Carnegie Mellon   CAPD CENTER   Braskem

C3 Feedstock Optimization for Multiproduct Polypropylene Production

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Center for Advanced Process Decision-making
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Motivation

- Most previous work in planning or scheduling type decisions involve very simple process models (fixed processing rates, fixed processing times, etc).
- Continuous chemical processes require more detailed models.
- **Goal:** Develop scheduling model in which the process model must be explicitly incorporated in the formulation.
- **Application:** Polypropylene production

Project Overview

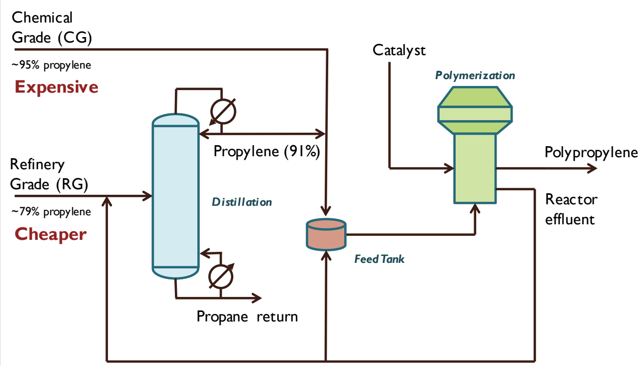
Polypropylene production facility

- Main equipment: distillation unit and polymerization reactor.
- Feedstocks: chemical and refinery grade propylene, with different prices and propylene purities.
- Best operation will balance production rate with costs of feedstocks, maximizing plant throughput.

Objectives:

- Maximize benefits by obtaining the optimal balance of RG and CG feedstocks for single/multiple production orders.
- Determine production rates for a schedule of multiple production orders within a given time horizon.

Process and Problem Description



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

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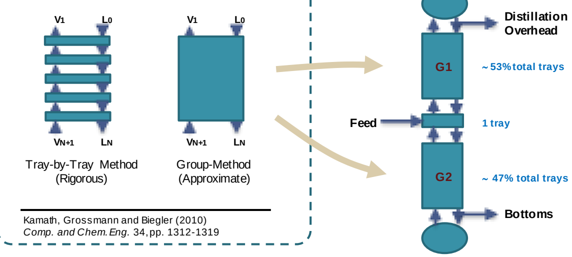
Distillation Model

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**

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

C3 Splitter modeled with Group-Method



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

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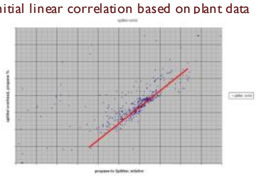
Distillation Model

Parameterization and Validation

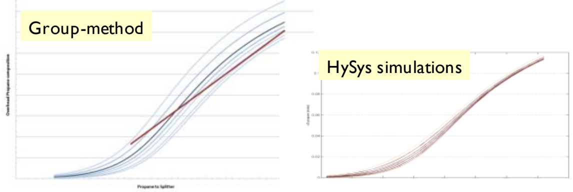
Initial linear correlation based on plant data



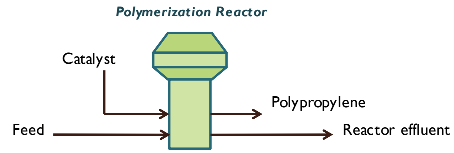
Degrees of freedom:
- **Reflux rate**
- **Bottoms composition**

<u>Additional Assumptions</u>
- **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)



Simplified Kinetic Model



Ziegler-Natta Catalysis

Kinetic parameters determined for each product family based on plant data.

Main assumptions:

- Polymerization rate proportional to monomer concentration and catalyst flow
- Single-site model, unimodal operation

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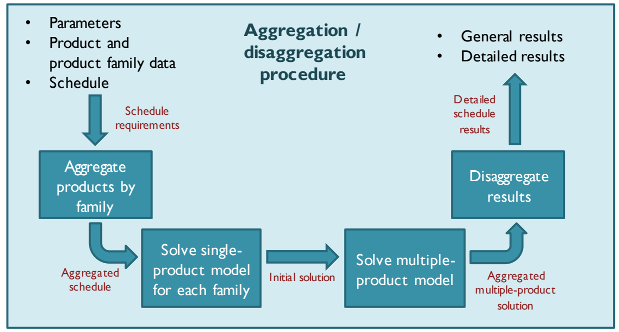
Single/Multiple Product Models

- **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

Multiple Product Model

Aggregation/disaggregation procedure allows to handle large scale test cases.

