Integrated C3 Feedstock and Aggregated Distillation Model for Polypropylene Production

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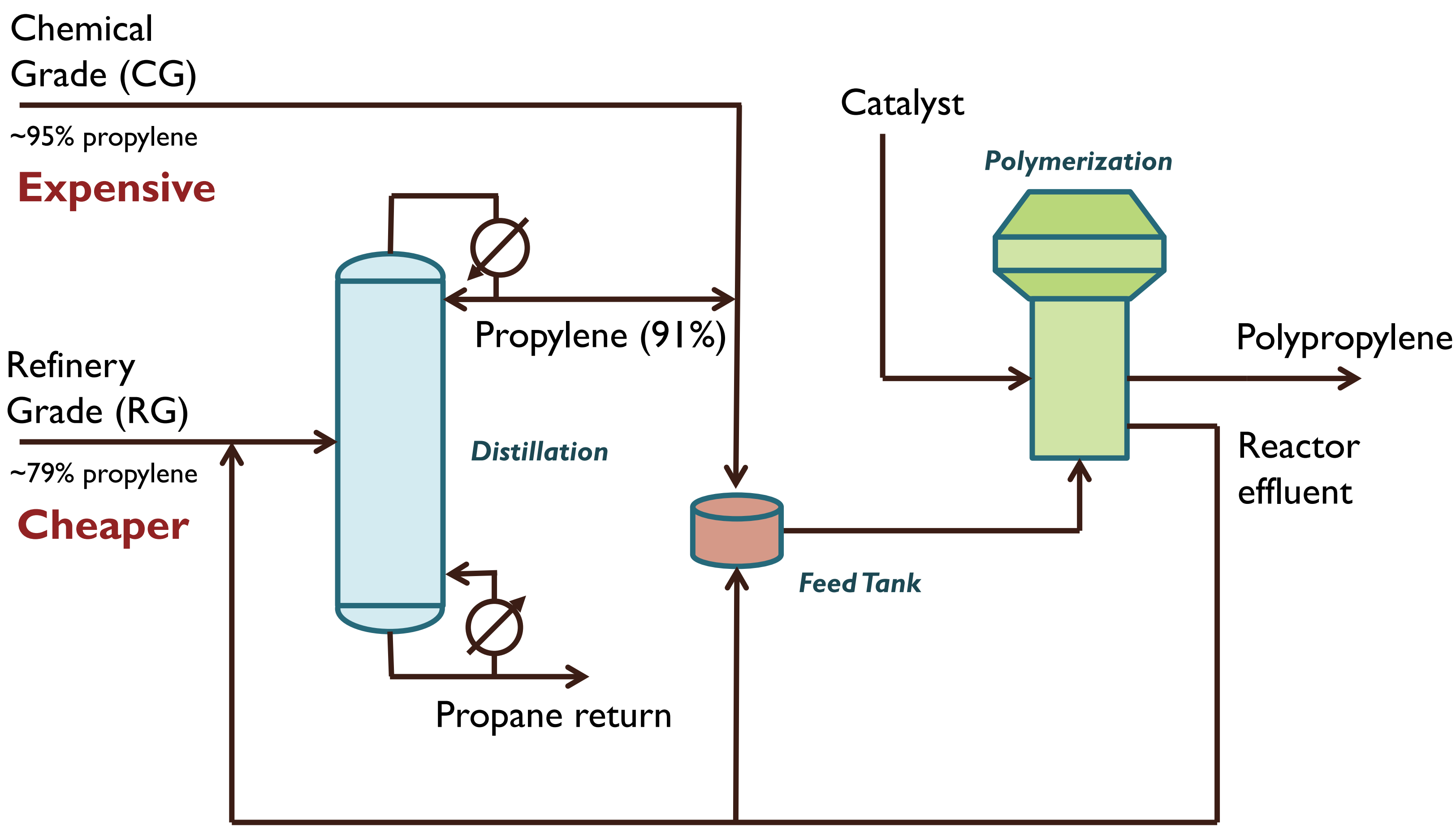
Motivation

- 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

Process and Problem Description



Goal: Select optimal mix of chemical and refinery grade propylene

Mathematical Model (***NLP***)

