C3 Feedstock Optimization
for Multiproduct Polypropylene Production

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Center for Advanced Process Decision-making
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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.
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.

- 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

Catalyst

Polymerization

Polypropylene

Reactor effluent

Feed Tank

Propane return
Process and Problem Description

Chemical Grade (CG)
- ~95% propylene
- Expensive

Refinery Grade (RG)
- ~79% propylene
- Cheaper
Goal: Select optimal mix of chemical and refinery grade propylene
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/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: 149 variables, 146 constraints
- Solved with CONOPT and BARON in less than 1 CPU s.
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: 149 variables, 146 constraints
    - Solved with CONOPT and BARON in less than 1 CPU s.

- **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
  - Products of the same family feature same kinetic properties.
  - Aggregation/disaggregation allows to handle large scale test cases.

Models implemented with GAMS
Distillation Model

**Objective:**

- Approximate 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
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Aggregated group-method of Kamath et al. (2010)

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

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• **Approximate 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**

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**Aggregated group-method of Kamath et al. (2010)**

- Tray-by-Tray Method (Rigorous)
- Group-Method (Approximate)

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C3 Splitter modeled with Group-Method

Kamath, Grossmann and Biegler (2010)

*Comp. and Chem. Eng. 34*, pp. 1312-1319
Distillation Model

Parameterization and Validation

Initial linear correlation based on plant data
Distillation Model

Parameterization and Validation

Initial linear correlation based on plant data

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
Distillation Model

Parameterization and Validation

Initial linear correlation based on plant data

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

Comparison of different column efficiencies against rigorous tray-by-tray simulations (Aspen HySys)

Group-method

HySys simulations
Multiple Product Model

- Parameters
- Product and product family data
- Schedule

**Aggregation / disaggregation procedure**

- General results
- Detailed results
Multiple Product Model

- Parameters
- Product and product family data
- Schedule

Aggregation / disaggregation procedure

- General results
- Detailed results
Multiple Product Model

- Parameters
- Product and product family data
- Schedule

**Aggregation / disaggregation procedure**

 Aggregate products by family

 Solve single-product model for each family

 Solve multiple-product model

- General results
- Detailed results

Disaggregate results
Multiple Product Model

- Parameters
- Product and product family data
- Schedule

Aggregation / disaggregation procedure

- Solve single-product model for each family
- Solve multiple-product model

- Aggregate products by family

Schedule requirements

- General results
- Detailed results

Disaggregate results
Multiple Product Model

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Aggregation / disaggregation procedure

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Solve single-product model for each family

Solve multiple-product model

Disaggregate results

Aggregated schedule
Multiple Product Model

- Parameters
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Aggregation / disaggregation procedure

- Aggregate products by family
- Solve single-product model for each family
- Solve multiple-product model

- Schedule requirements
- Initial solution
- Disaggregate results

- General results
- Detailed results
Multiple Product Model

- Parameters
- Product and product family data
- Schedule

**Aggregation / disaggregation procedure**

- Schedule requirements
- Aggregate products by family
- Solve single-product model for each family
- Aggregated schedule
- Initial solution
- Solve multiple-product model

**Results**

- General results
- Detailed results
- Disaggregate results
- Aggregated multiple-product solution
Multiple Product Model

- Parameters
- Product and product family data
- Schedule

Aggregation / disaggregation procedure

- Schedule requirements
- Aggregate products by family
- Solve single-product model for each family
- Aggregated schedule

Solve multiple-product model
- Initial solution
- Detailed schedule results
- Detailed results

General results
- Disaggregate results
- Aggregated multiple-product solution
Multiple Product Model

- Parameters
- Product and product family data
- Schedule

Aggregation / disaggregation procedure

- General results
- Detailed results

Schedule requirements

Aggregate products by family

Solve single-product model for each family

Aggregated schedule

Initial solution

Solve multiple-product model

Disaggregate results

Detailed schedule results

Aggregated multiple-product solution

Mid-size example (20 products, 5 families)
- Model size: 750 variables, 736 constraints
- Solved by CONOPT in ~9 seconds.
- Preliminary results show realistic tradeoff on feedstocks costs vs production rates (depending on available time).
Multiple Product Model - Example

Different time horizons tested to measure the tradeoff of feedstock costs versus production rates.
Multiple Product Model - Example

Different time horizons tested to measure the tradeoff of feedstock costs versus production rates.
Multiple Product Model - Example

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Different time horizons tested to measure the tradeoff of feedstock costs versus production rates.

![Diagram showing 20 products and tradeoff between feedstock costs and production rates.]
Multiple Product Model - Example

Different time horizons tested to measure the tradeoff of feedstock costs versus production rates.
Multiple Product Model - Example

Different time horizons tested to measure the **tradeoff** of **feedstock costs** versus **production rates**.
Multiple Product Model - Example

Different time horizons tested to measure the tradeoff of feedstock costs versus production rates.

