APPLICATION OF MODELING AND SIMULATION IN PROCESS SYNTHESIS AND OPTIMIZATION

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Application of Modeling and Simulation in Process Synthesis and Optimization

COMPETITIVE INTEGRATION

**EXTRACTION**
Feedstocks

**1st GENERATION**
Basic petrochemicals
- Naphtha
- Natural gas
- Ethanol
- Brine

**2nd GENERATION**
Thermoplastic resins
- Ethylene
- Propylene
- Chlorine
- Caustic soda
- PE
- PP
- PVC

**3rd GENERATION**
Consumer products
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BASIC PETROCHEMICALS

- Olefins
- Aromatics
- Solvents

- Fuels
- Specialties

POLYMERS

- PE
- PP
- Green PE

- EVA
- PVC
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**Steady-State Models**
- Process synthesis
- Off-line optimization
- On-line optimization

**Dynamic Models**
- Reactor design
- Control strategy design
- Flare system evaluation

**Computational Fluid Dynamics**
- Special flow conditions that can affect equipment performance
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Commercial software (Aspen Plus)

Application to process optimization

STEADY-STATE MODELS
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STEADY-STATE MODELS

Application to process synthesis

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1st step: thermodynamic modeling

- Identification of the significant system components
- Selection of a thermodynamic model
- Checking of accuracy of pure component vapor pressure data
- Identification of the most important component pairs
- Checking of accuracy of vapor-liquid equilibrium curves

If necessary, acquisition of pure vapor pressure data
If necessary, acquisition of binary vapor-liquid equilibrium data

Opportunity to a joint development with an university or a research institution: experimental measurement of phase equilibrium and pure component data
Collection of plant data of a similar system

Tuning of the model with plant data

Checking of mass and energy balances

Checking of key component separations

Consolidation of a base-case model

2nd step: process modeling

If necessary, data reconciliation to reduce balance gaps

If necessary, revision of thermodynamic modeling

3rd step: application of the model
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**Application to process design and optimization: dehydration of ethanol**

- 4 pairs furnace-reactor in series
- Ethanol is fed to the 4 reactors
- Ethylene is the main product
- Ethane is an important product contaminant
- Besides ethane, many oxigenated contaminants have to be taken into account
- Applications of the model:
  - Catalyst volume calculation for a capacity expansion project
  - Real-time optimization

Model developed at UFRJ
Kinetic data from laboratory

Development of a model with laboratory data

Improvement of the model with pilot plant data

Scale-up

Consolidation of a base-case model

Opportunity to a joint development with an university or a research institution: development of the model; experimental measurement of kinetic data

If necessary, more data from laboratory

Parameter adjustment to consider catalyst deactivation
Computational Fluid Dynamics

Applications

- Temperature calculations in furnaces
- Air and fuel flow in burners
- Two-phase flow patterns: evaluation of risk of erosion
- Design of mixing devices for two different streams
- Safety valves discharge flow rates
- Scale-up

Points of attention

- Internal expertise still being developed
- Technical assistance from the software licensor still very important
- Hardware requirements

Commercial software (Star - CCM+)