

# **Chemistry - Process Engineering**



#### In brief

> Course langage: French

## Presentation

### Learning objectives

In chemistry:

- know the general principles of chemical kinetics and thermodynamics as well as structure-property relationships of molecules
- Know the reactive molecular entities
- Know the general concepts of organic reactivity

In process engineering:

- Know how to apply material and energy balances, with and without chemical reaction, in steady state on a on a system
- Know and know how to calculate the volume of ideal reactors (closed reactor, perfectly agitated, piston) in simple cases.
- In the case of perfectly stirred reactors, know how to calculate the adiabatic temperature
- To approach the transient regime
- Apply this knowledge to the distillation of a binary mixture
- Know the thermodynamics of liquid/vapor equilibrium
- Know how to dimension a tray rectification column in continuous and batch modes.

### Description of the programme

In Chemistry:

Molecular Structure:

1. Chemical element and atom - Electronic configurations - Lewis theory - Geometry of molecules Molecules - Quantum model of the atom - Molecular orbitals - Hückel's method



2. Formal chemical kinetics - Speed and order of reaction and rate constant - Kinetics of complex reactions (parallel, consecutive reactions) - Mechanics - Activation thermodynamics Thermodynamics of activation - Kinetic/thermodynamic control

3. Chemical thermodynamics - Standard state - State functions

First principle and applications - The chemical potential - Second principle and evolution of chemical systems Second principle and evolution of chemical systems

#### Organic reactivity:

- 1. Static stereochemistry (central and axial chirality) Dynamic stereochemistry (conformational analysis)
- 2. Reactivity of alkanes and halogeno-alkanes, reactive species Nucleophilic substitution Elimination
- 3. Kinetic control, thermodynamic control orbital control, charge control, steric control

#### In Process Engineering:

- 1. Balances and reactor:
- Introduction to process engineering and unit operations
- Global analysis of a manufacturing process
- Application of global and partial balances without chemical reaction
- Application of global and partial balances with chemical reaction
- Energy balance, with and without chemical reaction
- Introduction to reactors (process & technology aspects)
- Particular case of ideal reactors
- 2. Distillation of a binary mixture:
- Introduction to separative methods
- Thermodynamics of liquid/vapour equilibrium
- Flash distillation
- Rectification in continuous mode: sizing by the Mac Cabe and Thiele method
- Rectification in batch mode: Rayleigh equation and sizing.

### Generic central skills and knowledge targeted in the discipline

#### In Chemistry:

- Be able to understand the kinetics and thermodynamics of molecular transformations
- Know how to identify the reactive species of a chemical system, know how to formulate hypotheses for a reaction mechanism
- Predict the selectivity and stereochemistry of a molecular transformation.

### How knowledge is tested

DS Chimie (2/3) - GP (1/3) : 50 % CC (TD + TP + TA) Chimie (2/3) - (TD + TA) GP (1/3) : 50 %

### Bibliography



Online resources on the Ecole Centrale pedagogical portal Books (documentation center)

## Teaching team

#### Chimie:

- \* Bastien Chatelet
- \* Laurent Giordano
- \* Alexandre Martinez
- \* Didier Nuel
- \* Innocenzo De Riggi
- \* Anne-Doriane Manick
- \* Cédric Colomban
- \* Louise Miton
- \* Emile Vandeputte

#### Génie des procédés :

- \* Pierrette Guichardon
- \* Pascal Denis
- \* Nelson Ibaseta
- \* René Arnaud

## Sustainable Development Goal



Responsible consumption and production

Total des heures		96h
CM	Master class	36h
TD	Directed work	32h
TP	Practical work	4h
AA		24h

# Useful info



# Name responsible for EU

#### **Lead Instructor**

Alexandre Martinez

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