Integrated C3 Feedstock and Aggregated Distillation Model for Multiproduct Polypropylene Production Optimization

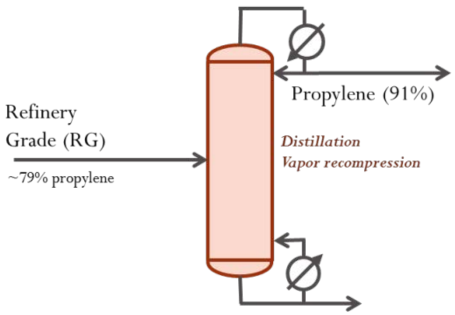
Miguel Zamarripa, Pablo A. Marchetti, Ignacio E. Grossmann
Department of Chemical Engineering
Carnegie Mellon University

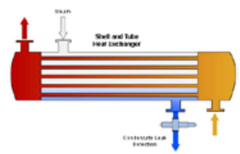
Wiley A. Bucey, Rita A. Majewski, Bobby Balsom, George Ostace
Braskem America

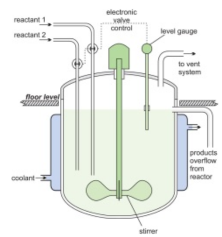
Center for Advanced Process Decision-Making,
Enterprise Wide Optimization Meeting, September 17-18, 2014

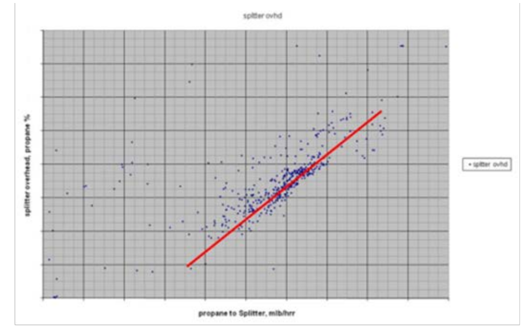
Motivation

- Most previous work in planning or scheduling type decisions involve very simple process models (fixed processing rates, fixed processing times, etc.).



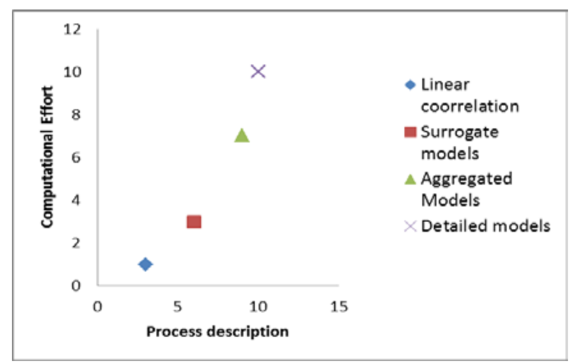






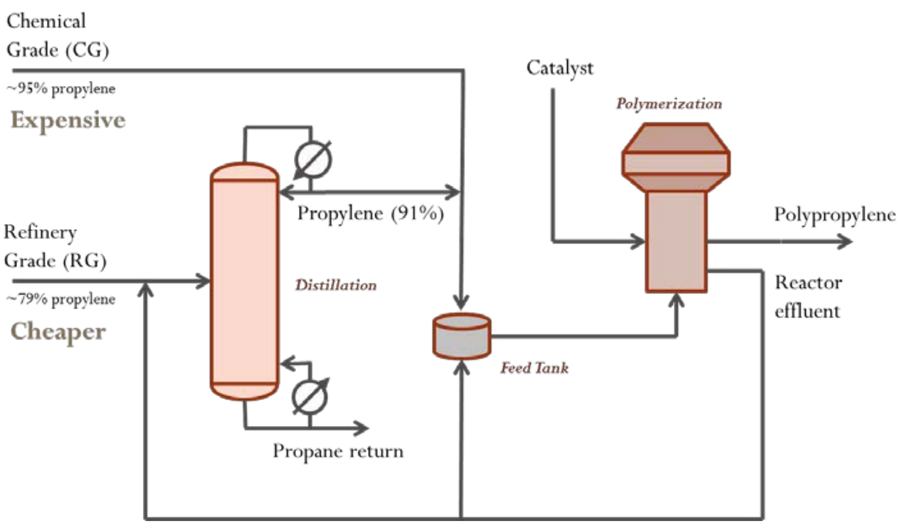
Relates overhead composition of propane with flowrate of propane feed to the splitter.

- Continuous chemical processes require more detailed models.
  - **Non-linear (non-convex)**
  - **Large computational effort**
  - **We need to provide 'good' initial solution**



- **Goal:** Develop a scheduling model in which the process model complexity must be explicitly incorporated into the problem formulation.

Problem Statement and Main Assumptions



- Maximize Profit

  Selecting the optimal mix of propylene from chemical and refinery grade

- Constraints on each time interval:
  - Material balances
  - Min/Max flow rates
  - Limits on catalyst yield and flow
  - Availability of Chemical Grade
  - Specifications on splitter feed and recycle rate
  - Mass and Energy balances (distillation column)
  - Absorption and stripping constraints (distillation column)

- Given
  - Network superstructure
    - Distillation column, Mixers, and Polymerization reactor.
  - Production demands
  - Products and Families
  - Maximum and Minimum
    - CG and RG purchase
    - Production rate
    - Propylene composition (DO and MR and Bottoms)

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

Aggregated group method (Kamath et al. 2010):

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

- Models a counter-current cascade of trays
- It is an alternative for detailed tray by tray distillation model:

