Operational Model for C3 Feedstock Optimization on a Polypropylene Production Facility

Pablo A. Marchetti, Ignacio E. Grossmann
Department of Chemical Engineering
Carnegie Mellon University
marchet@andrew.cmu.edu

Wiley A. Bucey, Rita A. Majewski
Braskem America

Center for Advanced Process Decision-making
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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- Chemical and refinery grade feedstocks with different prices and propylene purities.
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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

Catalyst

Polymerization

Polypropylene

Feed Tank

Propylene (91%)

Distillation

Propane return

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

- Maximize Profit
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
Mathematical Model (NLP)

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- 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.
Single/Multiple Product Models

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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
User Interface via Excel Worksheet

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

- Allows definition of input data and model parameters
- Presents results (output) in different levels of detail
- VBA code takes care of validation, running GAMS, and updating results.
- Flexibility to easily test different production schedules with alternative parameters.
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Specific parameters for testing gain/loss scenarios:
- Time horizon
- Addition of slack product (yes/no)
Overview of GAMS/Excel integration

**MS Excel**
- Parameters
- Product and product family data
- Schedule
- General results
- Detailed results

**GAMS Code**
- Aggregate products by family
- Solve single-product model for each family
- Solve multiple-product model
- Disaggregate results

- GDX input file
- GDX output file
User Interface via Excel Worksheet

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Schedule requirements

GDX input file

GDX output file
User Interface via Excel Worksheet

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Aggregated schedule
User Interface via Excel Worksheet

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GDX input file

Aggregated schedule

GAMS Code

Aggregate products by family

Solve single-product model for each family

Initial solution

Solve multiple-product model

Disaggregate results

GDX output file
User Interface via Excel Worksheet

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GDX input file

GDX output file

Schedule requirements

Detailed schedule results
User Interface via Excel Worksheet

Screenshots
## User Interface via Excel Worksheet

### Screenshots

### Feedstock Optimization Model

<table>
<thead>
<tr>
<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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**Schedule Data**  
**Schedule Results**  
17 Jun, 08:30 AM

**Run Feedstock Model**

**Update Results**

**Time Horizon:** 50 days

**Add SACK Product**

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**Braskem America - Neal Plant**
# User Interface via Excel Worksheet

## Screenshots

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## Multiple-product Feedstock Model - Detailed Results

### Time Horizon = 50 days

#### TIME SLOTS

<table>
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#### Production Requirements

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#### Results Summary

- Production rate (lb/hr)
- Time (hr)
- Use of product

#### Refinery Grade

<table>
<thead>
<tr>
<th>% Propane</th>
<th>Propane</th>
<th>% Propylene</th>
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#### Chemical Grade

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Improvements on Distillation Model

Objective:

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

- Models a counter-current cascade of trays

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

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

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Improvements on Distillation Model

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

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Parameterization and Validation

- Comparison against rigorous tray-to-tray simulations (Aspen / HySys) based on plant data.

Comparison of different column sizes (or efficiencies) against linear correlation

Tray-to-tray relative volatilities predicted by rigorous model
Conclusions and Future Work

CONCLUSIONS

- Single and multiple-product feedstock optimization models including distillation and polymerization processes.
- User interface through MS Excel developed and being tested (with promising initial results).
- Proposed method handles gain/loss scenarios and large schedules (through aggregation/disaggregation).
- Distillation model reformulated using aggregated group-method based on work of Kamath et al. 2010.
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FUTURE WORK

- Final deployment of computational tool to assess monthly feedstock purchase decisions.
- Parameterization of aggregated group-method, and integration with overall plant model.