MULTIPHASE MASTER

Erasmus Mundus

Course description

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Contents

Overview

Successful students will receive following diploma:

- MSc in Chemical and Biochemical Engineering delivered by Mines Saint-Etienne
- Laurea Magistrale (Master of science-level) in Chemical and Sustainable Processes Engineering, Chemical Engineering degree class delivered by the Polytechnic University of Turin
- MSc. In Materials Science and Engineering delivered by Technical University of Munich

The programme spreads over two years (4 semesters), during which MULTIPHASE students will visit three universities:

- one semester in Mines Saint-Etienne (France)
- one semester in Polytechnic University of Turin (Italy)
- one semester in Technical University of Munich (Germany)

Two winter schools and an 18 months-long project driven by industrial partners are also offered.

The fourth semester is devoted to an internship with MSc thesis, in industry or academia.

Please, note that this program is subject to (minor) changes to reflect the evolution of the state-of-the-art disciplines and the multiple constraints experienced by the Consortium's institutions.

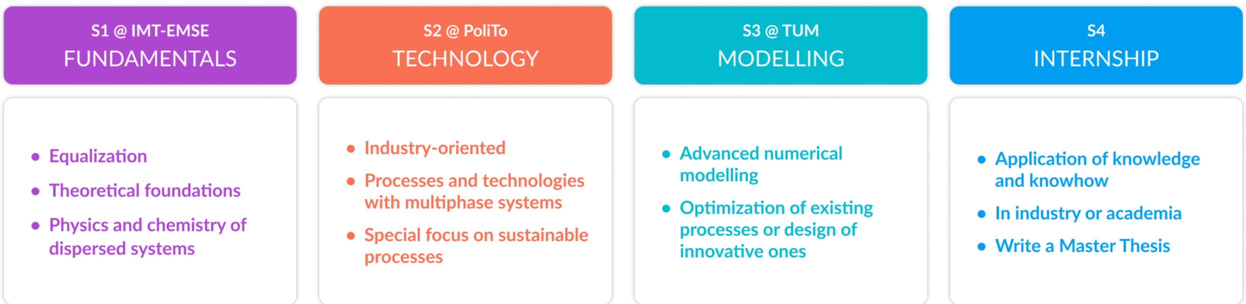

Figure 1: Overview of the curriculum.

1. Semester 1 in Saint-Etienne, France

1.1 CS01: Fluid dynamics (10 ECTS)

Content: Physics of fluids, micro-, meso- and macroscale, transport phenomena, constitutive equations, complex fluids, rheology, conservations laws (local and global), turbulence, boundary layer, RANS, LES, k-epsilon models, combustion and reactive flows, liquid-gas or liquid-vapor flows, flow regimes map and correlations, suspension flows

Learning outcomes:

- explain the link between microscopic properties of a fluid and its rheological and thermal behaviour
- choose and implement the appropriate method for modelling turbulent flows
- explain the Finite Volume Method, write a toy code and critically
- evaluate the influence of material properties and operating conditions on the flow regime

1.2 CS02: Physical chemistry (5 ECTS)

Content: Transport phenomena (momentum, mass, heat), homogeneous reactors (CSTR, plug flow), heterogeneous reactors (catalytic or not), crystallization, germination, growth, agglomeration, reaction kinetics and thermodynamics

Learning outcomes:

- describe the main transport phenomena and propose their modelling equations
- write and solve equations to predict a concentration or temperature evolution in a reactor
- differentiate the different crystallization processes at play during precipitation or solid-state transformations

1.3 CS03: Experimental characterization methods of solids and fluids (2,5 ECTS)

Content: Radiation-matter interaction, X-ray diffraction, Scanning and Transmission Electron Microscopy, Elementary surface analysis, specific surfaces, porosity, thermal stability,

Learning outcomes:

- understand the theory underlying the experimental characterization tools
- know the working principles and the limits of the main characterization methods of dispersed systems (solids, fluids)
- operate some of these instruments, in autonomy or under guidance

1.4 CS04: Particulate processes (5 ECTS)

Content: Physics of granular matter, mechanical, thermal and chemical transformations, size reduction (grinding, abrasion, attrition) and enlargement (agglomeration, granulation, caking), compaction and sintering, pneumatic transport and fluidization, ..