Main Assumptions

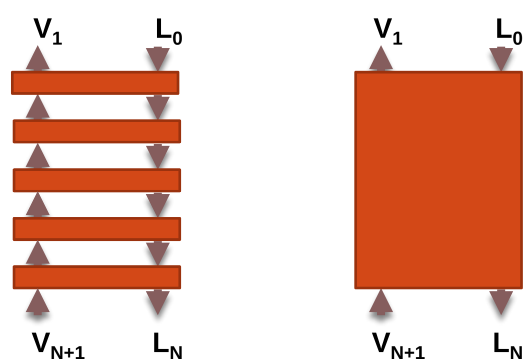
- Adiabatic and isobaric operation

Variables

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

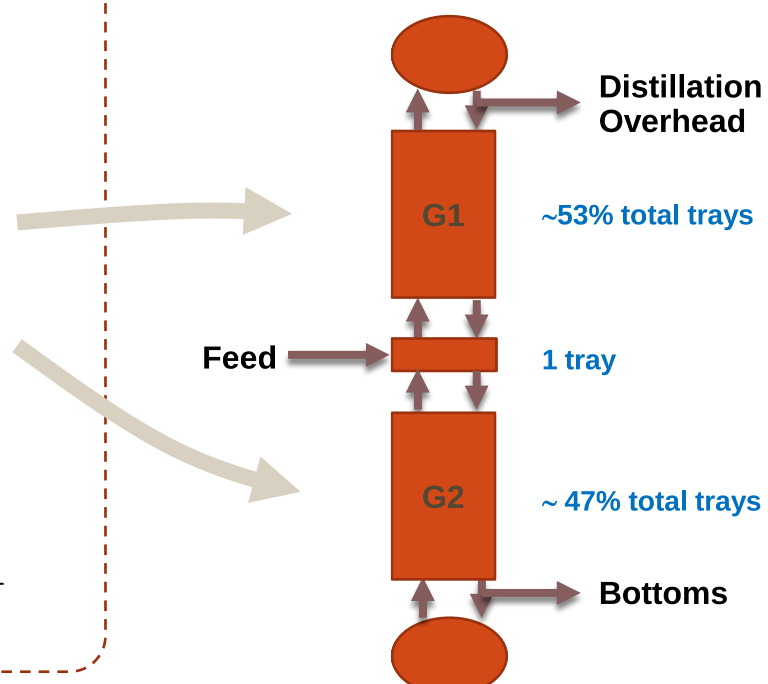
Distillation Model

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



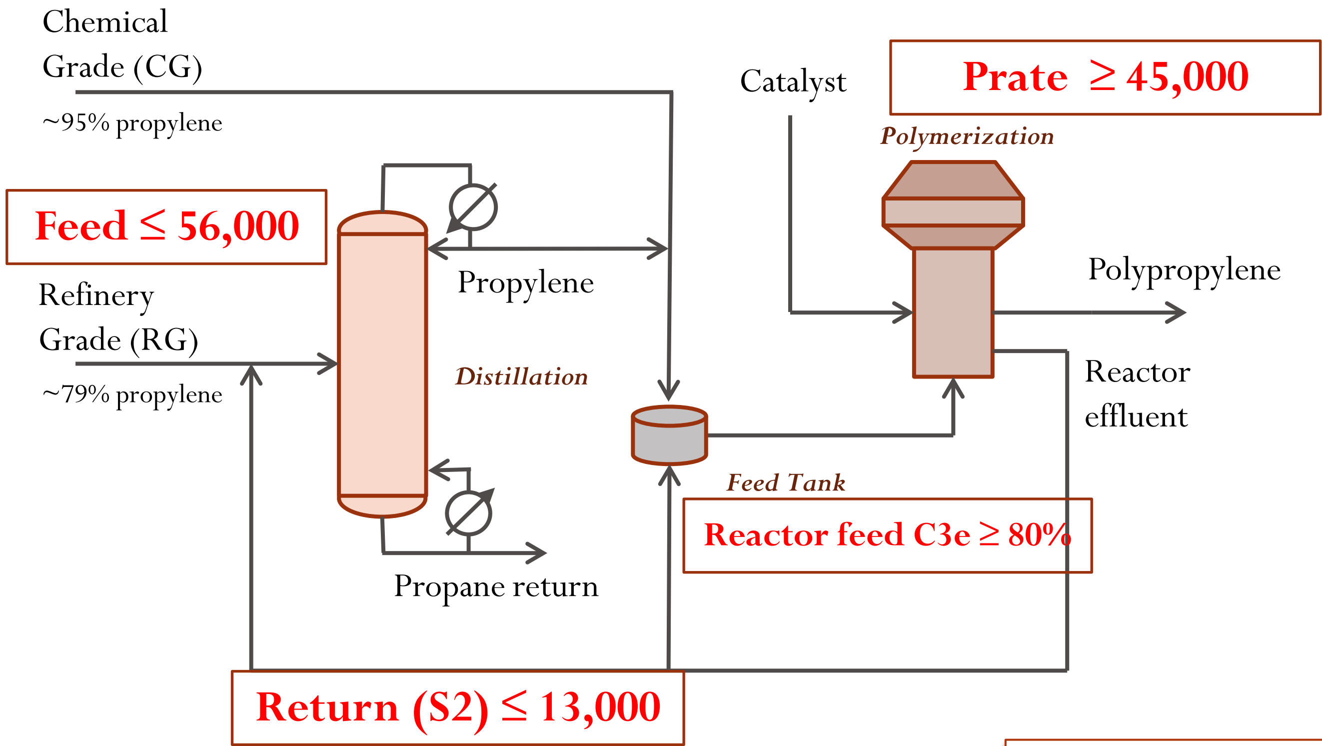
Tray-by-Tray Method (Rigorous)

