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Integrated C3 Feedstock and Aggregated Distillation Model for Polypropylene Production

Miguel Zamarripa, Pablo A. Marchetti, Ignacio E. Grossmann

Department of Chemical Engineering
Carnegie Mellon University

Wiley A. Bucey, Rita A. Majewski

Braskem America

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

Process and Problem Description

Chemical
Grade (CG)

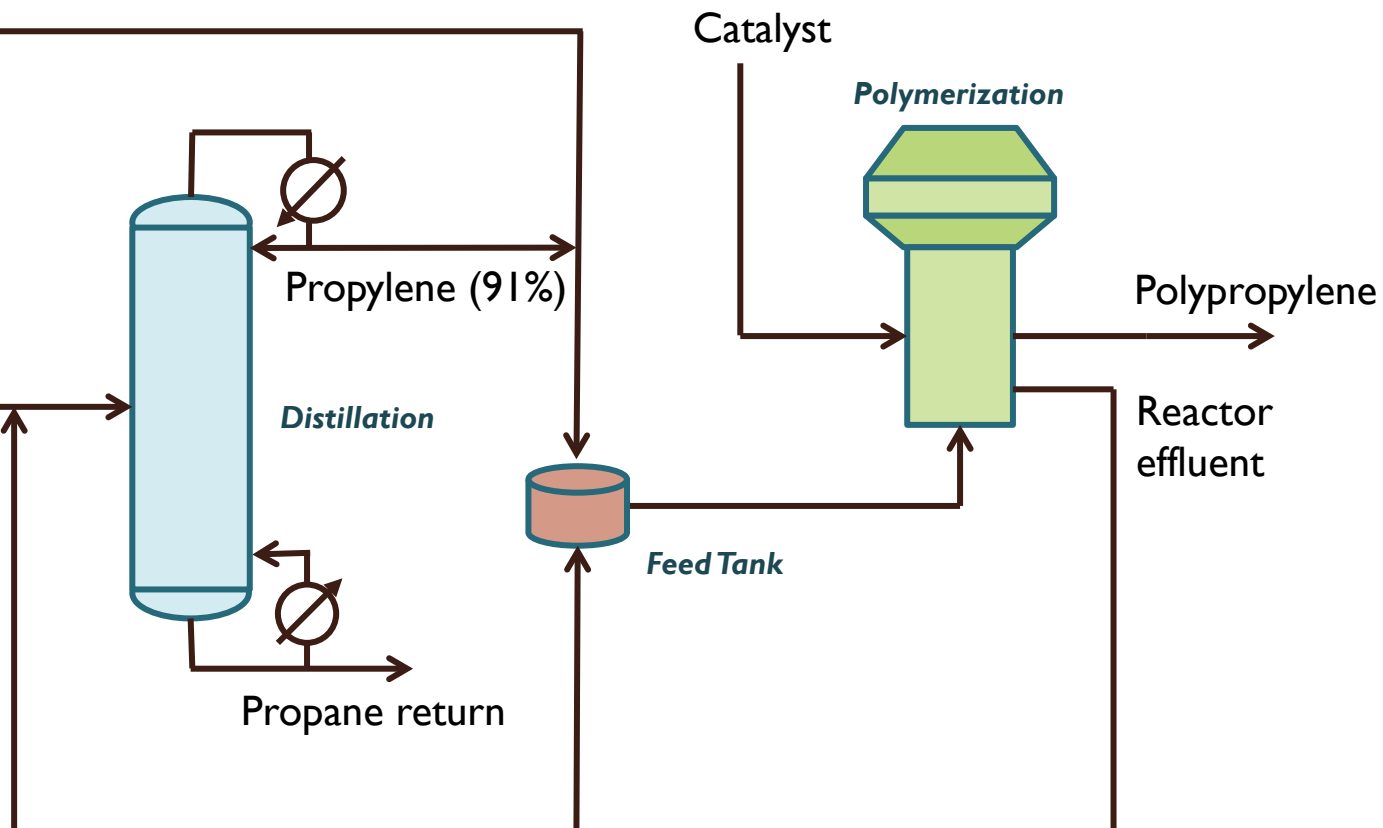
~95% propylene

Expensive

Refinery
Grade (RG)

