## Chemical Reaction Engineering

### Overview

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<th>LEVEL</th>
<th>Expert</th>
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**PURPOSE**

This course aims to impart the method for selecting the adequate reactor and determine the necessary data for design or performance optimization.

**LEARNING OBJECTIVES**

Upon completion of the course, the participants will be able to:

- understand the characteristics of chemical reactions, operating parameters and their impact on the conversion and yield,
- estimate the characteristics of the various technologies of the reactor (catalytic or otherwise),
- select the technology and optimal operating conditions.

**WAYS AND MEANS**

Numerous examples from the refining and chemical industry, based on real cases.

Emphasis on exchanges between participants.

Extensive use of case studies, based on experience feedback, to illustrate the topics covered in the course.

**LEARNING ASSESSMENT**

Quiz.

**PREREQUISITES**

No prerequisites for this course.

### Agenda

**CHEMICAL REACTIONS**

Thermodynamics and kinetics of the chemical reactions.

Consecutive, competitive reactions. Selectivity, yield and conversion.

Catalysts: main characteristics, shape, structural, textural and mechanical properties. Activity and selectivity.

Kinetics of the catalytic reactions: adsorption, on-surface reaction and desorption. Deactivation. Simplified mechanisms and kinetic laws.

Multiphase reactions: mass transfer at the interface. Intra-granular diffusion for catalytic reactions with a solid catalyst. Importance of specific interfacial area for liquid-liquid reactions.

Notion of chemical regime, external mass transfer or intragranular limitation.

Heat of reaction: production, temperature gradients, diffusion and elimination.

The different parameters are studied using examples from the chemical industry, with one selected case study (“training case study”) followed through the training session.

**MAIN CHARACTERISTICS OF CHEMICAL REACTORS**

Batch, semi-batch or continuous reactors: management of productivity, control of the yield.
Control of the temperature profiles in reactors: adiabatic behavior, with thermal exchange. Influence on the results.
Stability of the exothermic reactions.
Criteria of choice: this part is covered through analysis of situations, including the training case study.

TECHNOLOGICAL FEATURES OF THE REACTORS
Performances of mass and heat transfer. Monitoring the type of flow. Constraints in the catalyst formulations.
Consequences on technological choice:
Fixed beds, fluidized or circulating beds for gas-solid reactors.
Bubble columns, reactive absorption columns, etc., for gas-liquid systems.
Stirred reactors, single or multiphase; criteria for choosing of the impeller.
Up-flow or trickle bed for 3 phase fixed beds.
Criteria for technological choice, basic design rules.
This section is mainly covered through the use of case studies, including the training case study.

FROM THE SELECTION OF THE REACTOR TO THE OPTIMIZATION OF THE OPERATING CONDITIONS
This chapter is divided into different parts within the train case study. This implies an active involvement of each part and allows an application of the different steps of the method.
Approach of the design of a reactor:
Analysis of the thermodynamic, kinetic and thermal characteristics of the desired transformation.
Advantages and the drawbacks of the possible technologies of reactors.
Selection criteria.
Use of several reactors.
Choice of the operating conditions.
Expected performances.