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

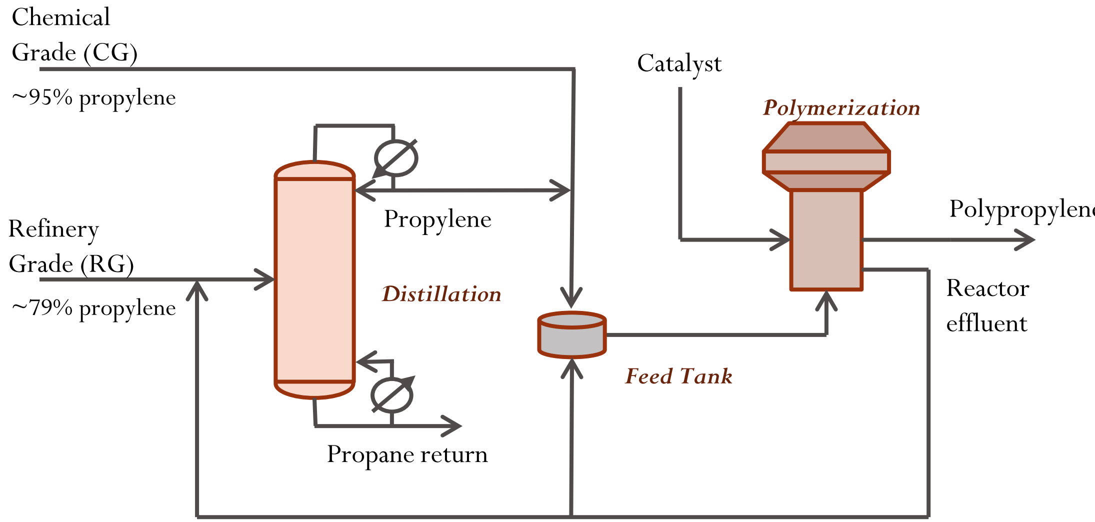
  Reactor feed and catalyst flow

  Reflux rate (min/max 300,000 – 400,000 lb/hr)

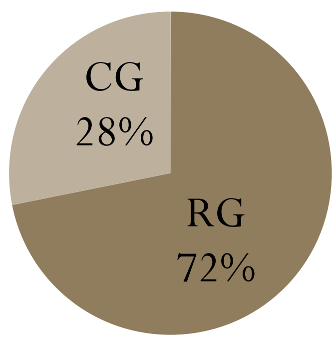
Additional Assumptions

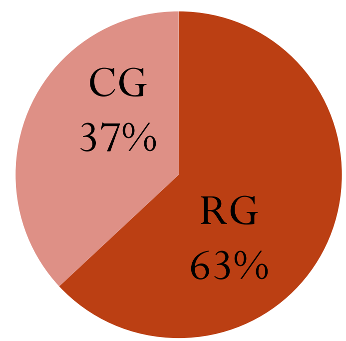
- **Fixed pressure for the whole column = 9.778 atm**
- **Total condenser (top)**
- **Total reboiler (bottom)**
- **Single feed**
- **Bottoms composition (5% propylene)**

Single Product Model - Example



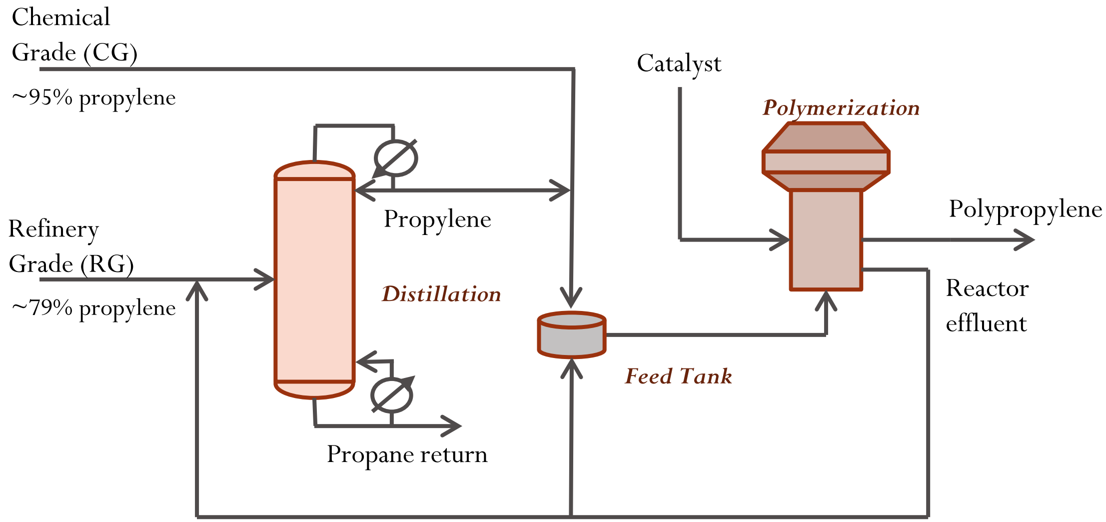
Propylene Source	Empirical model	Kamath model (160 trays)





	Empirical model	Kamath model (160 trays)
Optimal Solution (PROFIT, $)	**11, 042**	**10,576**
Cpu time (cpu s)	**0.031**	**0.156**
Variables	**33**	**172**
Constraints	**43**	**161**

Single Product Model - Example



Propylene Source	Empirical model	Kamath model (160 trays)
Optimal Solution (PROFIT, $)		
Cpu time (cpu s)		
Variables		
Constraints	43	161