~79% propylene

Cheaper



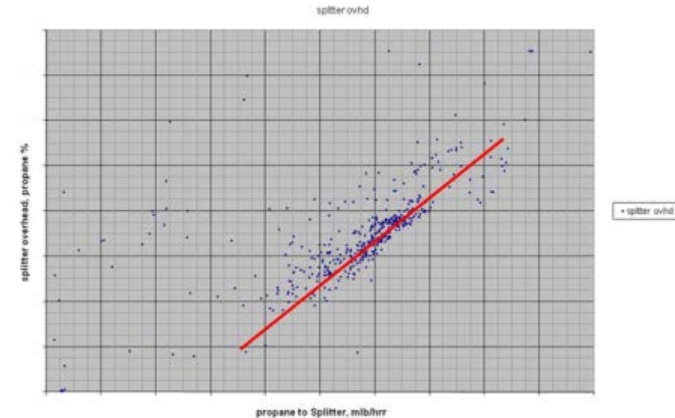
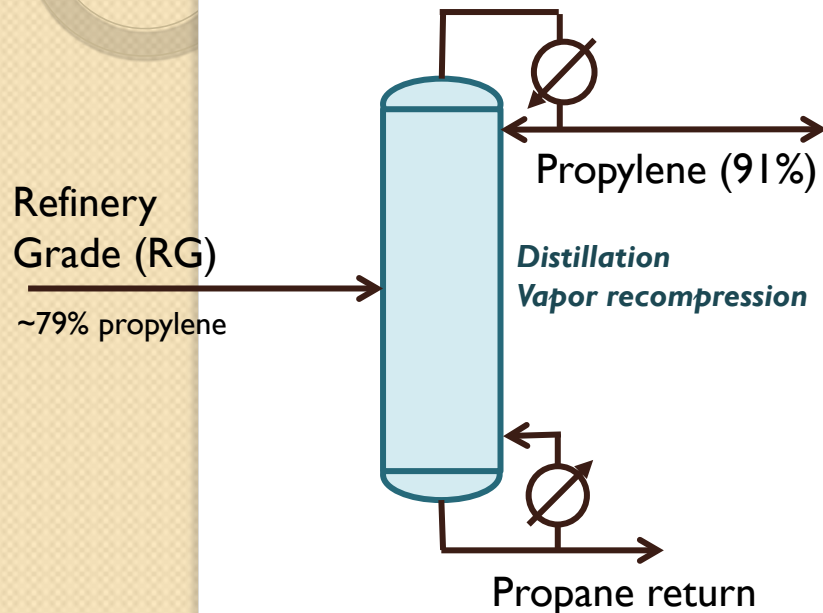
Goal: Select optimal mix of chemical and refinery grade propylene

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
 - 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.**

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)

