# Introduction to “Synthesis and Simulation of Chemical Processes” (Simulation module)


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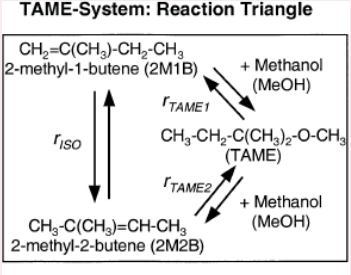
# Outline

1. What is process analysis?
   - Production of fuel ethers
   - HydroDeAlkylation process
   - Objectives of process analysis
2. Process simulators: an overview
3. Course presentation
   - Objectives
   - Syllabus
   - Course material

# What is process analysis? ...Example 1: fuel ethers

## TAME/MTBE production reactions

- Fuel ethers such as tert-amyl-methylether (TAME), or methyl-tert-butylether (MTBE), are used as additives to gasoline because of their anti-knocking properties
- TAME is formed from methanol and the two isomers 2-methyl-1-butene (2MB1) and 2-methyl-2- butene (2MB2) according to:

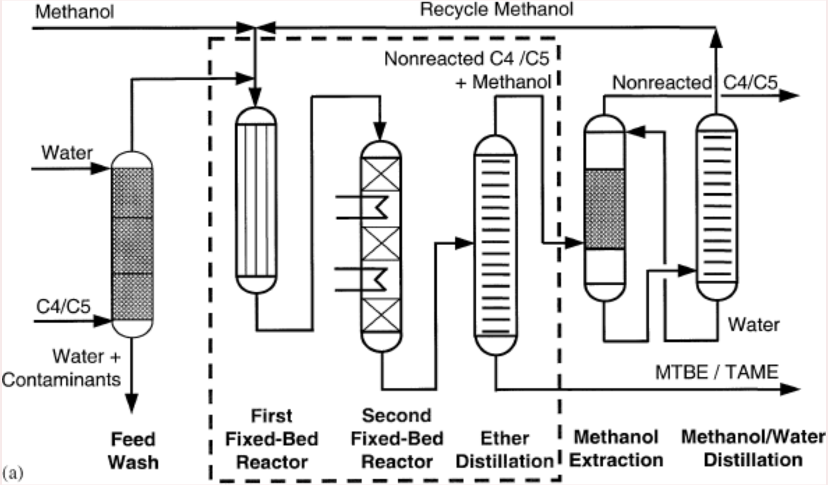



- Additional side reactions can occur, e.g.:

$$2CH_3OH \rightleftharpoons CH_3{-}O{-}CH_3 + H_2O$$

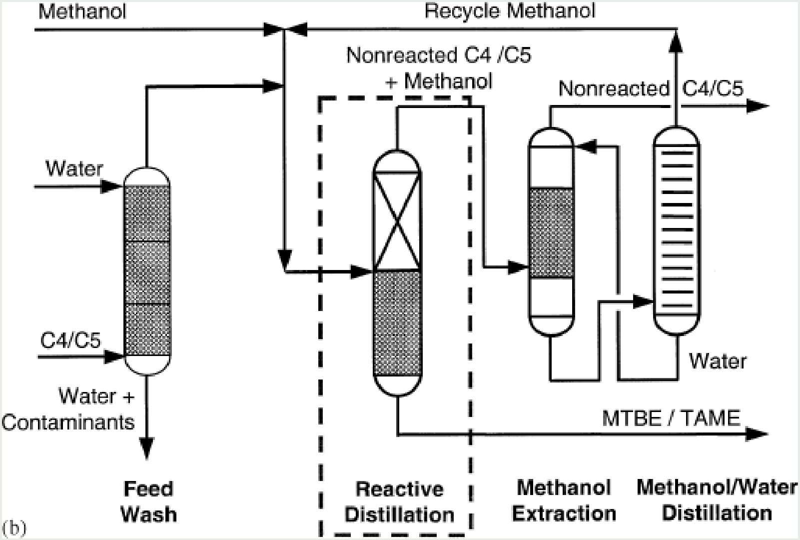
# What is process analysis? ...Example 1: fuel ethers

## TAME production conventional process



# What is process analysis? ...Example 1: fuel ethers

## TAME production process including a reactive distillation column



# What is process analysis? ...Example 2: HDA

## HDA process reactions and conditions

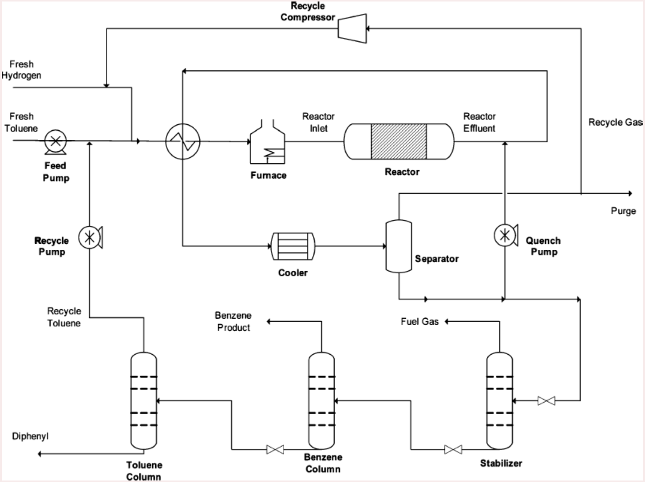
- The production of benzene from toluene, known as HydroDeAlkylation (HDA) process, involves two main reactions:

$$C_6H_5{-}CH_3 + H_2 \longrightarrow C_6H_6 + CH_4 \qquad \text{(desired)}$$
$$2C_6H_6 \rightleftharpoons C_6H_5{-}C_6H_5 + H_2 \qquad \text{(undesired)}$$

