Computer Aided Process Design (courses taught in English)

Specialisation of ENSGTI Final year Program
(2^{nd} year MSc in Chemical Engineering)

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ÉCOLE D'INGÉNIEURS

INDUSTRIAL RISK MANAGEMENT

Subject Information	
Code	**EP3OC1**
Credits (ECTS)	1
Semester	Spring
Time Allocation (Lec. / Prac. / Lab.)	24h / - / -
Lecturers	T. Baron (Total)
Pre-requisites	
Assessment	Group Project: Oral Presentation (1/3) and written evaluation (2/3)

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description	
Introduction	Process engineers are expected to make decisions either for the building of a new process or for revamping of an old one. The process engineer should make these decisions considering the social, environmental and economic context. This lecture, given by a highly experienced industrial partner aims at preparing future process engineers to industrial risk management
Learning outcomes	**After this course, students will:** • Be aware of issues and risks (economic, social, environmental...) associated with the conception or the revamping of an industrial unit • Know the main steps in a design project • Be able to estimate the results of an industrial activity
Contents	**I Economics of an industrial activity** • Variable expenses of process • Estimation of a margin upon variable expenses • Capital expenses of a process • Results of an industrial activity **II Design and risks management** • Production of new products. Definition and adjustment of this product (R&D, industrial trials, management) • Revamping of an existing process • Price trend analysis of the different steps in the project • Risk Management: preliminary questions….

PROCESS SYNTHESIS

Subject Information	
Code	**EP3OC2**
Credits (ECTS)	1
Semester	Autumn
Time Allocation (Lec. / Prac. / Lab.)	6h / 12h / -
Lecturers	Dr. S. Sochard
Pre-requisites	Unit Operation, mass and heat balances
Assessment	project

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description	
Introduction	Process synthesis is a methodology based on the experience and know-how of engineers. These qualitative procedures lead to an acceptable (from a technical and economic point of view) process predesign using heuristic rules.
Learning outcomes	**After this course, students will:** - know the main steps of the hierarchical procedure proposed by Pr. Douglas - know the main heuristics for each step - be able to pre design a process based on these rules
Contents	1. Definition of process inputs (raw materials) and outputs, 2. General process structure 3. Reactive zone: heat effect, reactor type 4. Design of gas and liquid separation, 5. Heat exchanger network design.
Literature	**Conceptual Design of Chemical Processes ;** J.M. Douglas; McGraw-Hill, Inc.; New York, 1988 **Process Design Principles**; W.D. Seider, J.D. Seader, D.R. Lewin. J Wiley&Sons 1999 Analysis, Synthesis and Design of chemical Processes**; R. Turton, RC Bailie, W.B. Whiting, J.A. Shaeiwitz. Prentice Hall 1998**

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PROCESS OPTIMIZATION

Subject Information	
Code	**EP3OC3**
Credits (ECTS)	1
Semester	Spring
Time Allocation (Lec. / Prac. / Lab.)	4h / 16h / -
Lecturers	Prof. J-M. Reneaume
Pre-requisites	Optimization Methods (GC2MI2)
Assessment	Project

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description	
Introduction	Optimisation is one of the major quantitative tools for decision-making in Chemical Engineering. Students are familiarized with Process Optimization (operating and design parameter optimization) using flowsheeting environments (ProSim Plus and/or Pro II).
Learning outcomes	**After the course the students will:** - have advanced knowledge about optimization algorithms (SQP) and solution strategies (Feasible or Infeasible Path) - be able to formulate and solve a process optimisation problem within a flowsheeting environment
Contents	Theoretical concepts are presented: Feasible or Infeasible Path, SQP algorithm During the proposed project, the students will have the opportunity to formulate and solve a parametrical optimization process. Considered examples are: HDA process or Cyclohexane plant. ProSim Plus and ProII are the selected optimization tools.
Literature	Optimization of Chemical Processes **T.F. Edgar, D.M. Himmelblau –** ***McGraw Hill International Edition***

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INDUSTRIAL OPTIMIZATION PROBLEMS: SCM, SCHEDULING

Subject Information	
Code	**EP3OC4**
Credits (ECTS)	2
Semester	Autumn
Time Allocation (Lec. / Prac. / Lab.)	30h / - / -
Lecturers	Dr. Zoltan LELKES (OPTASOFT)
Pre-requisites	Optimisation methods (GC2MI2)
Assessment	- written: test 20% - oral: participation in classes 40 % - project: Software development with AIMMS 40%.