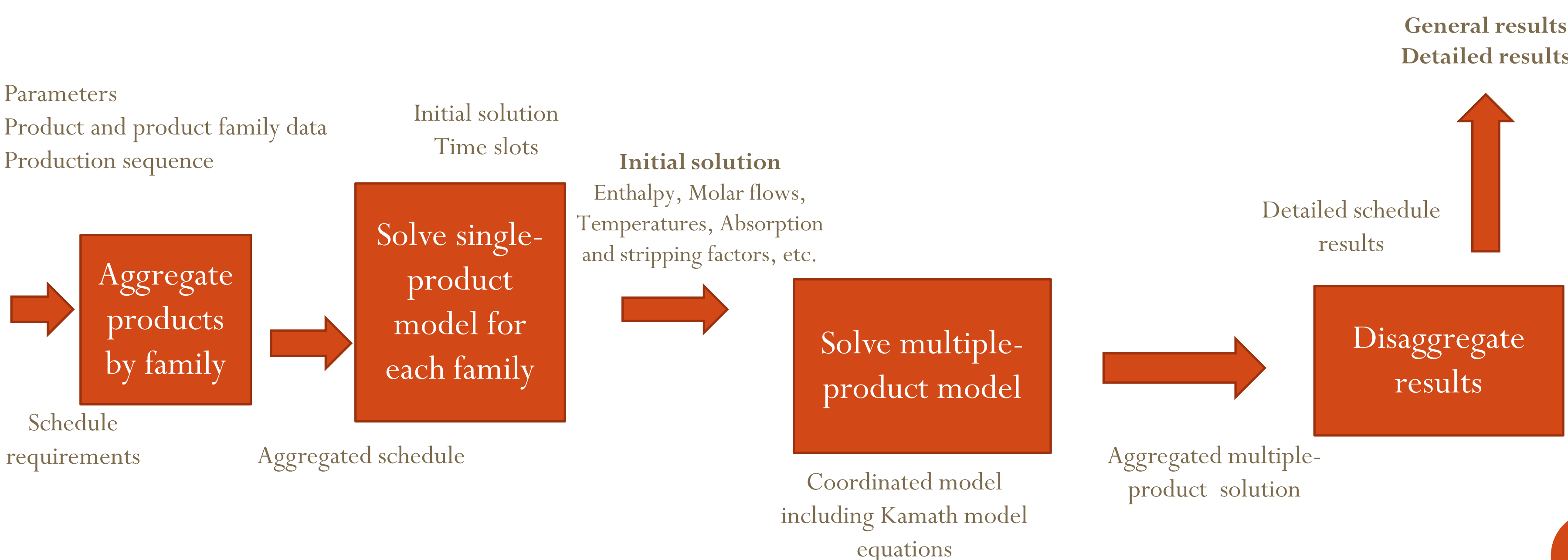
Tradeoff:

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

Multiple Product Model Framework

Multiple Product Model

- Multiple orders of different products over a specified horizon
- Production sequence given
- Profit ($) = selling prices – feedstock costs
  + propane return – others
- Solution yields **optimal production rates** with minimum costs for each product
- Products of the same family feature same kinetic properties.
- Aggregation/disaggregation allows to **handle large scale problems**.



Multiple Product Model - Example

Maximize profit

Decision variables:

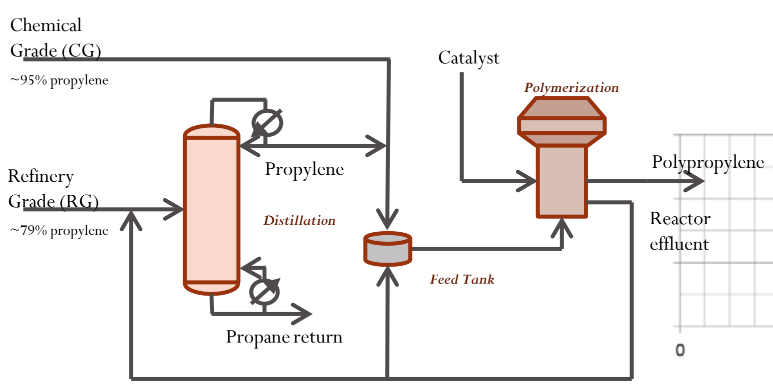
k production slots (for each family of products)
Production rate of polypropylene at each time slot (k)
RG and CG feed rates at each time slot (k)
Distillation overhead flow and composition at slot (k)
Reactor feed and catalyst flow at each time slot (k)
Production time; Time(k)*Prate(k)=Demand(k)

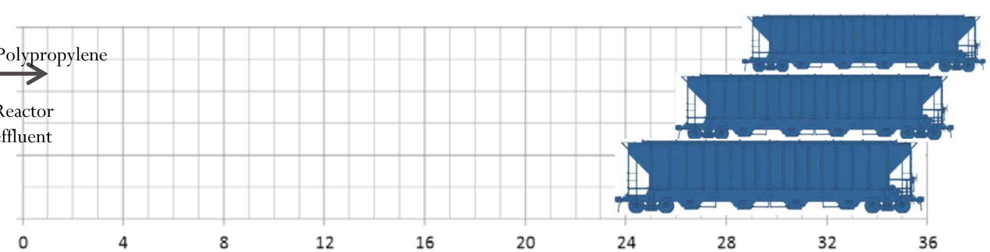
Additional Assumptions

- **Fixed pressure for the whole column = 9.778 atm**
- **Total condenser (top)**
- **Total reboiler (bottom)**
- **Single feed**
- **Bottoms composition (5% propylene)**
- **Reflux rate (min/max 300,000 – 400,000 lb/hr)**

Mid-size example

- 20 products belonging to 5 families (k= 5, model constraints and variables)
- 189 railcars (190,000 lbs. each)
- Time horizon: 25, 27, 31 and 34 days