Learning outcomes:

- choose the appropriate sequence of unit operations to handle and transform powders and grains
- describe the main phenomena at play in these devices/reactors
- design some reactor properties and operating conditions to handle a particular granular matter
- critically identify the advantages and drawbacks of a unit operation

1.5 CS05: Discrete Element Method (3 ECTS)

Content: Event driven, soft sphere and hard sphere approaches, algorithmic implementation for soft spheres, contact laws and calibration, scale-up, coarse graining and homogeneization

Learning outcomes:

- write a toy code implementing the basic physical laws
- use a highly parallelised research code and/or an industrial one
- propose a method to calibrate the numerical parameters and guarantee the validity of the simulation outputs
- customize an existing code to take into account new phenomena

1.6 CS06: Introduction to CFD (2 ECTS)

Content: Mesh-based methods (FDM, FVM, FEM), Particle-based methods, Explicit vs. Implicit solvers, CFL stability condition, algorithm, time stepping methods, visualization

Learning outcomes:

- discretize an EDP according to a given numerical scheme
- write a toy code to compute flow field on benchmark configuration
- use the different softwares on the chain (geometry, mesh generation, solver, visualization)
- know the main open-source and industrial codes

2. Semester 2 in Turin, Italy

2.1 CT01: Sustainability in the chemical industry (8 ECTS)

Content: Impact of sustainability of anthropogenic activities, multiphase production systems, optimization matter and energy consumption, use of renewable materials, Energy Sustainability Index (ESI), Energy Return On Investment (EROI) and Energy Payback Time

Learning outcomes:

- design of new approaches for the development of sustainable production processes
- assess the interaction between natural cycles and anthropic activities
- perform analysis on energy and production processes sustainability e.g. Life Cycle Analysis (LCA)

2.2 CT02: Fixation and recycle of CO2 for Green House Gas mitigation (6 ECTS)

Content: Carbon cycle, main greenhouse gases, CO2 sequestration and conversion processes, synthesis of urea, dry reforming, conversion of CO2 into inorganic carbonates, power-to-X, photo-catalytic, electro-catalytic and photo- synthetic processes

Learning outcomes:

- nature and chemistry of the natural carbon cycle on the planet
- properties of the CO2 molecule and the consequent poor chemical reactivity
- CO2 capture processes, chemical reactivation through the use of renewable energy and H2, CO2 entrapment in "end-of-life" compounds

2.3 CT03: Multiphase chemical reactors (8 ECTS)

Content: Gas-liquid and liquid-liquid reactors, catalytic heterogeneous reactors, porous catalysts, modelling of multiphase chemical reactors, three-phase chemical reactors, mixing and scale-up

Learning outcomes:

- master and control mixing in multiphase chemical reactors

- design multiphase chemical reactors with optimal mass, momentum and energy transfer
- design multiphase chemical reactors for sustainable engineering applications

2.4 CT04: Hydrogen for sustainable mobility (3 ECTS)

Content: Energy transition, hydrogen economy, production, storage and use of H2 through electrolysers and fuel cells. Basic theory on electrochemistry. Momentum, mass, heat, charge transport phenomena

Learning outcomes:

- explain the basic fundamental aspects of electrochemistry
- understand the working principles, advantages and drawbacks of electrolysers and fuel cells (mainly PEMFC and SOFC)
- use models to evaluate the influence of the materials on electro- catalytic properties

2.5 CT05: Population balances (3 ECTS)

Content: Definition of population balances, application of population balances to multiphase systems for sustainable engineering applications, solution methods and coupling with CFD

Learning outcomes:

- ability to formulate and solve a population balance
- numerical solution of population balances with different methods
- coupling of population balances with CFD

3. Semester 3 in Munich, Germany

3.1 CM01: Multiscale modelling (5 ECTS)

Content: Systematic overview of the developments and challenges in multiscale modeling with emphasis on fundamental principles and overaching issues

Learning outcomes:

- master numerical models from scale-separation analysis
- ability to compute coarse-grained (CG) models for molecular dynamics
- use CG models for general applications in science and engineering

3.2 CM02: Mathematical modelling of materials (5 ECTS)

Content: Linear FEM for elasticity with volume locking, error estimators and non-linear analysis, discussion of limits for phase transition and fracture problems

Learning outcomes:

- understand and apply linear and nonlinear FEM
- apply FEM using advanced software packages
- master FEM for continuum mechanics, phase transitions and fracture mechanics

3.3 CM03: Computational thermo-fluids dynamics (4 ECTS)

Content: Overview of fundamental numerical methods used in thermo-fluid dynamics and introduction to high-level programming

Learning outcomes:

- understand and solve partial differential equations
- write high-level language solver (Matlab) for Fourier equations
- combine mathematical, numerical and physical analysis of PDEs

3.4 CM04: Multiphase flows CFD (4 ECTS)

Content: Introduction to state-of-the-art numerical methods for multiphase flow simulations using sharp- and diffuse-interface models

Learning outcomes:

- understand multiphase systems and their challenges on numerical methods
- use diffuse-interface (vof) and sharp-interface (level-set) methods for compressible and incompressible flow problems
- critically assess validity, efficiency and accuracy of opposed methods in different flow configurations

3.5 CM05: Particle-simulation methods for Fluid Dynamics (3 ECTS)

Content: Introduction on theoretical basics of Particle- Simulation Methods for Fluid Dynamics ranging from molecular dynamics (MD), Monte-Carlo methods (MC) over Lattice-Gas automata (LGA)/Lattice-Boltzmann methods (LBM) to continuum methods (Navier-Stokes)

Learning outcomes:

- understand basics and principles of microscopic methods (MD, MC)
- understand basics and principles of mesoscopic methods (LGA, LBM, DSMC, DPD)
- understand basics and principles of macroscopic methods (Navier- Stokes, SPH, PIC)

3.6 CM06: Artificial Intelligence in Engineering (5 ECTS)

Content: A deepened understanding of the basic techniques in artificial intelligence and its application for engineering problems

Learning outcomes:

- knowledge on localization filters (Bayesian, Kalman, particle)
- knowledge on ML algorithms (linear NN, Kohonen maps, reinforcement learning)
- apply ML to engineering applications like robotics

4. Semester 4 for internship

The Internship will last 5 months, during which the student will work on his/her Master Thesis. It is the opportunity for the students to apply the knowledge and know-how delivered during the 3 first semesters of the MULTIPHASE master to a challenge which is both involving a multiphase system and an application oriented towards sustainable engineering.

Students will have the choice to join an academic laboratory, especially among the full partners and the academic Associated Partners, or to go for an internship in an industrial environment.

5. Green Line Research Project (GLiP)

Groups of three students will work to solve a real-life challenge provided and supervised by an industrial partner, with a special focus on sustainable development. It will be the opportunity to establish a durable and interactive relationship with an industrial Associated Partner and:

- experience a collaborative work over a long period of time (18 months)
- learn how to manage human relationships in a team
- learn how an industrial company is leading an R&D project with scientific and economic aspects
- have the opportunity to report their work in a professional environment (oral presentation, written report)

The different phases of the GLiP are synchronized with the overall curriculum:

- S1: in-depth study of the product or material to be manufactured (physico-chemical properties and theories underlying these properties and the experimental characterization methods)
- S2: technological implementation, physical and chemical phenomena involved during the manufacturing, Life Cycle Analysis and identification of innovative production ways with an improved sustainability
- S3: identification of all reasonable modelling approaches to design and optimize the production process, selection of one of them and development of the associated computer model

Students will have the possibility to go in the industrial partner buildings during two periods of 6 weeks each.

The results of the GLiP will be presented during the September week, just before the graduation, in presence of the industrial Associated Partners and the incoming cohort.

Students will present their results in the form of a scientific article, that will be critically reviewed and published in the internal "MULTIPHASE master Journal". This will be a good preparation for students willing to engage in a PhD after the Master.

6. Application seminars

Two Applications seminars are proposed to students every semester. An application seminar consists of 3-to-5 days focused on an application field.

Morning presentations are given by renowned researchers and/or invited scholars. They will giveinsight in a specific theory related to multiphase systems and describe novel methods and applications published in the field.

Afternoon presentations will be delivered by industrial representatives explaining the practical and technological challenges they are facing.

Below is the provisional planning for the first three semesters. Attention has been brought to present scientific state-of-the-art challenges and their impact on society. Provisional agenda includes:

- Societal and technological impacts of nuclear fuel for CO2-free electricity and health diagnosis
- Critical metals processing and recycling + Society readiness to open new mines
- Bio-refinery and bio-fuels
- Catalysis, Hydrogen and fuel cells. Impact on transportation and way of living
- Sustainable development, climate resilience and smart industry
- High-Performance Computing, Data Center and digital twins

7. Winter schools

In a mountain village, two successive cohorts of students will spend 5 days.

The program is:

- morning for hard-skills: scientific lectures delivered by top international experts in multiphase systems for sustainable engineering
- afternoon: team building activities
- evening for soft skills: entrepreneurship, innovation methods, ethics and how-to-find-a-job, …