![Graph showing feedstock costs and production rates over time.](image)
Multiple Product Model - Example

Different time horizons tested to measure the tradeoff of feedstock costs versus production rates.

- 3days

Ref

% of Max Production Rate

0 4 8 12 16 20 24 28 31

0 20 40 60 80 100

0 4 8 12 16 20 24 28 31

0 20 40 60 80 100
Multiple Product Model - Example

Different time horizons tested to measure the \textit{tradeoff} of \textbf{feedstock costs} versus \textbf{production rates}.

- 3 days
- Ref

![Graph showing different production rates over time.](image-url)
Multiple Product Model - Example

Different time horizons tested to measure the **tradeoff** of **feedstock costs** versus **production rates**.

![Graph showing different time horizons tested for feedstock costs versus production rates.](image-url)
Multiple Product Model - Example

Different time horizons tested to measure the tradeoff of feedstock costs versus production rates.

- 3 days
- Ref
- + 3 days

% of Max Production Rate

Idle time
Multiple Product Model - Example

Different time horizons tested to measure the **tradeoff** of **feedstock costs** versus **production rates**.

Propylene Source

- **CG** 37%
- **RG** 63%

Optimal Solution (PROFIT)

- **CG** 23%
  - **RG** 77%
  - **Idle time**
  - 3 days

- **CG** 19%
  - **RG** 81%

- **CG** 31
  - **RG** 34

- **Idle time**
- 3 days

**Idle time**

- 28
- 31
- 34

- 88.1 MU
- 100.0 MU
- 103.2 MU
Multiple Product Model - Example

Added “slack” product to assess the benefits of extra production when schedule finishes early ➔ gain/loss opportunity
Multiple Product Model - Example

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Multiple Product Model - Example

Added “slack” product to assess the benefits of extra production when schedule finishes early ➔ gain/loss opportunity

Propylene Source

Optimal Solution (PROFIT)

100.0 MU

109.1 MU
User Interface via Excel Worksheet

User interface for GAMS multiple-product model developed in MS Excel

- Flexibility to easily test different production schedules with alternative parameters.
User Interface via Excel Worksheet

User interface for GAMS multiple-product model developed in MS Excel

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<table>
<thead>
<tr>
<th>Order</th>
<th>Product</th>
<th>Order</th>
<th>Product</th>
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<th>Duration</th>
<th>Production Rate</th>
<th>Profit</th>
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Feedstock Optimization Model

<table>
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<th>Order</th>
<th>Product</th>
<th># Cars</th>
<th>Start Time</th>
<th>Duration</th>
<th>Production Rate</th>
<th>Profit</th>
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</table>

Multiple-product Feedstock Model - Detailed Results

Time Horizon = 50 days

<table>
<thead>
<tr>
<th>TIME SLOTS</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
</table>

Production Requirements

<table>
<thead>
<tr>
<th>Product</th>
<th># Cars</th>
</tr>
</thead>
<tbody>
<tr>
<td>Product Family</td>
<td># Cars</td>
</tr>
<tr>
<td># Cars</td>
<td>10</td>
</tr>
</tbody>
</table>

Results Summary

<table>
<thead>
<tr>
<th>Production rate (lb/hr)</th>
<th># Cars</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time (hr)</td>
<td># Cars</td>
</tr>
<tr>
<td>Use of product</td>
<td># Cars</td>
</tr>
</tbody>
</table>

Refinery Grade

<table>
<thead>
<tr>
<th>% Propylene</th>
<th># Cars</th>
</tr>
</thead>
<tbody>
<tr>
<td>% Isobutane</td>
<td># Cars</td>
</tr>
</tbody>
</table>

Chemical Grade

<table>
<thead>
<tr>
<th>% Propylene</th>
<th># Cars</th>
</tr>
</thead>
<tbody>
<tr>
<td>% Isobutane</td>
<td># Cars</td>
</tr>
</tbody>
</table>
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Conclusions and Future Work

CONCLUSIONS

- Multiple-product feedstock optimization nonlinear programming model developed. Process models include distillation and polymerization units.
- Proposed method handles gain/loss scenarios and large schedules (through aggregation/disaggregation).
- Distillation model formulated using aggregated group-method based on work of Kamath et al. 2010.
- Deployment of computational tool to assess monthly feedstock purchase decisions.
- Initial tests show large potential for savings in feedstock cost.
Conclusions and Future Work

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• Initial tests show large potential for savings in feedstock cost.

FUTURE WORK

• Improvements on distillation model parameters.
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Thanks for your attention!
Questions?