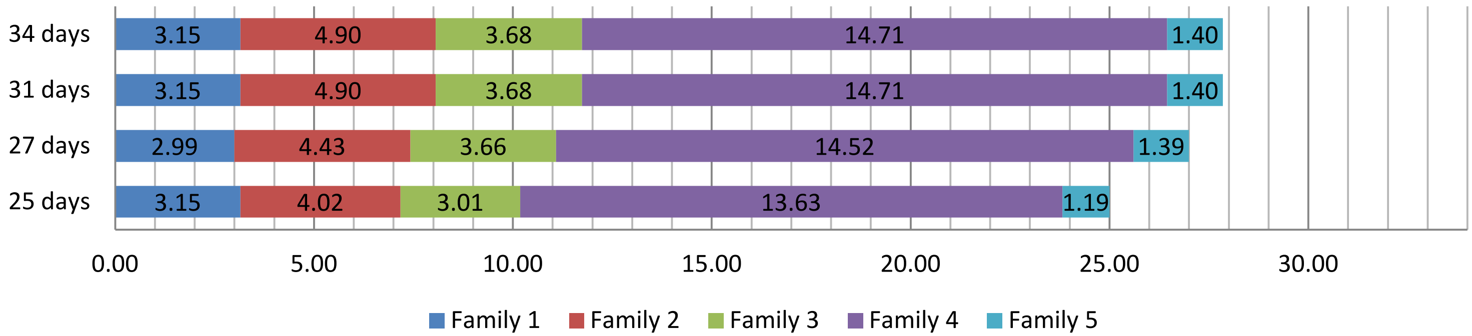




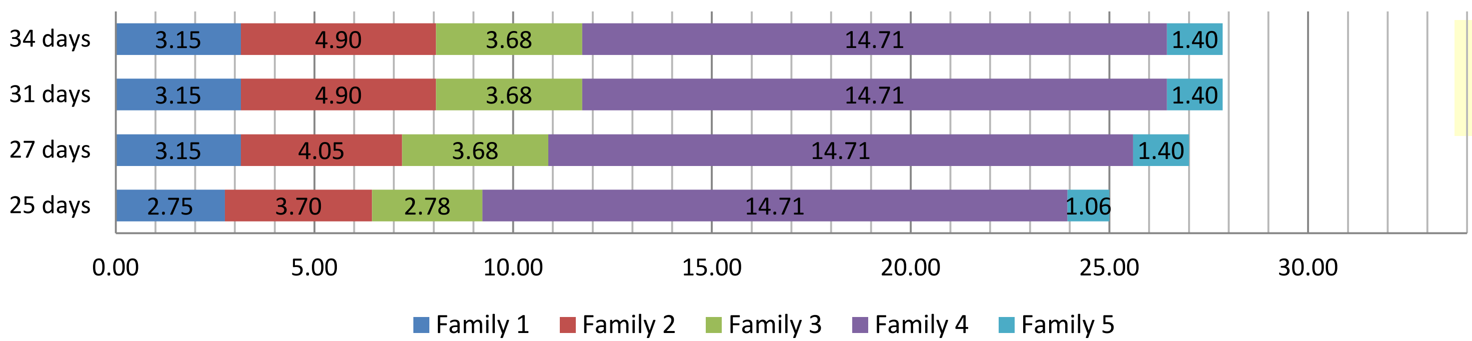
Multiple Product Case Study - Results

Production Scheduling

Empirical model



Kamath model (160 trays)



Statistics (Empirical model)

Model size: 192 variables, 166 constraints

Solved by CONOPT in ~ 60 cpu seconds. (including initialization) .

Statistics (Kamath model 160 trays)

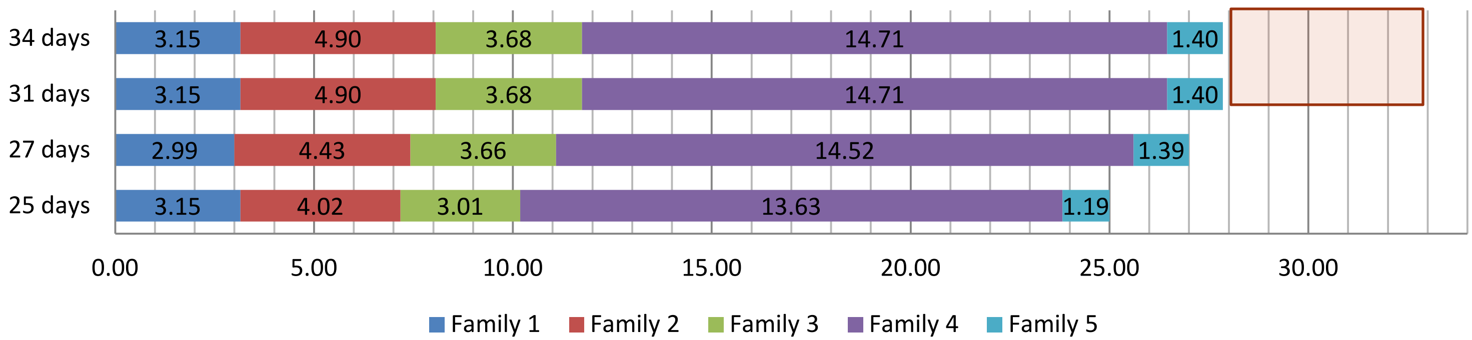
Model size: 882 variables, 798 constraints

Solved by CONOPT in ~120 seconds. (including initialization)