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description	
Introduction	The aim of the course is to familiarize the students with the AIMMS optimization platform. Understanding the SCM and scheduling problems (capacity optimization, short term planning, flow-shop, job-shop).
Learning outcomes	**After the course the students will be able to :** • Use AIMMS platform for optimization • Formalize of Supply Chain optimization problem • Know different heuristics and meta-heuristics methods for scheduling optimization • Understand the parts of a complete scheduling planning system (capacity planning, operation scheduling optimization, reactive scheduling)
Contents	During the course we will present the followings: • AIMMS optimization platform • AIMMS project, model tree, algorithmic features, GUI, integration • Case study: SCM optimization problem in SAB Miller company • Programming a simple SCM optimization problem in AIMMS • Programming rolling horizon optimization in AIMMS • Flow-shop, job-shop scheduling, heuristics and meta-heuristics methods • Case study: a simple job-shop scheduling problem in AIMMS • Case study: Scheduling in Graboplast company
Literature	Johannes Bisschop: AIMMS Optimization Modeling Marcel Roelofs, Johannes Bisschop: AIMMS User's Guide

DATA RECONCILIATION

Subject Information	
Code	**EP3OC5**
Credits (ECTS)	1
Semester	Spring
Time Allocation (Lec. / Prac. / Lab.)	6h / 4h /-
Lecturers	Dr S. Sochard
Pre-requisites	Statistical tests, nonlinear optimisation
Assessment	project

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description	
Introduction	In a wide range of situations, chemical engineers point out differences between experimental result and theory. So the main question is: "are my experiments wrong or did I use an inappropriate theory?". This course answers this central question through a systematic approach.
Learning outcomes	**After this course, students will:** • Be able to derive a consistent set of measurements • Be able to use gross error detection algorithms • Have basic knowledge on observability and redundancy
Contents	• Introduction • Steady state detection • Consistent set of measurements derivation • Sensor fault diagnosis • Data reconciliation on partial observable systems
Literature	**Validation de données et diagnostic ;** J. Ragot, D. Maquin, G. Bloch, M. Darouach ; HERMES, Paris 1990. **Ensembles et statistique ;** C. Tricot, J.M. Picard ; Mac Graw Hill, Montréal, 1969. **Modélisation et estimation des erreurs de mesure ;** M. Neuilly ; Tech. et Doc., Lavoisier, 1993. Méthodes numériques appliquées ; **A. Gourdin, M. Bouhmeurat ; Tech. et Doc., 1983.**

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MODELLING PROCESS OPERATION II

Subject Information	
Code	**EP3OM1**
Credits (ECTS)	2
Semester	Autumn
Time Allocation (Lec. / Prac. / Lab.)	2h / 22h / -
Lecturers	Pr. F. Marias
Pre-requisites	Thermodynamics-Process operation, Modelling process operation I
Assessment	Project

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description	
Introduction	This lecture gives insights on the skills and knowledge needed in the topic of modelling process operation. During this course, students will be able to derive a mathematical model for a multistage and multi components distillation column.
Learning outcomes	**After the lecture, students will know how to:** • derive equations translating mass, species and energy conservation in a distillation column. • Formulate the mathematical model in a way that it can be solved using a Newton Raphson algorithm • use the numerical tools (developed during the lecture) to strengthen their knowledge in the field of distillation
Contents	**Numerical skills reminder in order to solve linear systems** • Modelling of multistage and multi components separation process • Solving • Conclusion
Literature	**Techniques de l'ingénieur (J1076, J1021, J 2623)** Process modeling simulation and control for chemical engineers, **W.L. Luyben,** ***Mc Graw-Hill 1990***

MODELLING AND SIMULATION USING COMPUTATIONAL FLUID DYNAMICS

Subject Information	
Code	**EP3OM2**
Credits (ECTS)	2
Semester	Autumn
Time Allocation (Lec. / Prac. / Lab.)	6h / 18h / -
Lecturers	Pr. F. Marias
Pre-requisites	Basics in Fluid Dynamics. Numerical Methods
Assessment	Project