- Operating temperature above 600°C but below 700°C to avoid cracking
- Operating pressure around 35-40 bar

# What is process analysis? ...Example 2: HDA

## HDA process scheme



# What is process analysis? ...Comments

## Understanding the process

- In the previous examples many different unit operations are involved, e.g. heating/cooling, fixed-bed reactions, compression, pumping, partial condensation, extraction, multi-component distillation
- These unit operations are highly interconnected (recycles, bypass, purge) and integrated (heating/cooling)
- To understand a process:
  - each UO needs to be understood from a qualitative point of view
  - each UO needs to be described from a quantitative point of view
  - the effect of interconnections must be taken into account

# What is process analysis? ...Goals

## Objectives

1. Evaluation of the degrees of freedom for each UO, i.e. variables and relations
2. Mathematical modeling and computational solution of each UO
3. Individuation of process bottlenecks and identification of strategies for removal of such bottlenecks
4. Evaluation of optimal operating conditions for each UO and for the overall process

*The above goals can be achieved only by means of modern process simulators*

# Process simulators: an overview

## What can process simulators do?

- Process simulators are able to evaluate the operating conditions (flow rates, temperatures, compositions, etc.) of UO arranged in a Process Flow Diagram (PFD) and interconnected by material and energy streams
- Process simulators evaluate the energy requests of the UOs
- Process simulators can perform sensitivity analysis and optimization
- Process simulators typically work in steady state conditions but many can also perform dynamic simulations

## How do they work?

- Process simulators are complex computational programs
- Process simulators must solve a large number of (linear and nonlinear) equations, even for simple UO (e.g. a multi-component flash calculation)
- Process simulators often rely on iterative methods
- In dynamic mode, process simulators usually integrate Ordinary Differential Equations (ODEs)

# Objectives of the course

1. Understand the computational foundations of process simulators
2. Understand the fundamentals of numerical computation and mathematical programming
3. Learn how to use process simulators effectively to build, simulate and optimize complex processes

# Course syllabus (1/3)

## Part I: theory

1. Introduction to Process Simulation (1 hours)
   1. What is process analysis?
   2. Process simulators: an overview
   3. Course presentation
2. Review of Numerical calculus (3 hours)
   1. Linear systems: review of basic concepts
   2. Solving linear systems: Gaussian elimination, LU decomposition, forward/back substitution, pivoting, iterative methods
   3. Eigenvalue problems and decompositions
   4. Special linear cases: positive definite systems and least-squares problems
   5. Nonlinear equations: bisection and Newton's method
   6. Nonlinear systems: Newton's method, quasi-Newton's methods
   7. Numerical integration: quadrature formulas
   8. Ordinary differential equations: Euler's method (explicit and implicit), Runge Kutta methods, multi-step methods

# Course syllabus (2/3)

## Part I: theory (cont.)

1. Numerical optimization (6 hours)
   1. Introduction to optimization: variables, objective function and constraints
   2. Unconstrained optimization: line search and trust region methods
   3. Constrained optimization: optimality KKT conditions
   4. Linear Programming (LP) and Quadratic Programming (QP) methods
   5. Nonlinear optimization via Sequential Quadratic Programming (SQP) methods
2. Process simulation with UniSim Design: theoretical foundations (6 hours)
   1. Thermodynamics: VLE calculations, EOS and activity models
   2. Basic UOs: degrees of freedom, material and energy streams, valves, pipes, compressors, turbines, heat exchangers, reactors
   3. Kinetics: reaction types and reactor models
   4. Stage-wise unit operations (distillation columns)

# Course syllabus (3/3)

## Part II: applications and examples

3. Numerical computations and programming using Python (12 hours)
   1. Overview of Python: installation, basic commands and scripts
   2. Solving linear and nonlinear systems
   3. Integrating ODEs and quadrature
   4. Fundamentals of programming and examples
   5. Numerical optimization examples
4. Steady-state simulation with UniSim Design (16 hours)
   1. Fluid-Package definition and flash calculations
   2. PFD construction, adding UOs and understanding the solver principles
   3. Recycle, Adjust, Set, Balance
   4. Spreadsheet, Case study, Reporting
   5. Distillation columns and stage-wise operations
   6. Optimization
   7. Examples

# Course material

## What?

1. Lecture slides
2. UniSim Design documentation
3. Python documentation
4. Supplementary material (examples, articles, etc.)

## Where?

- All material will be made available at the Elearning site:

  `http://elearn.ing.unipi.it/course/view.php?id=1119`

- Registration to the course at the Elearning site is required!

# Student office hours and list

## Student office hours

- GP will be available for questions and clarifications on Monday 14:30-16:30
- Presence must be confirmed by email at `gabriele.pannocchia@unipi.it`
- Quick questions can also be asked by email

## Student list

- Each student must be enrolled in the course at the E-learning site
- All communications will be sent via email from E-learning (make sure your address at E-learning is up to date)

# Examination

## Examination scheme

- Step 1 - Home works (Python, UniSim Design):
- Step 2 - Written exam (Theory, both Synthesis and Simulation):