Operational Model for C3 Feedstock Optimization on a Polypropylene Production Facility

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Center for Advanced Process Decision-making
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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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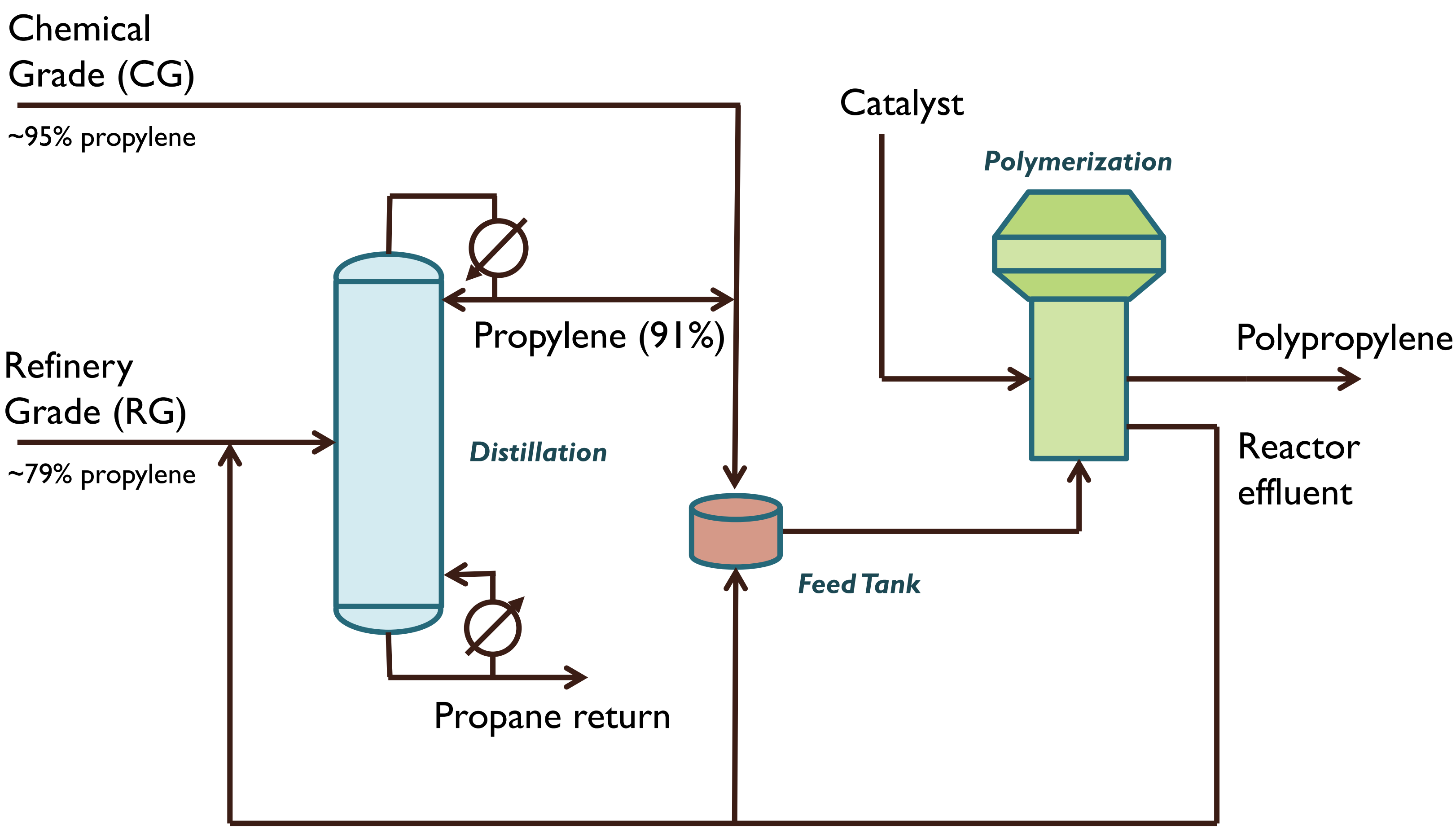
- Objectives:
  - Development of a Non-linear Programming (NLP) model to maximize benefits by obtaining a better balance of RG and CG feedstocks for single or multiple production orders.
  - Determine operation rates for a schedule of multiple production orders within a 3-month timeframe.
  - Implement user-friendly interface (GAMS model / MS-Excel)