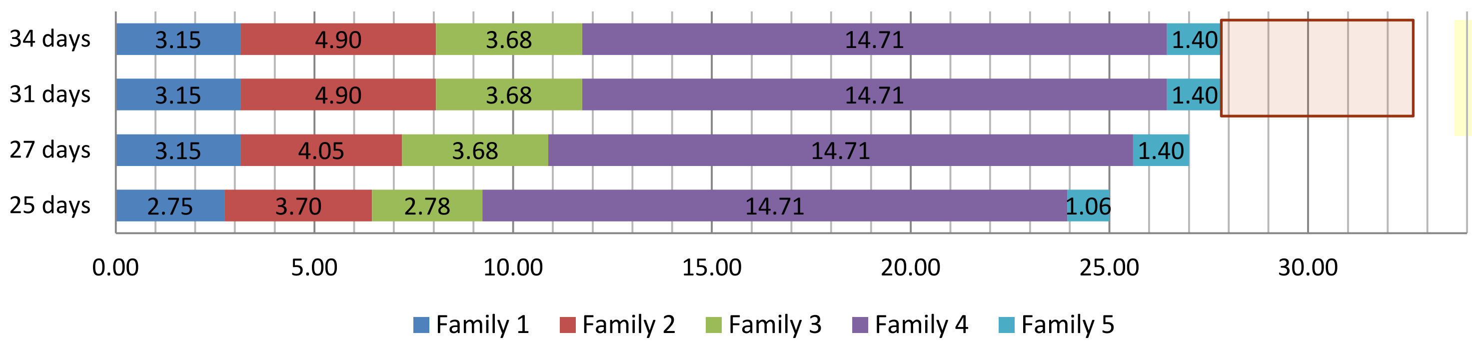
Multiple Product Case Study - Results

Production Scheduling

Empirical model



Kamath model (160 trays)



Tradeoff : produce more and provide more **idle time**, or produce at the faster production rate and finish earlier.

Statistics (Empirical model)

Model size: 192 variables, 166 constraints

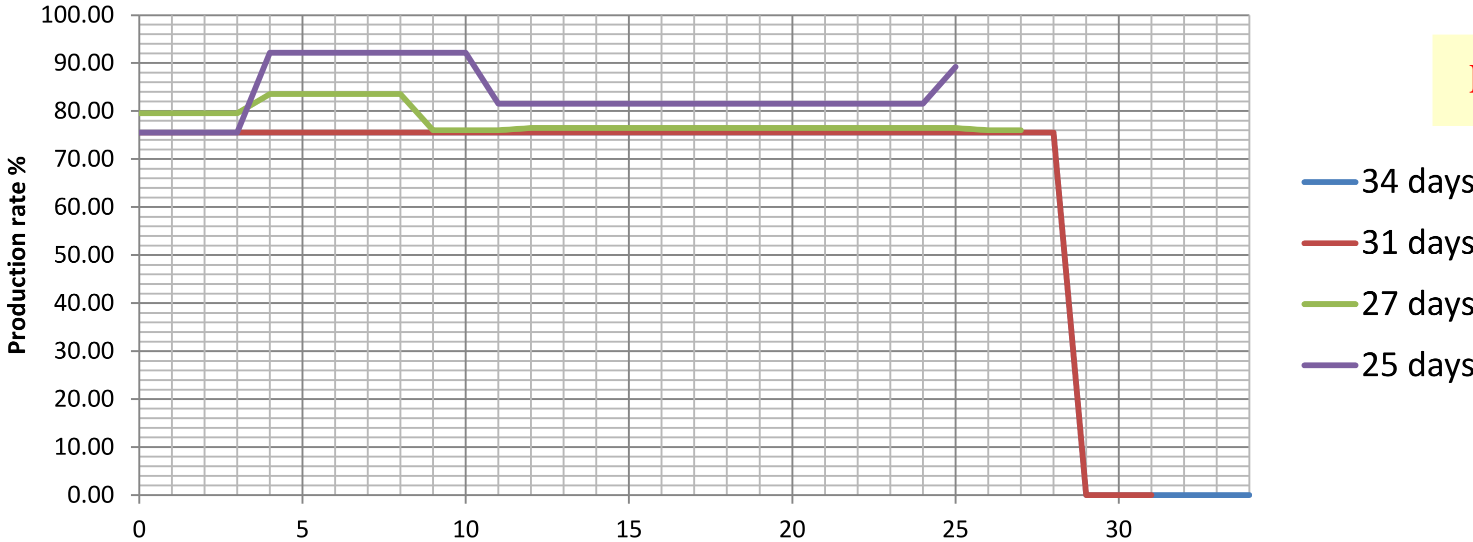
Solved by CONOPT in ~ 60 cpu seconds. (including initialization) .

Statistics (Kamath model 160 trays)

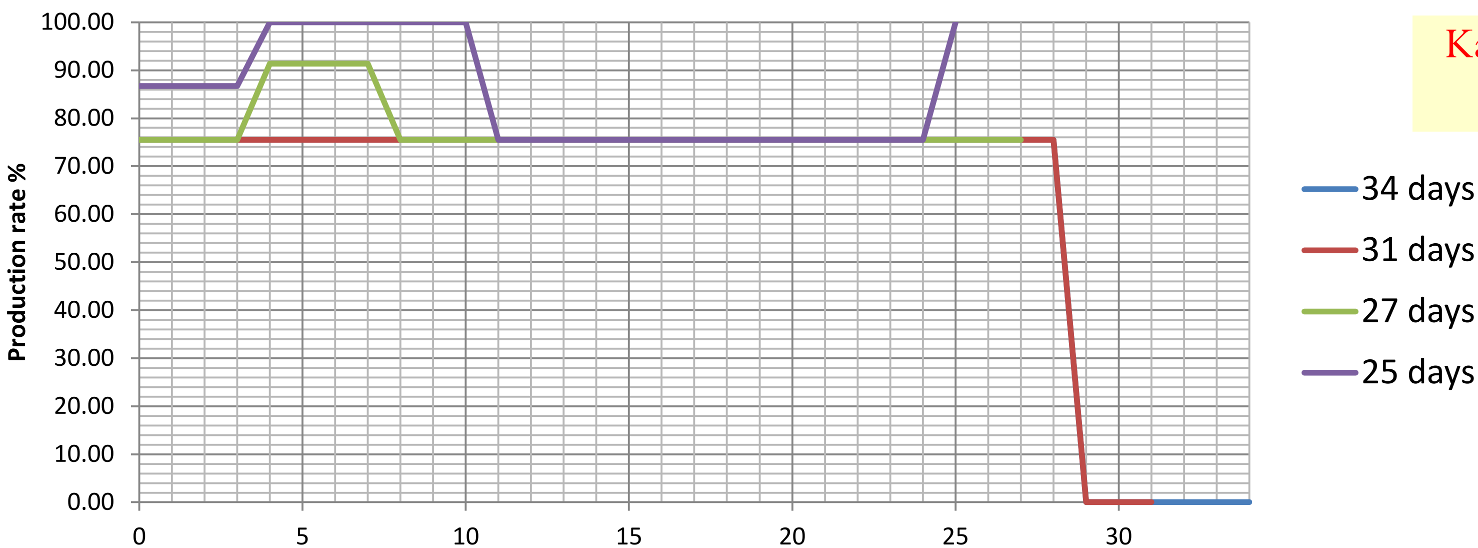
Model size: 882 variables, 798 constraints