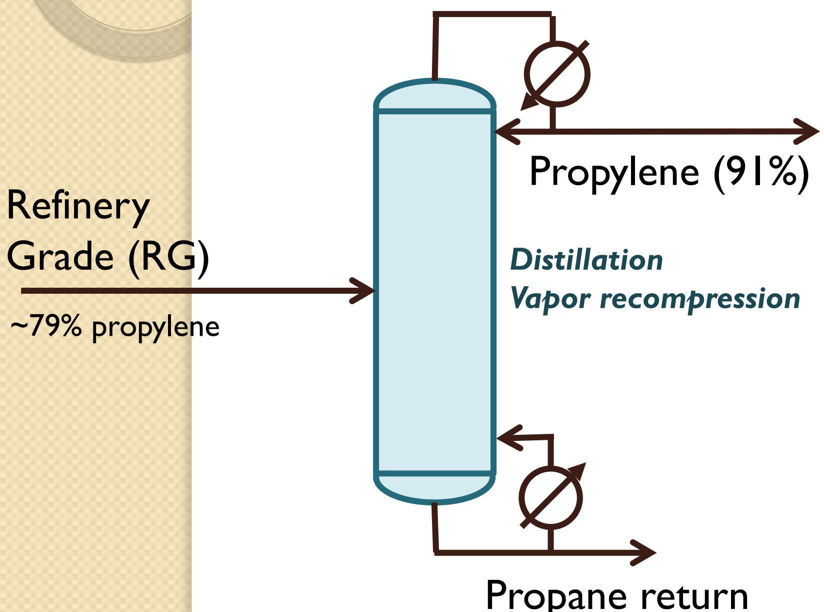
- Maximize Profit

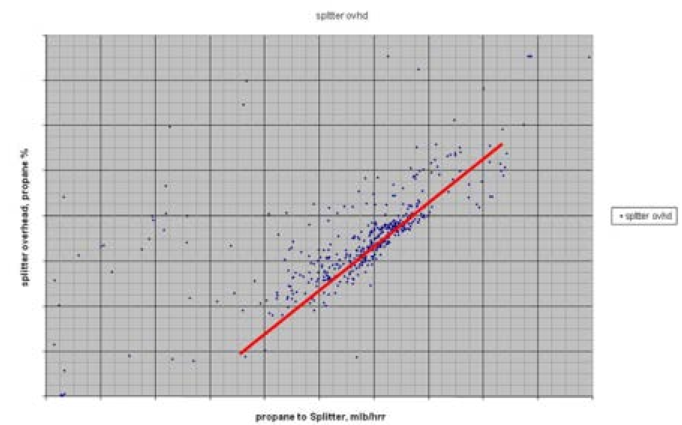
- Constraints on each time interval:
  - Material balances
  - Min/Max flow rates
  - Constraints on composition of Propane Return, Distillation Overhead & Reactor Feed
  - Limits on catalyst yield and flow
  - Availability of Chemical Grade
  - Specifications on splitter feed and recycle rate
  - Mass and Energy balances (distillation column)

- Decision variables:
  - Production rate of polypropylene
  - RG and CG feedrates
  - Distillation overhead flow and composition
  - Reactor feed and catalyst flow
  - Reflux ratio

Empirical Distillation Model

Previous model uses an **empirical linear correlation** to compute the overhead and bottoms flows/compositions obtained from plant data.





Relates overhead composition of propane with flowrate of propane feed to the splitter.

Objective:

- **Develop an 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 treatable.**

Distillation Model

Aggregated group method (Kamath et al. 2010) is an alternative for detailed tray by tray distillation model:

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

❖ **Models a counter-current cascade of trays**

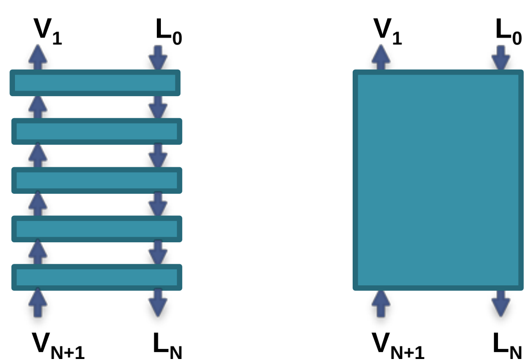
Main Assumptions

- Adiabatic and isobaric operation

Variables

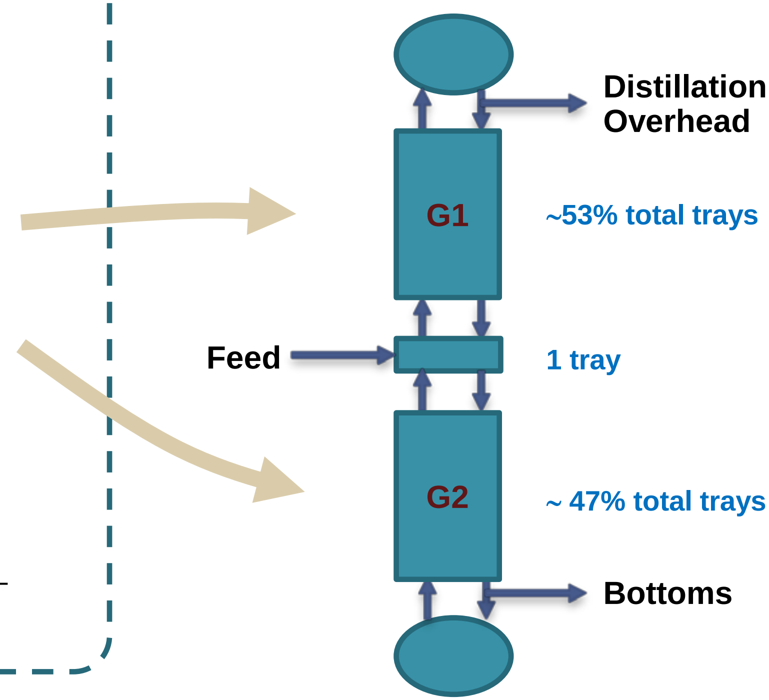
- Molar flows and compositions
- Temperatures
- Absorption and stripping factors

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

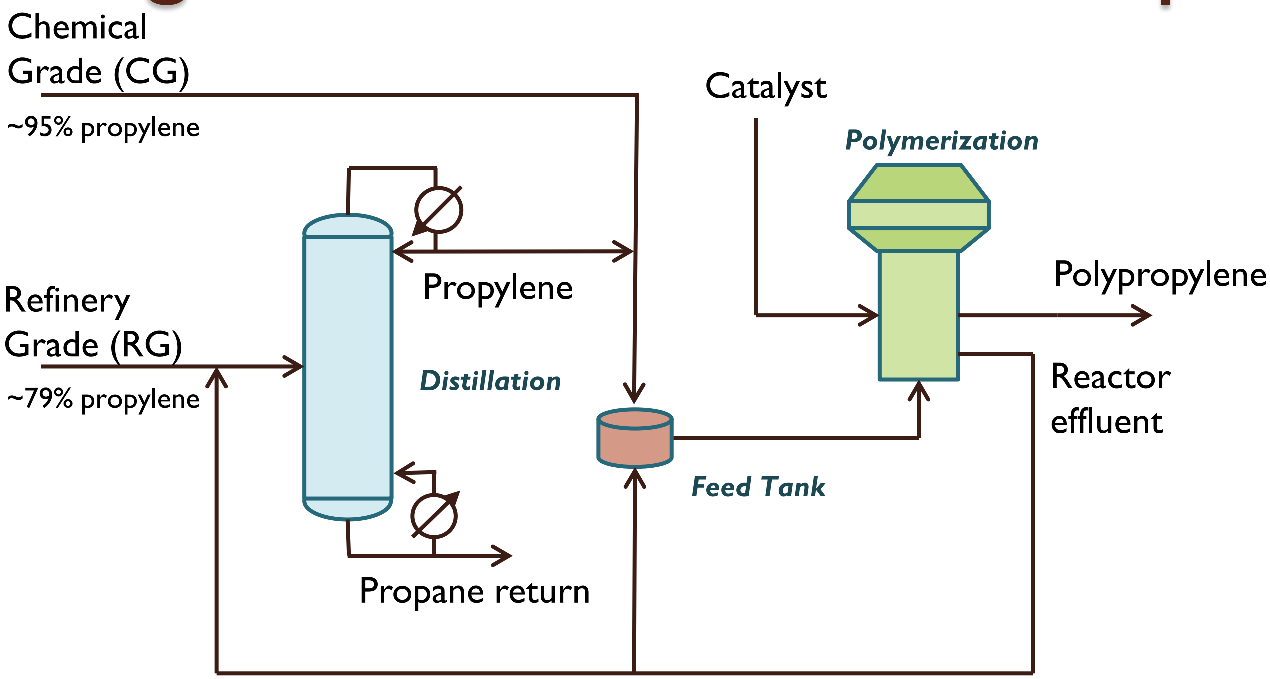


Tray-by-Tray Method (Rigorous) | Group-Method (Approximate)