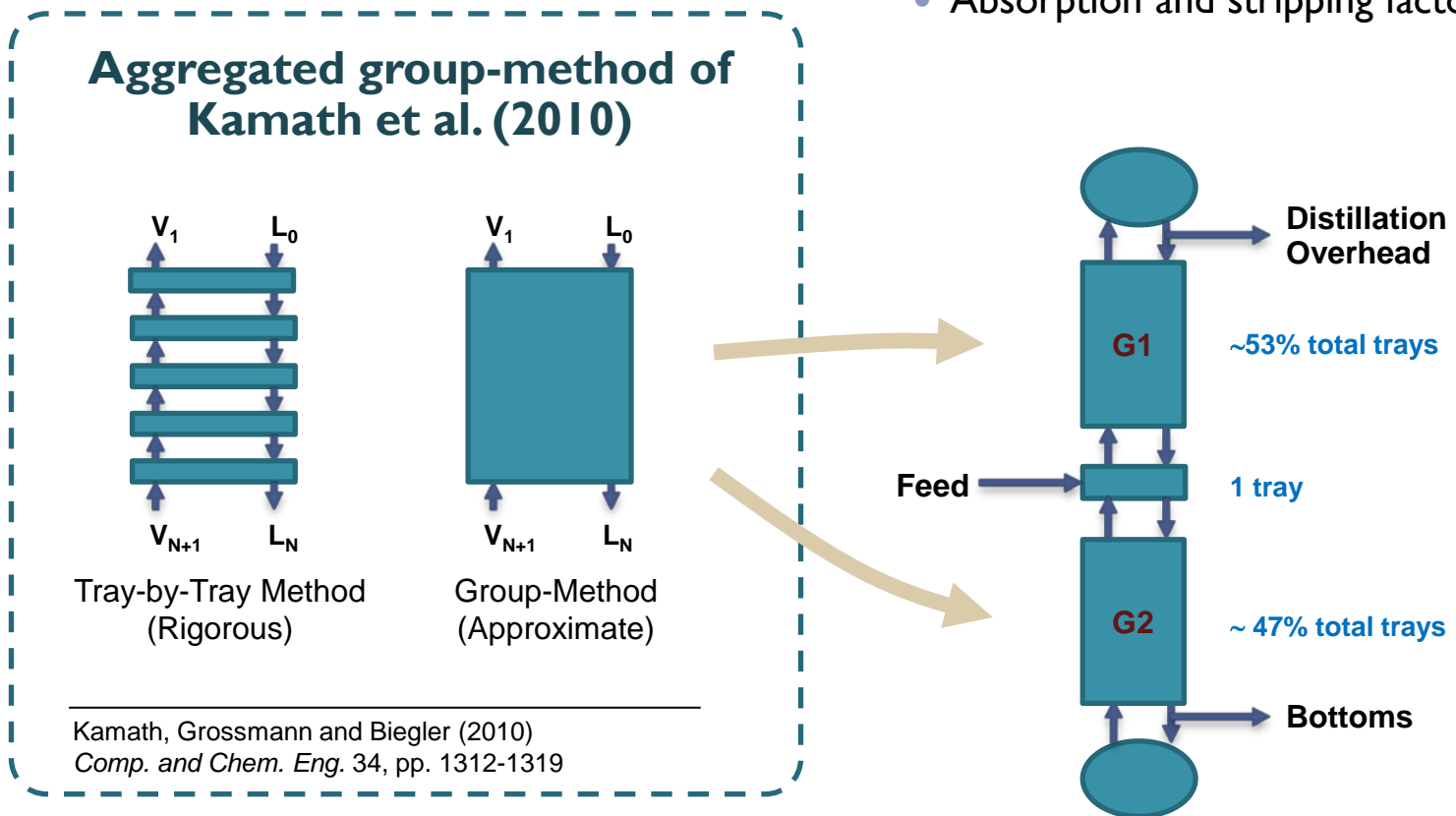
❖ Models a counter-current cascade of trays

