Optimisation in a Process Engineering Context

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Product and Process Systems Engineering

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Our key areas of research:

- Competence Areas
  - Product and Process Design
  - Operations and Control
  - Modelling and Model Solution Tools

Application Domains

- Chemical Manufacturing Systems
- Biological Systems Engineering
- Supply Chains of the Future
- Energy Systems Engineering
• **Process Systems Engineering** is concerned with the improvement of decision making processes for the creation and operation of the chemical supply chain.

• It deals with the discovery, design, manufacture and distribution of *chemical products* in the context of many conflicting goals.

Grossmann and Westerberg, Carnegie Mellon University
“Chemical products”
“Chemical products”

Application Domains:

- Chemical Manufacturing Systems
- Molecular Systems Engineering
- Biological Systems Engineering
- Supply Chains of the Future
- Energy Systems Engineering
Process Engineering pipeline

- **Product & Process Development**
  - Detailed design of complex units

- **Process flowsheeting**
  - Process flowsheeting

- **Detailed design of process plant**
  - Detailed design of process plant

- **Model-based automation applications**
  - Model-based automation applications – performance monitoring and decision support

- **Troubleshooting**
  - Troubleshooting with detailed predictive models

- **Design of operating procedures**
  - Design of operating procedures

- **Simultaneous design of equipment and control**
  - Simultaneous design of equipment and control
Distillation column design
Distillation column design contd.

TRADE OFF

Minimum capital costs

Minimum operating costs

Minimum ANNUALISED costs

Energy
Distillation column design *contd.*

- Minimum ANNUALISED costs
- Minimum ENVIRONMENTAL impact

? Energy

Diagram showing processes A, A & B, and B.
Column scheduling
The use of **validated predictive** models for...

- Quantified uncertainty in the model predictions
- Quantification of technological risk involved in model-based decisions
- Effective targeting of experimental R&D towards minimisation of this risk
- Quantitative prediction of the effects of design & operating decisions on KPIs, within the accuracy necessary to achieve the business objectives
- Optimisation of process design & operation by comprehensive exploration of alternatives
Model?

Catwalk!

Synthesis  Process Design  Mechanical Design
Model?

Catwalk!

Mechanical Design
Mathematical mass and energy balances

MODEL:
Accumulated = In - Out + Generated - Consumed
Model details - distillation

Simplified Models

Rigorous Models

Detailed Models

Rate-based Models

Column

FUG

Reboiler

Stage

MESH
Tray model

\[ \frac{dM_{i,j}}{dt} = L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} - L_j x_{i,j} - V_j y_{i,j} \quad , \quad i = 1, \ldots, NC \]

\[ \frac{dU_j}{dt} = L_{j-1}h_{j-1}^L + V_{j+1}h_{j+1}^V - L_j h_j^L - V_j h_j^V \]

\[ M_{i,j} = M_j^L x_{i,j} + M_j^V y_{i,j} \quad , \quad i = 1, \ldots, NC \]

\[ U_j = M_j^L h_j^L + M_j^V h_j^V - P_j v_j \]

\[ \frac{M_j^L}{\rho_j^L} + \frac{M_j^V}{\rho_j^V} = v_j \]

\[ \sum_{i=1}^{NC} x_{i,j} = \sum_{i=1}^{NC} y_{i,j} = 1 \]

\[ y_{i,j} = K_{i,j} x_{i,j} \quad , \quad i = 1, \ldots, NC \]

\[ h_j^L = h_j^L(T_j, P_j, x_j) \quad ; \quad h_j^V = h_j^V(T_j, P_j, y_j) \]

\[ \rho_j^L = \rho_j^L(T_j, P_j, x_j) \quad ; \quad \rho_j^V = \rho_j^V(T_j, P_j, y_j) \]

\[ K_{i,j} = K_i(T_j, P_j, x_j, y_j) \quad , \quad i = 1, \ldots, NC \]

Single tray only!!!!
Model details – spatial variations

Properties vary with respect to one or more spatial dimensions as well as with time:

- Tubular reactors
- Packed bed columns (adsorption/absorption/distillation/chromatography)
- Pipelines
- *etc*
Model details – Probability density

• Probability density functions instead of single scalar values:
  – Crystallisation units (size of crystals)
  – Polymerisation reactors (length of polymer chains)
• For such processes, the properties may also vary with both time and spatial position.
Optimisation Problem Formulation

**Minimise**
Objective function 1 & **Minimise**
Objective function 2

**Subject to:**
- Model equations: DAE/PDAE, nonlinear
- Design variable bounds: discrete and continuous
- Operational variable bounds: continuous

**To determine:**
- Design variables (constant)
- Operation variables (time dependent)
EXAMPLES
Multi-scale considerations
Micro distillation

• To fabricate micro-distillation chips based on zero-gravity distillation

• To demonstrate fluid separation and assess separation performance
Compute optimal gene delivery profile to maximise efficacy and minimise toxicity subject to model equations and constraints.
Recall: Multi-scale considerations
Water Resource Management

- Non-conventional water resources are crucial to water deficient areas
  - Desalinated water
  - Treated wastewater
  - Reclaimed water

- MIP approaches proposed for integrated water resources management

- Decisions:
  - Plants locations, capacities and productions
  - Pipeline networks and flows
  - Pumping stations
  - Storage tanks

- Objective: annualised total cost
  - Capital costs (plant/pipeline/pumping station/storage tank)
  - Operating costs (production/pumping)
Global Supply Chain Planning

- Three key supply chain performance metrics are considered:
  - Cost
  - Responsiveness (flow time)
  - Customer service level (lost sales)

- Two solution approaches for multiobjective MILP model:
  - $\epsilon$-constraint method $\rightarrow$ Pareto solutions
  - Lexicographic minimax method $\rightarrow$ Fair solution
Recall: Multi-scale considerations
Main constraints

PHYSICS/CHEMISTRY

RISK ???

SAFETY

SUSTAINABILITY
Optimisation problem

Integer:
# columns
# plants
etc

Continuous:
Energy
Flowrates
etc

Integer:
# columns
# plants
etc

Continuous:
Energy = f(t)
Flowrates = f(t)
etc

MINLP

MIDO
Product and Process Systems Engineering

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