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description	
Introduction	Computational Fluid Dynamics is a recent tool which is commonly used for the design of new unitary operations (reactors, separators, heat exchangers…). The knowledge of such a tool is important for students that aim at designing new processes.
Learning outcomes	**After the course the students will be able to:** • know the numerical methods used in Computational Fluid Dynamics • know the main mathematical models allowing the description of physical phenomena • handle a complete simulation using Fluent (sketching, CAD, Meshing, solving) • know the influence of the main parameters allowing the simulation to converge (meshing, relaxation, interpolation) • Analyse and validate the results
Contents	**1) Introduction to computational Fluid Dynamics** • Main goals of CFD • Main strategies used in CFD • Discretisation using finite volume methods • Examples • Turbulence modelling **2) Software environment Ansys WorkBench** **3) Case Studies**
Literature	**An Introduction to Computational Fluid Dynamics : 2nd Edition (**H. Henk Kaarle Versteeg, Weeratunge Malalasekera) Pearson Education **Ansys Fluent User Guide**

INDUSTRIAL PROCESS SIMULATION

Subject Information	
Code	**EP3OM3**
Credits (ECTS)	1
Semester	Spring
Time Allocation (Lec. / Prac. / Lab.)	20h / - / -
Lecturers	O. Baudouin (ProSim SA)
Pre-requisites	VB Language
Assessment	Project (study report for the gas treatment unit)

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description	
Introduction	The main objective of this course is to train students to perform some relatively complex steady state process simulation problems. This course is built around the process simulation of a gas treatment unit. Several thermodynamical models will be used and students will analyse the effects of the choice of such models. ProSimPlus will be the steady state process simulation software that they will work with.
Learning outcomes	**After this course, abilities acquired by students:** • Distillation curves (TBP, ASTM…) and pseudo-components • Selection of thermodynamics models • Phase envelope and equilibrium curves analysis (retrograde condensation) • Methodology for modelling of complex units with a steady state process simulation software (numerous cycling networks, process constraints, absorbers, distillation columns, user defined unit operations…)
Contents	During this course, students will concentrate on the material system modelling, linked to unit operations used in the simulation file (streams characteristics from a distillation curve, acid gas treatment with amine solutions, liquid phase splitting with water presence…) A methodology for the creation of a complex simulation file will be presented and the complexity of unit operation modelling will be introduced step by step. A case study of a user defined unit operation with a windows script module (VBS language) will also be conducted by students (this kind of unit operation is often used in the industry to introduce its know-how in a commercial simulation software). Analysis tools, particularly thermodynamics tools, available in the process simulation software will be widely used.

MIXTURE PROPERTIES AND FLUID PHASE EQUILIBRIA CALCULATION

Subject Information	
Code	**EP3OM4**
Credits (ECTS)	1
Semester	Spring
Time Allocation (Lec. / Prac. / Lab.)	10h / 10h
Lecturers	Pr P. Cézac
Pre-requisites	Solution Thermodynamics
Assessment	Project

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description	
Introduction	Mixture properties and fluid phase equilibria calculations are an essential tool for the analysis of the real processes. The primary aim of this subject is to train students to use a thermophysical properties calculation server, Simulis Thermodynamics©.
Learning outcomes	• Partial Properties • Chemical Potential • Real Solution • gE models • EOS • Phases equilibria and thermo physical properties calculation.
Contents	After this course, students will: • have a great knowledge on thermodynamics models • be able to describe any thermodynamic equilibrium in a complex system. • know how to use Simulis Thermodynamics© and VBA
Literature	Vidal, Thermodynamique : application au Génie Chimique et à l'industrie pétrolière, Ed. Technip, 1997. Smith et Van Ness, Introduction to Chemical Engineering Thermodynamics, Ed. Mc Graw-Hill, Inc, 1987

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BATCH PROCESSES

Subject Information	
Code	**EP3OS1**
Credits (ECTS)	2
Semester	Spring
Time Allocation (Lec. / Prac. / Lab.)	8h / - / 16h
Lecturers	Dr JP Serin / Dr F Contamine / Pr P Cézac
Pre-requisites	Modelling, distillation, Kinetic, thermodynamic, thermochemistry
Assessment	Written report for each day of practical work