Solved by CONOPT in ~120 seconds. (including initialization)

Multiple Product Case Study - Results



Empirical model



Kamath model (160 trays)

Statistics (Empirical model)

Model size: 192 variables, 166 constraints

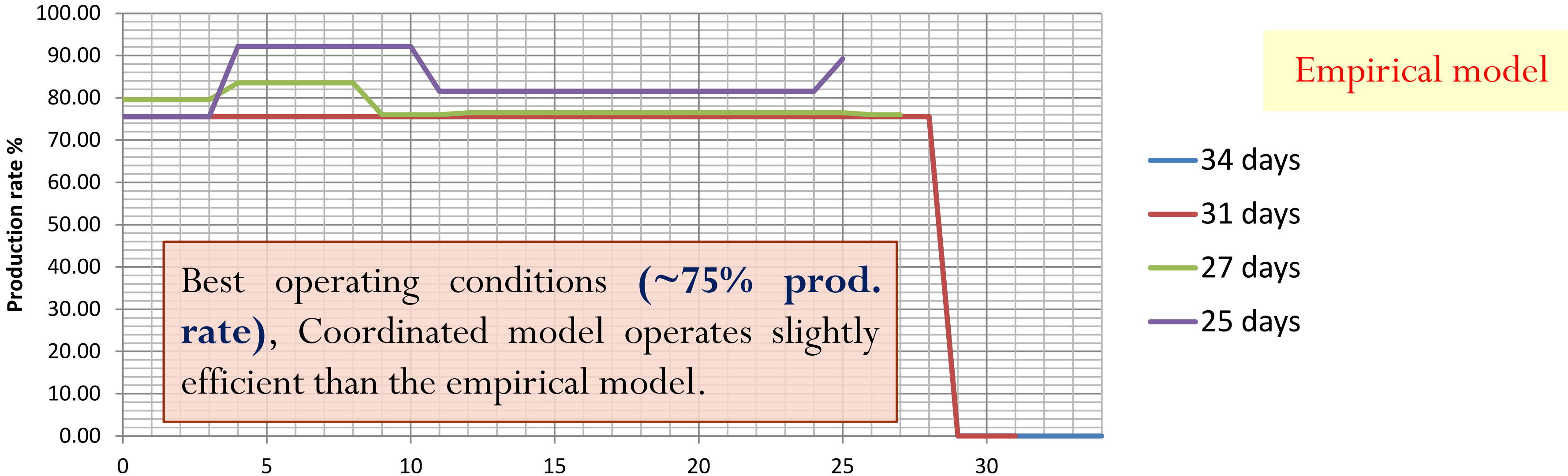
Solved by CONOPT in ~ 60 cpu seconds. (including initialization) .

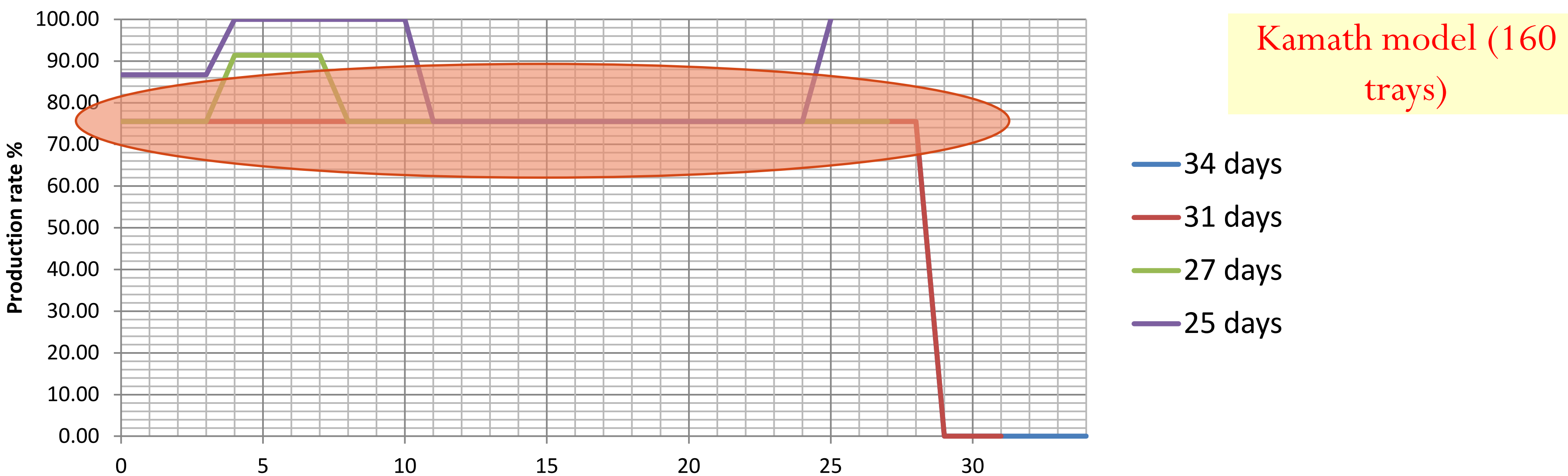
Statistics (Kamath model 160 trays)

Model size: 882 variables, 798 constraints

Solved by CONOPT in ~120 seconds. (including initialization)

Multiple Product Case Study - Results





Statistics (Empirical model)

Model size: 192 variables, 166 constraints

Solved by CONOPT in ~ 60 cpu seconds. (including initialization) .