Main Assumptions

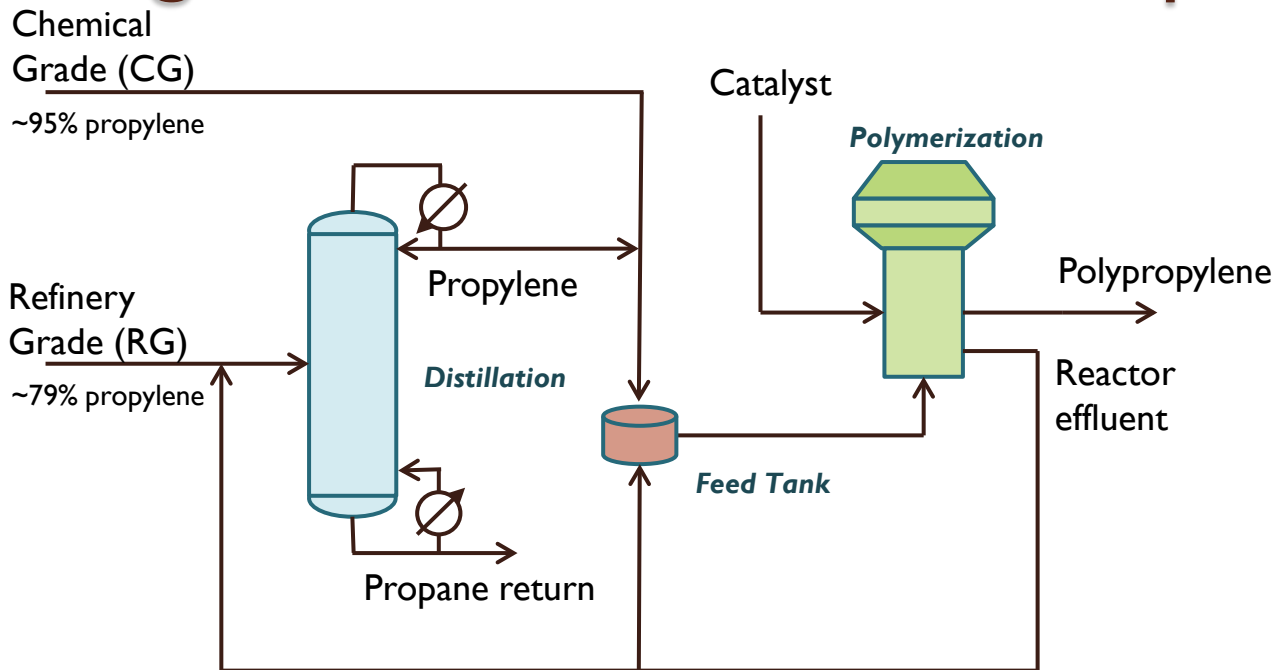
- Adiabatic and isobaric operation

Variables

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



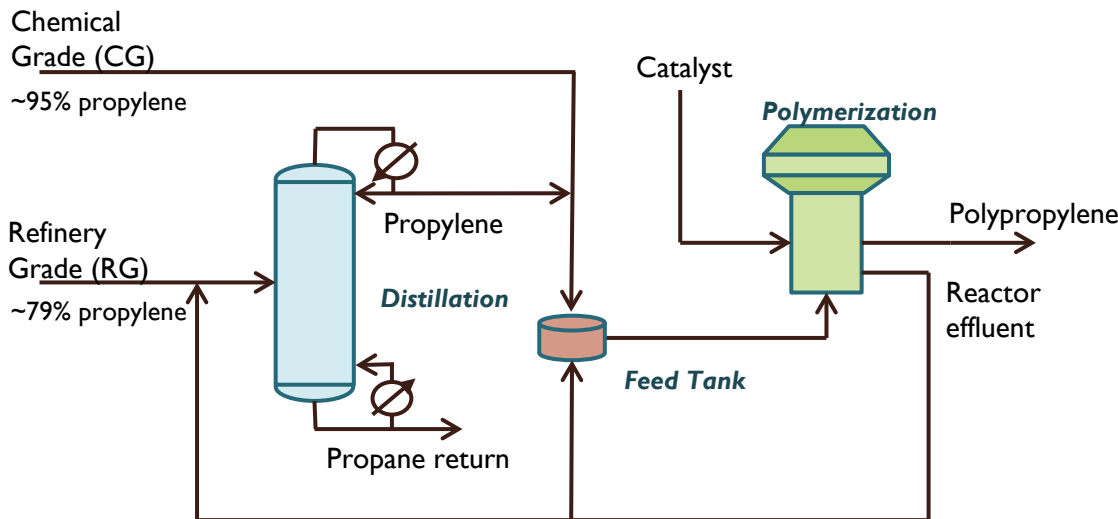
Single Product Model - Example



- 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)**

Additional Assumptions

- 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

Propylene Source

Er

Kamath model

Kamath model (90)

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**).