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



Single Product Model - Example

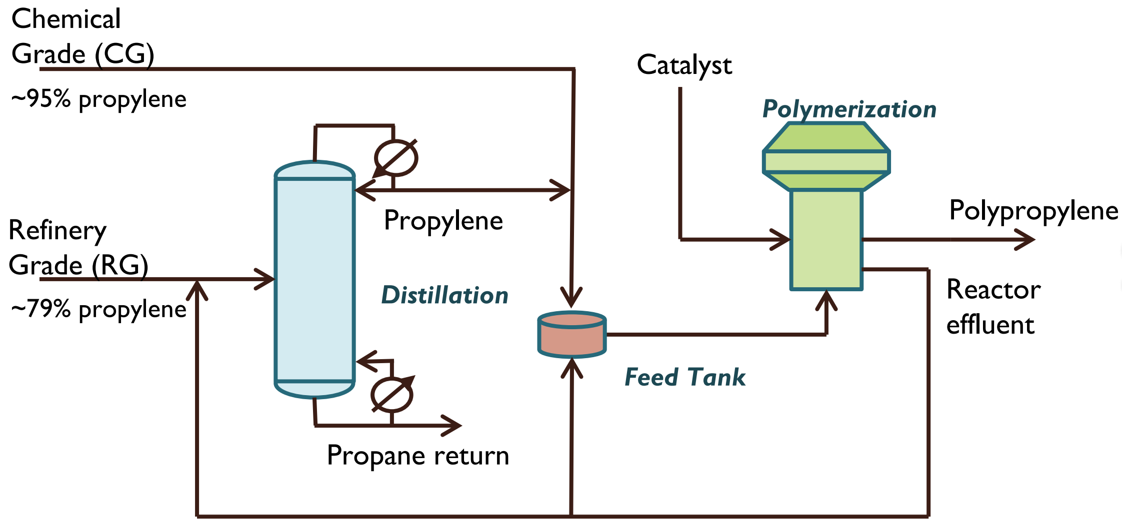


- Maximize profit
- Decision variables:

  Production rate of polypropylene
  RG and CG feed rates
  Distillation overhead flow and composition
  Reactor feed and catalyst flow
  Reflux rate (min/max 300,000 – 400,000 lb/hr)

<u>Additional Assumptions</u>

- **Fixed pressure for the whole column = 9.778 atm**
- **Total condenser (top)**
- **Total reboiler (bottom)**
- **Single feed**
- **Bottoms composition (5% propylene)**



Single Product Model - Example

	Em	Kamath model	Kamath model (80
Propylene Source			
Optimal Solution (PROFIT, $)			
Cpu time (cpu s)			
Variables	33	151	151
Constraints	43	154	154

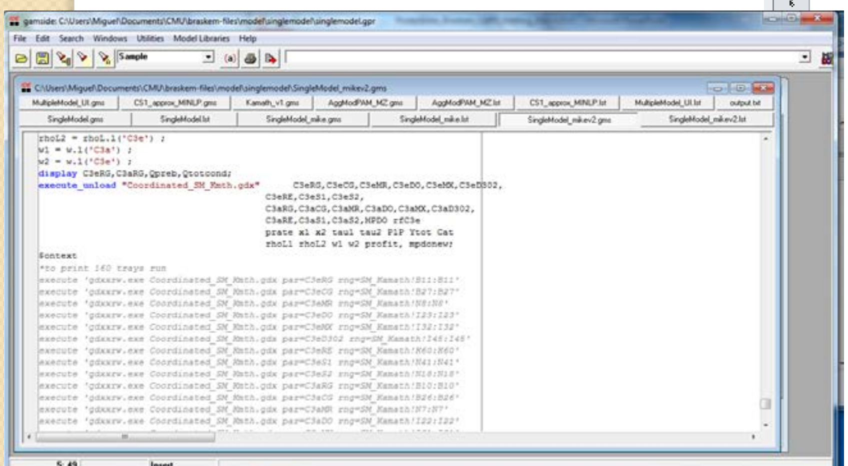
Tradeoff:

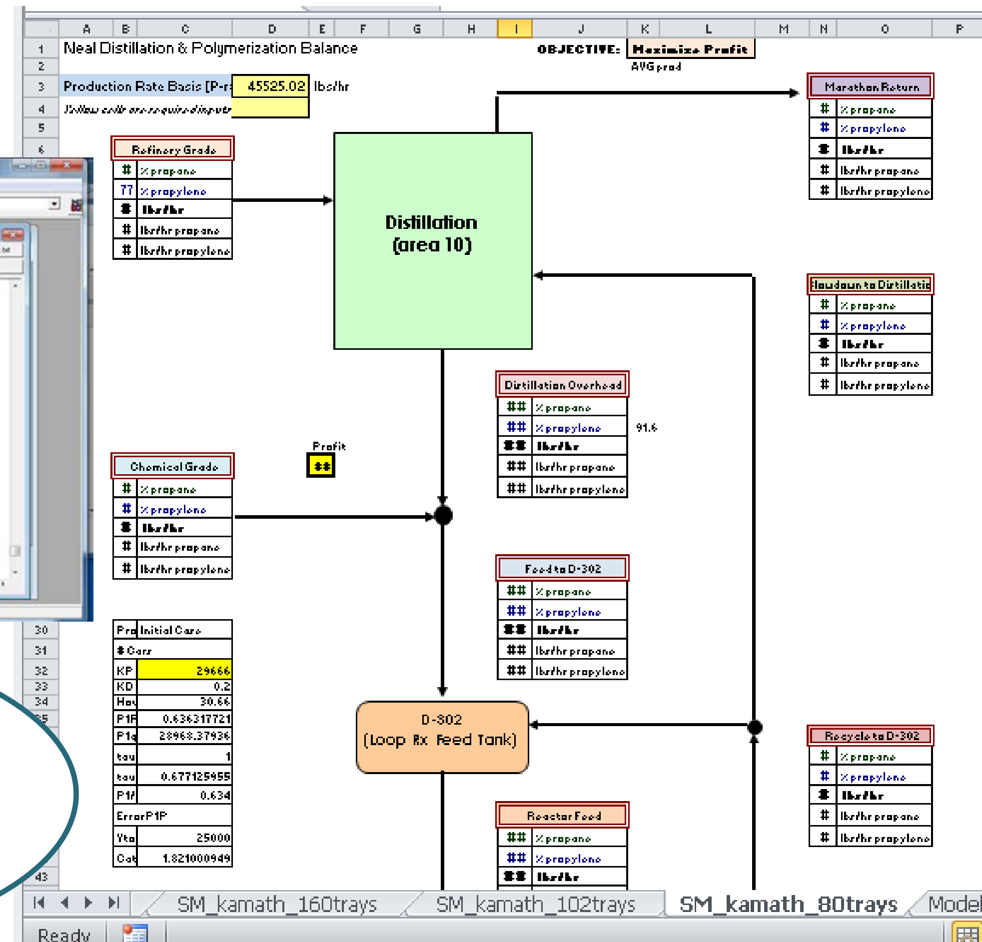
- Empirical model is **smaller and much more easier** but may be **infeasible**.
- Kamath model avoids unrealistic operation in the distillation column (**computationally more difficult**).

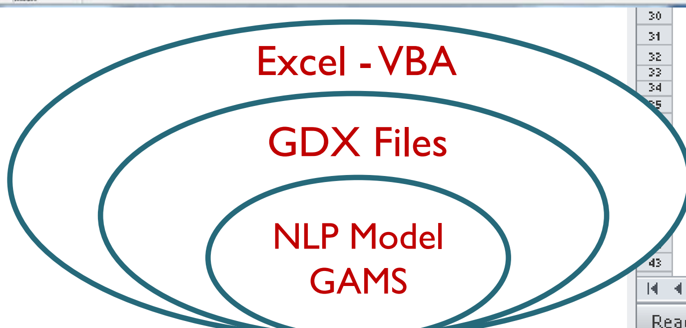
User Interface via Excel Worksheet

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

- Flexibility to easily test different column efficiencies.
  - 80 - 160 trays







Remarks and Future Work

Novelty of work

- Proposed work provides more accurate model that can be applied to scheduling of multiple grades of polypropylene.
- Single product feedstock nonlinear programming model has been implemented:
  - Aggregated group-method based on work of Kamath et al. 2010.
  - Initialization strategies developed for robust computations.

Potential benefit in application to industrial problems

- More accurate estimation of the profit
- Computational efficiency has been demonstrated for single product optimization (few cpu seconds).
- Conjecture: we expect new method will scale well with multiple-product grades.

Further work

- Integrate the aggregated model (Kamath method) for multiple-product scheduling.