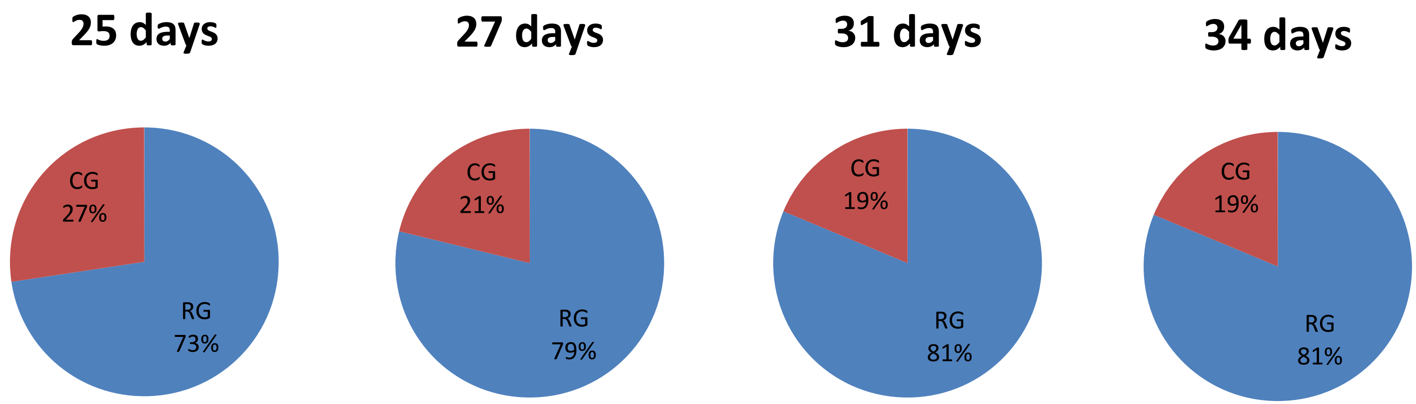
Statistics (Kamath model 160 trays)

Model size: 882 variables, 798 constraints

Solved by CONOPT in ~120 seconds. (including initialization)

Multiple Product Case Study - Results

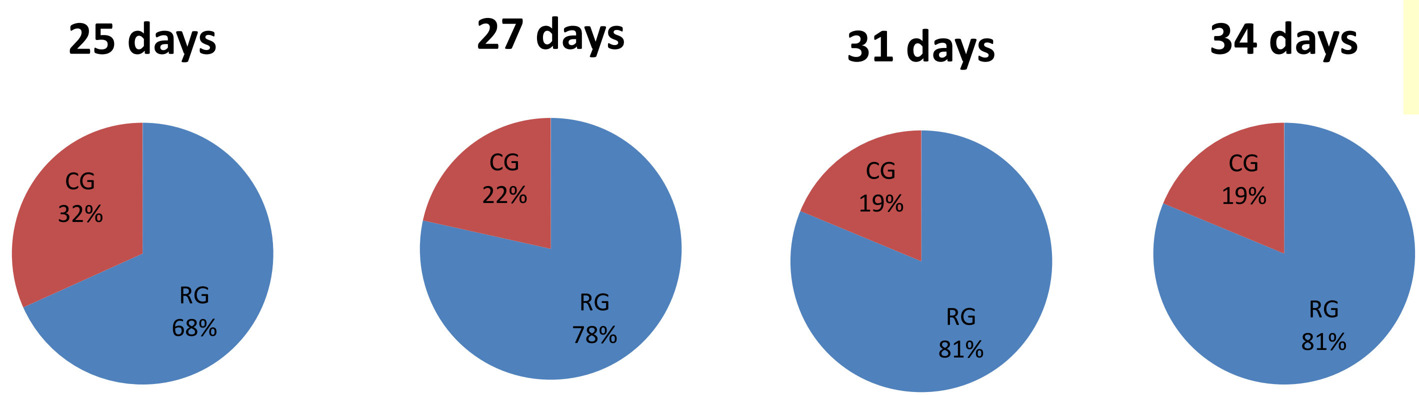
Empirical model



25 days	27 days	31 days	34 days
94.68	98.31	99.86	99.86

Profit (Normalized)

Kamath model (160 trays)



25 days	27 days	31 days	34 days
94.8	98.5	100	100

Profit (Normalized)

Statistics (Empirical model)

Model size: 192 variables, 166 constraints

Solved by CONOPT in ~ 60 cpu seconds. (including initialization) .

Statistics (Kamath model 160 trays)

Model size: 882 variables, 798 constraints

Solved by CONOPT in ~120 seconds. (including initialization)

Remarks and Future work

Novelty of work

- Proposed work provides an accurate model 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.
- Multiple product feedstock nonlinear programming model has been implemented
  - Linear correlation → aggregated group-method

Potential benefit in application to industrial problems

- More accurate estimation of the profit
- Computational efficiency has been demonstrated for single and multiple product optimization (few cpu seconds).
- Schedule of multiple-product grades has been obtained.
- Profit: slightly better solutions have been obtained.