Optimal Solution (PROFIT, \$)

Cpu time (cpu s)

Variables

Constraints

33

151

151

43

154

154

User Interface via Excel Worksheet

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

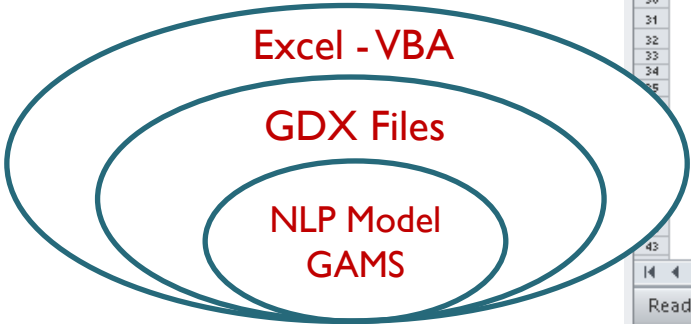
- Flexibility to easily test different column efficiencies.
 - 80 - 160 trays

```

gamside: C:\Users\Miguel\Documents\CMU\braken-files\model\singlemodel\singlemodel.gpr
File Edit Search Windows Utilities Model Libraries Help
Sample
C:\Users\Miguel\Documents\CMU\braken-files\model\singlemodel\singlemodel.gpr
MultipleModel_UI.gms  CS1_appox_MNLP.gms  Kamath_v1.gms  AggModPAM_M2.lst  AggModPAM_M2.lst  CS1_appox_MNLP.lst  MultipleModel_UI.lst  output.txt
SingleModel.gms  SingleModel.lst  SingleModel_nike.gms  SingleModel_nike.lst  SingleModel_nike2.gms  SingleModel_nike2.lst

rhol2 = rhol1*(C3e) ;
w1 = w1*(C3e) ;
w2 = w1*(C3e) ;
display C3eR,C3eG,C3eB,C3eD,C3eM,C3eS,C3eO,C3eX,C3eD00,
C3eR,C3eS1,C3eS2,
C3eR,C3eG,C3eM,C3eD,C3eX,C3eD00,
C3eR,C3eS1,C3eS2,W00 rhol;
prate xl x2 tau1 tau2 FIP Ytot Cat
rhol1 rhol2 w1 w2 profit; mpdnew;

Fonttext
**o print: 160 trays run
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eR eng=SM_Kamath1821:821';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eG eng=SM_Kamath1827:827';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eM eng=SM_Kamath197:897';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eD eng=SM_Kamath129:129';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eX eng=SM_Kamath1232:1232';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eO eng=SM_Kamath1248:1248';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eS eng=SM_Kamath190:190';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eS1 eng=SM_Kamath103:103';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eS2 eng=SM_Kamath181:181';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eR eng=SM_Kamath1810:1810';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eG eng=SM_Kamath186:186';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eM eng=SM_Kamath197:197';
execute 'gdx.exe Coordinated_SG_Nick.gdx par=C3eD eng=SM_Kamath1232:1232';
    
```



Excel Worksheet: Neal Distillation & Polymerization Balance

OBJECTIVE: Maximize Profit
AVGprod

Production Rate Basis [P-r] 45525.02 lb/hr

How can we require inputs

Distillation (area 10)

Marathon Return

Headman to Distillate

Distillation Overhead

Feed to D-302

D-302 (Loop Rx Feed Tank)

Recycle to D-302

Reactor Feed

Chemical Grade

Refinery Grade

Profit

Prod Initial Cost

Carz	296.66
KP	0.2
KD	30.66
tau	0.636317121
Pf1	28968.37936
tau	1
tau	0.677125955
Pf1	0.634
Error Pf1	25000
Ytot	1.821000949
Cat	

SM_kamath_160trays SM_kamath_102trays SM_kamath_80trays Model

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.