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description	
Introduction	The aim of this course is to familiarize students with the simulation of a batch process. The coupling of the simulation with two practical study cases (distillation column, reactor) will allow them to compare the numerical approach and experimental constraints
Learning outcomes	At the end of this course, students will be able to use simulators (BATCHREACTOR © and BATCHCOLUMN) to simulate the operation of a distillation column and a reactor in batch mode.
Contents	• Modelling • Presentation of batch reactor© and batch column © • Application: o Dynamic simulation of the thermal runaway of a reactor o Simulation and optimization of a distillation column for the mixture Acetone / Water / IPA
Literature	**Process modelling, simulation, and control for chemical engineers** W.L. Luyben *McGraw-Hill, 1990*

MODELLING, SIMULATION AND OPTIMISATION USING gPROMS

Subject Information	
Code	**EP3OS3**
Credits (ECTS)	2
Semester	Autumn
Time Allocation (Lec. / Prac. / Lab.)	- / 32h / -
Lecturers	Dr Maarten Nauta, Process Systems Enterprise Ltd. (London, UK)
Pre-requisites	Basic understanding of first-principles modelling of transient behaviour of chemical processes
Assessment	2 hour individual examination (using computer)

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description	
Introduction	This course introduces the students to the use of the gPROMS® software tool for the modelling of the steady-state and transient behaviour of chemical processes.
Learning outcomes	At the end of the course, the students will be able to : • translate a mathematical model expressed in terms of a mixed system of integral, ordinary and partial differential, and algebraic equations (IPDAEs) to a working gPROMS model • use the above model to perform steady-state and dynamic simulations • express operating procedures in the gPROMS language • perform steady-state and dynamic optimisation calculations in gPROMS • estimate model parameters using data from steady-state and dynamic experiments • use the gPROMS Model Builder to build, debug and manage models.
Contents	This involves a number of topics that are closely aligned with the above Learning Outcomes.
Literature	gPROMS Introductory Training Course notes gPROMS Dynamic Optimisation/Parameter Estimation Training Course notes.

PROCESS AUTOMATION AND CONTROL METHODS

Subject Information	
Code	**EP3OS4**
Semester	Spring
Time Allocation (Lec. / Prac. / Lab.)	10 h / 20 h / -
Lecturers	M. Ricarde, Pr. F. Marias
Pre-requisites	Basic regulatory control (PID loop)
Assessment	2-hour examination

Lec. : Lectures *Prac. : Practical works ("small classes")* *Lab.: Laboratories*

Subject Description

Introduction

Process automation and control methods: theory and use for petrol, chemical and pharmaceutical industries.

Learning outcomes

This education allows students to plan and to specify process control systems:
- safety controls,
- regulatory controls,
- chronological sequences,
- alarm and event monitoring,
- system architecture.

Contents

Basic and advanced regulatory methods:
- PID,
- split-range,
- ratio control,
- cascade control,
- feed forward control.

Safety Loops
- Matrix representation
- Safety shutdown system
- Safety Integrity Level

Software INDISS RSI

Examples and applications: Boiler, heat exchanger, distillation colon…

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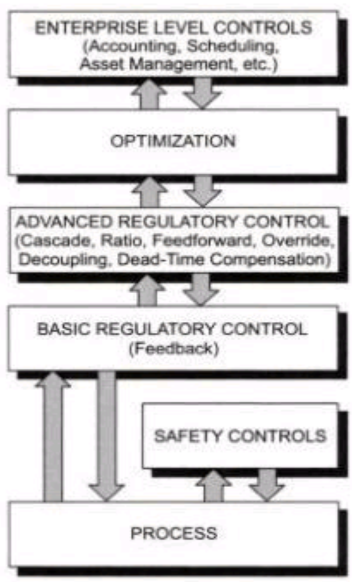

Literature

Régulation industrielle, Emmanuel Godoy, Collectif Dunod, L'Usine Nouvelle.
Régulation P.I.D, Daniel Lequesne, Lavoisier.
Régulation de chaudières (Conférence Framatome).
Système et instrumentation de sécurité (Yokogawa, Triconex, ICS…).
RsBatch (Rockwell).

SIMATIC Safety Matrix (Siemens)