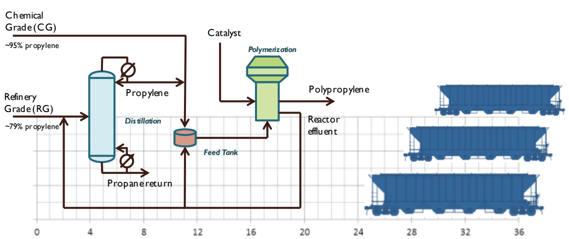


Model size depends on number of product families (only 5-15 aprox).

Multiple Product Model - Example

Mid-size example

- 20 products belonging to 5 families
- 188 railcars (190,000 lbs. each)
- Time horizon: 31 days (reference)

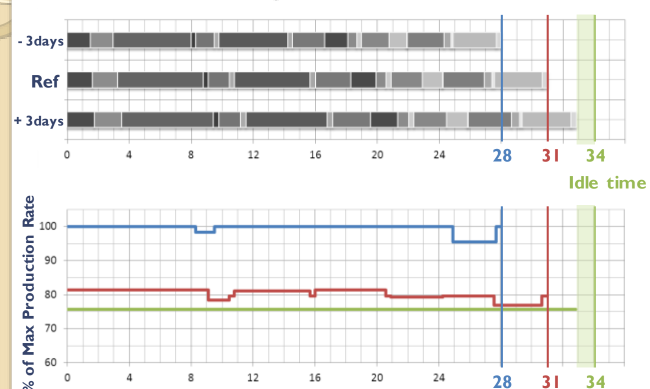


Statistics

- Model size: 750 variables, 736 constraints
- Solved by CONOPT in ~9 seconds.

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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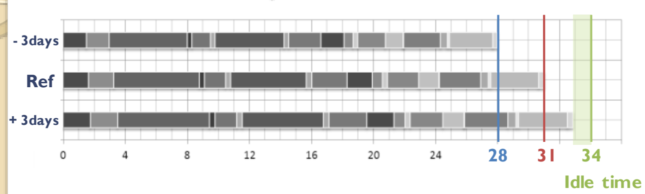
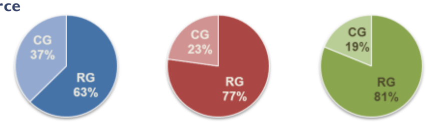


Propylene Source

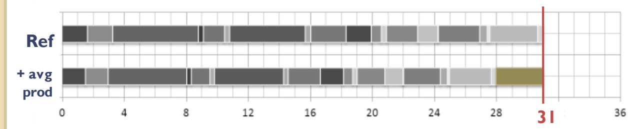


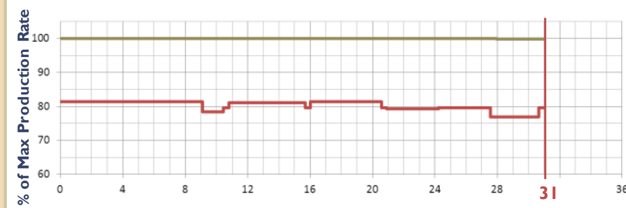
Optimal Solution (PROFIT)

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**





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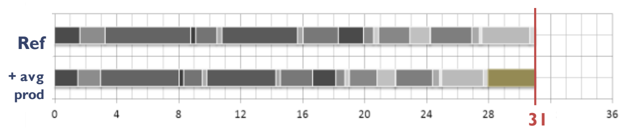


Propylene Source

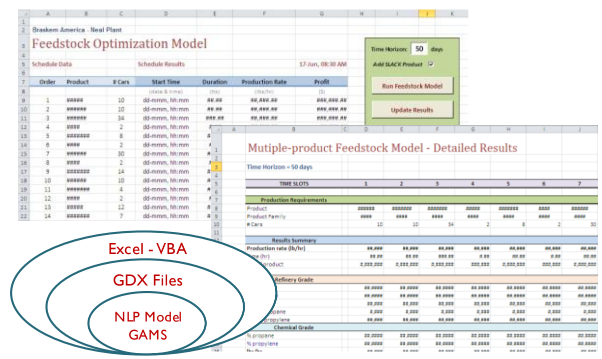
Optimal Solution (PROFIT)

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.



Final Remarks

Model results show:

- **A realistic tradeoff on feedstocks costs vs production rates** (depending on available time).
- **The overall convenience of running the plant at maximum capacity whenever possible** (depending on market conditions).
- **Using a feedstock mix and operating conditions that are not economically optimal for a given monomer spread can have large effect on feedstock costs.**

Potential annual savings:
$0.4 - $16 MM depending on monomer spread.

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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.

FUTURE WORK

- Evaluation of capacity expansions for current plant.
- Application of the proposed framework to additional facilities.

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