Operational Model for C3 Feedstock Optimization on a Polypropylene Production Facility

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Project Overview

Polypropylene production facility

- Chemical and refinery grade feedstocks with different prices and propylene purities.
- Best operation will balance production rate with costs of feedstocks, maximizing plant throughput.
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Objectives:

- Development of a Non-linear Programming (NLP) model to maximize benefits by obtaining a better balance of RG and CG feedstocks for single or multiple production orders.
- Determine operation rates for a schedule of multiple production orders within a 3-month timeframe.
- Implement user-friendly interface (GAMS model / MS-Excel)
Process and Problem Description

Chemical Grade (CG)

~95% propylene

Refinery Grade (RG)

~79% propylene

Propylene (91%)

Distillation

Propane return

Catalyst

Polymerization

Polypropylene

Reactor effluent

Feed Tank
Chemical Grade (CG)

~95% propylene

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Catalyst

Polymerization

Polypropylene

Reactor effluent

Maximizing the amount of RG may not be the best economic option
Mathematical Model (NLP)

• Maximize Profit

• Constraints on each time interval:
  ◦ Material balances
  ◦ Min/Max flow rates
  ◦ Constraints on composition of Propane Return, Distillation Overhead & Reactor Feed
  ◦ Limits on catalyst yield and flow
  ◦ Availability of Chemical Grade
  ◦ Specifications on splitter feed and recycle rate

• Decision variables:
  ◦ Production rate of polypropylene
  ◦ RG and CG feedrates
  ◦ Distillation overhead flow and composition
  ◦ Reactor feed and catalyst flow
Single/Multiple Product Models

- **Single Product Model** (one time interval)
  - Maximize profit in terms of $/hr
  - Best production rate with minimum cost of feedstocks.
    - Model size: 31 variables, 40 constraints
    - Solved with CONOPT and BARON in less than 1 CPU s.
    - Improved hourly profit by ~1.5% (compared with previous Excel-based model)
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- **Multiple Product Model**
  - Multiple orders of different products
  - Production sequence given beforehand
  - Profit ($) = selling prices – feedstock costs
    + propane return – others
  - Solution gives best production rates with minimum costs for each product
    - Mid-size example (20 products, 5 families)
    - Model size: 727 variables, 986 constraints
    - Solved by CONOPT in ~9 seconds.
    - Preliminary results show realistic tradeoff on feedstocks costs vs production rates (depending on available time).
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Models Implemented with GAMS
Improvements on Distillation Model

Current model is based on a **linear correlation** obtained from plant data, relating the overhead composition of propane with flowrate of propane feed to the splitter.
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Goal

- Develop an approximation procedure that provides overall treatment of the distillation (no details about flows, composition, temperatures, etc. for each individual tray)
- The number of variables and constraints must remain small
- The predicted outputs must closely match those of rigorous model (Aspen)
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**Aggregated group-method of Kamath et al. (2010)**

- Models a counter-current cascade of trays

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Kamath, Grossmann and Biegler (2010)
*Comp. and Chem. Eng.* 34, pp. 1312-1319
Improvements on Distillation Model

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• Aggregated group-method of Kamath et al.
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• Aggregated group-method of Kamath et al.
• Modified group-method using Fixed Relative Volatilities
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  • Can be accurately obtained using Peng-Robinson or other first-principle method.
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### C3 Splitter modeled with Group-Method

**Degrees of freedom:**
- Reflux rate
- Bottoms composition

**Additional Assumptions**
- Fixed pressure for the whole column = 9.778 atm
- Total condenser (top)
- Total reboiler (bottom)
- Single feed
Improvements on Distillation Model

Parameterization and Validation (Work in Progress)
- Comparison of results obtained by the Aggregated Group-Methods against rigorous tray-to-tray simulations (Aspen) and plant data.
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\[ \alpha = 1.1645 \]

Propylene composition in distillation overhead for different column efficiencies

Modified Group-Method - comparison of different column sizes (or efficiencies) against linear correlation

Aspen Simulation Results

RadFrac component
Peng-Robinson thermodynamics

Tray-to-tray relative volatilities predicted by rigorous model
Integrated Model and User Interface
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Integration of Group-Method Distillation Model in General Flowsheet Model (Work in progress)

- The new distillation model is being integrated within the single and multiple-product models.
- Initial point for multiple-product model obtained by the solution of several single product models, one for each product.
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User Interface for GAMS model being developed in Excel

- Excel and VBA as a front-end
- Excel as User Interface (UI) to define input data
- Excel used to display results
- Flexibility to manipulate input data/output results (tables, graphics)
Conclusions and Future Work
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CONCLUSIONS

- Integrated plant formulation developed including distillation and polymerization processes in a single model.
- Single and multiple-product models.
- Distillation model reformulated using aggregated group-methods (based on work of Kamath et al. 2010)
- Comparison with rigorous tray-to-tray simulation results (Aspen) and plant data to parameterize the models.
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FUTURE WORK

- Determine most accurate parameterization of aggregated group-methods to predict distillation column outputs
- Additional tests on larger problem instances
- Deployment of computational tool to assess monthly feedstock purchase decisions