous waste, aimed at the recovery of material and energy

Program
1. Sustainability, Circular Economy and Environmental protection. Waste minimization and clean technologies.
2. Water/Wastewater Advanced Tertiary treatment Processes: Membrane operations and MBR, Constructed wetlands, Wet Air Oxidation, Advanced Oxidation processes, Electrochemical processes, Photocatalysis, Biological electrochemical system and Microbial Fuel Cell.
3. Effluent disposal: direct and indirect toxicity in natural systems, dispersion models in water
4. Soil and groundwater characterization.

5. Principles of groundwater contamination: Causes, Fate, Transport of contaminants in groundwater
6. Soil and groundwater remediation: Soil Vapour Extraction, Biosparging, Bioventing, Thermal desorbing, Bioremediation, Multi Phase Extraction, Ex situ thermal treatments, Soil washing, Pump&Treat, Air Sparging, In situ chemical oxidation, In situ chemical reduction, Permeable Reactive Barrier, Plume Containment.
7. Solid and Hazardous waste treatment: Characterization, Landfilling, Composting, Thermal treatment, Stabilization and vetrification

Nanotechnologies and nanostructured materials for innovative wastewater treatment and soil remediation: application and environmental and toxicological issues.

Textbooks
L. Di Palma - Course materials available on Sapienza e-learning platform

Testi consigliati
M.L. Davies - Water and Wastewater Engineering: Design Principles and practice, 2010,

Prerequisites
Water characterization and chemistry – Wastewater Treatment Processes (Unit design and calculation)

Type of lectures
Front-end lectures and exercises

Attendance
Face to face (unless otherwise specified by Sapienza)

Final evaluation
Written test: two exercises and five theoretical open questions.
Evaluation criteria for the written test: procedure correctness, numerical results accuracy, correct results interpretation.
Oral test: discussion on theoretical aspects of environmental processes and remediation technologies and questionnaires on practical exercises.

Second year – second semester

Computational methods for chemical and biochemical reactor dynamics (6 CFU) - SSD ING-IND/26

Prof. Antonio Brasiello (antonio.brasiello@uniroma1.it)

Objectives
The course aims to broaden the skills in the theory of complex systems with particular reference to the non-linear dynamics of chemical and biochemical reactors. It also provides a critical approach to numerical techniques for dynamic analysis leading students to the development of algorithms and their translation into computational codes using high-level programming languages (e. g. Fortran, C ++, etc.).

Programme
Balance and constitutive equations for reacting systems.
Elements of chemical kinetics.
Linear and non-linear dynamical systems theory: elements and complex scenarios.
Chemical and biochemical reactors as dynamic systems: batch, semi-batch, CSTR, PFR, Packed bed

reactor, Reverse Flow Reactor.
Introduction to programming using high-level languages (e.g. Fortran, C ++, etc.).
Applications of numerical methods for dynamical systems analysis: equilibrium points calculation, numerical integration of systems of ordinary differential equations, numerical integration of systems of partial differential equations, parametric continuation.

Textbooks
Teacher's lecture notes
Bequette B. W., Process Dynamics Modeling, Analysis, and Simulation, Prentice Hall, 2002
Kuznetsov Y. A., Elements of applied bifurcation theory, Springer, 2004
Quarteroni A., Sacco R. Saleri F., Numerical Mathematics, Springer 2007
Parker T. S., Chua L. O., Practical numerical algorithm for chaotic systems, Springer-Verlag, 1991

Bibliografia
Strogatz S. H., Nonlinear dynamics and chaos: with application to physics, biology, chemistry and engineering, Addison Wesley, 1994 Hale J., Kocak H., Dynamics and Bifurcations, Springer, 1991 Wiggins S., Introduction to applied nonlinear dynamical systems and chaos, Springer, 2003 Nayfeh A. H., Balachandran B., Applied Nonlinear Dynamics - Analytical, Computational, and Experimental Methods, WILEY-VCH, 2004

Prerequisit
Good knowledge of calculus, linear algebra, and ordinary differential equations is required.

Type of lectures
Lectures and computer exercises

Attendance
not compulsory

Final evaluation
Evaluation of a project and oral exam

Sustainable design of materials (6 CFU) - SSD ING-IND/22
Prof. marco Valente (marco.valente@uniroma1.it)

Objectives
What is intended to be transferred as training objectives are the basic knowledge of the principles on which the analysis of the potential environmental impacts related to the production processes of the products and the growing problem of impacts on the environment is based. The above will be analyzed from the point of view of the different types and classes of materials in consideration of the volumes of use and the growing demand for energy involved in their production. A further objective of the course is to transfer to the students the approach of designing production processes and design choices aimed as much as possible at an evaluation of choices that allow a greater "circularity" of the resources used and a lower impact on the environment. . All this through an integrated vision between resource, contained energy and impact of production through the study and knowledge of the LCA philosophy.

Program
Basic analysis of the general characteristics of the various classes of materials: polymers, ceramic metals and composites, highlighting the strengths, criticalities and properties microstructure bonds of the various classes of materials. Subsequently, the production processes and especially the transformation of the different materials will be analyzed, which will be used in the second phase, relating to the LCA assessments.
In a second part 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 of the processes and the impacts they have on the global

costs of the processes and products; looking in particular at the entire life cycle of the components and the potential economic and industrial repercussions in terms of environmental costs. This last part will be addressed with the approach and philosophy of the Life Cycle Assessment.

Textbooks
Notes and texts by the teacher

Final evaluation
Oral exam

Theory & development of process design (6 CFU) - SSD ING-IND/26

Prof.ssa Alessandra Adrover (alessandra.adrover@uniroma1.it)

Objectives
1) analytical and numerical approaches for the characterization of dynamical behaviour of chemical engineering systems, with and without controls.
2) identification of the possible cohexistence of multiple steady states, limit cycles and attractors
3) Identification of model parameters controlling the asymptotic behaviour of chemical engineering systems and construction of bifurcation diagrams
Students should be able to apply analytical and numerical techniques for characterizing the dynamical behaviour of chemical engineering systems and for constructing bifurcation diagrams for dynamical systems operating with and without automatic controls.

Program
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.

Textbooks
Stephen Wiggins "Introduction to applied nonlinear dynamical systems and Chaos " ,II edition, Springer Verlag 2003
Steven Strogatz : "Nonlinear Dynamics and Chaos with applications to Physics, Biology, Chemistry and Engineering", Perseus Books Publishing L.L.C 1994
Teacher's handouts

Testi consigliati
Stephen Wiggins : " Introduction to applied nonlinear dynamical systems and Chaos " ,II edition, Springer Verlag 2003 Steven Strogatz : "Nonlinear Dynamics and Chaos with applications to Physics, Biology, Chemistry and Engineering", Perseus Books Publishing L.L.C 1994 Dispense preparate dal docente

Prerequisites
Calculus

Final evaluation
Written test and evaluation of a project

Transport phenomena in microsystems and micro-nano reactive devices (6 CFU) - SSD ING-IND/24

Prof. Massimiliano Giona (massimiliano.giona@uniroma1.it)

Objectives
The basic units of a microfluidic circuit are analyzed, namely micromixers, micro heat exchangers, and separation units. Background on the constitutive relationships governing molecular transport of momentum, mass and energy, and their use in local and macroscopic balances constitute the incipit of the course. Emphasis is focused on the interaction between mass and momentum transport and externally imposed electromagnetic fields (electroosmotic and magnetohydrodynamic pumps). Analytical solutions derived for simple geometries are used as a paradigm to orient the design of real world devices, the performance of which is established through commercial software.

Program
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.

Textbooks
1) G. Karniadakis, A. Beskok and N. Aluru, Microflows and nanoflows (Springer, New York, 2005).
2) H. C. Ottinger, Stochastic processes in polymeric fluids: tools and examples for developing simulation algorithms (Springer, New York, 2012).
3) Course notes edited by the instructor.

4) B. Gaveau, T. Jacobson, M. Kac and L.S. Schulman, "Relativistic extension of the analogy between quantum mechanics and Brownian motion, Phys. Rev. Lett. 53 (1984) 419-422.

Attendance
Participation to classes is not mandatory

Final evaluation
Oral exam with the possibility of developing a study project to be discussed with the instructor.

Seminars (Activities useful for entering the job market) (1 CFU)

Prof.ssa Cecilia Bartuli (cecilia.bartuli@uniroma1.it)

Program
Students must register to individual seminars in advance, and the attendance of students is recorded and transmitted to the President by the person in charge of the seminar.
The database reporting the attendance of students to the past seminars, updated monthly, is available in the Download Area at this link
Once the student has been certified the attendance of at least 8 seminars, he/she will register for the the exam "Altre attività utili all'inserimento nel mondo del lavoro" (1 CFU) on INFOSTUD platform. Exam sessions are opened about 1 month before the deadline for the application for the final thesis discussion. For more information, please contact Prof. Bartuli.

Final evaluation
Attendance and participation will be certified by the organizing commission.
A final evaluation will not be required