Process and Problem Description



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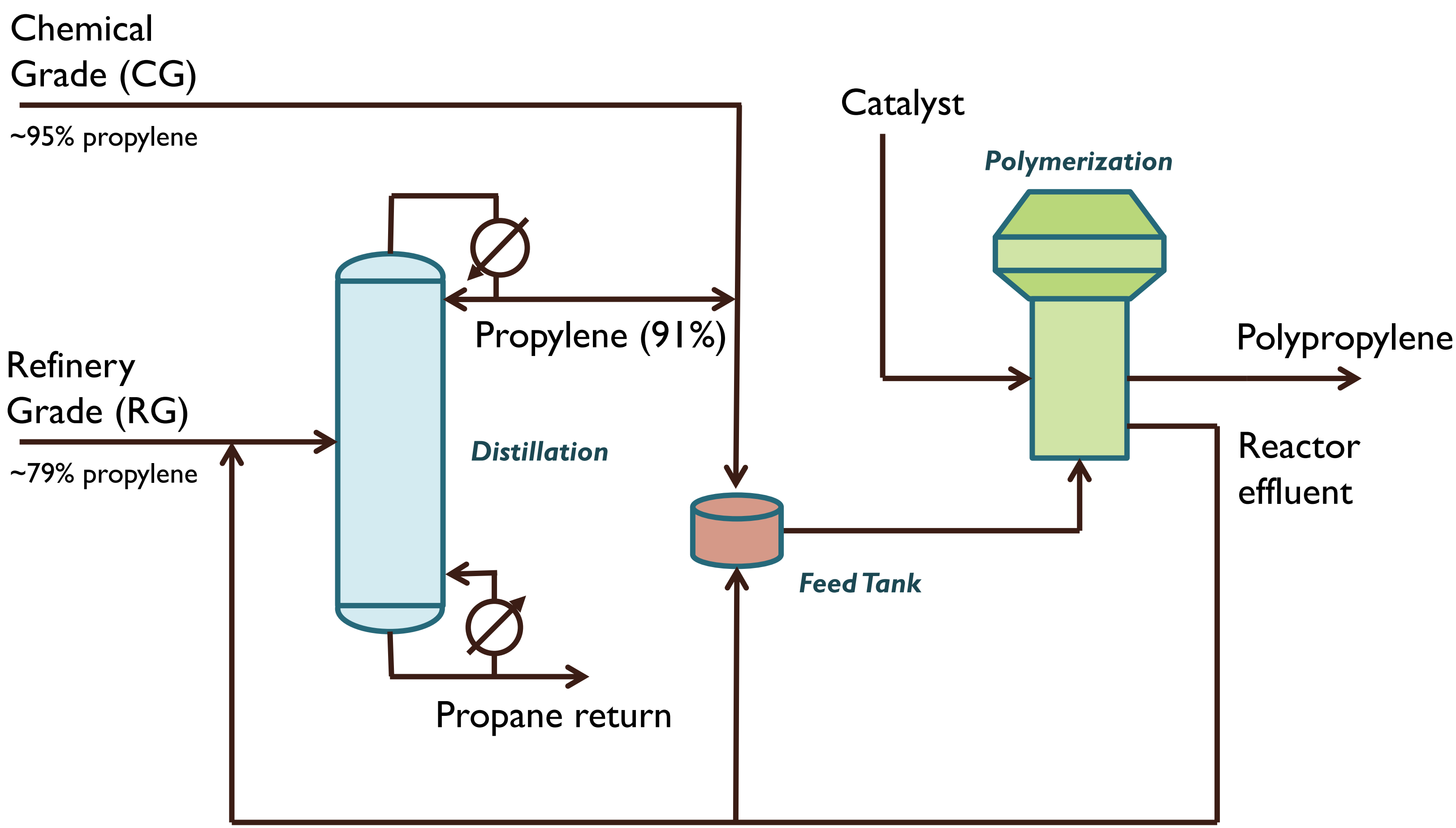

Maximizing the amount of RG may not be the best economic option

Mathematical Model (NLP)

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  - Material balances
  - Min/Max flow rates
  - Constraints on composition of Propane Return, Distillation Overhead & Reactor Feed
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  - Availability of Chemical Grade
  - Specifications on splitter feed and recycle rate

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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.

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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
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    - Preliminary results show **realistic tradeoff on feedstocks costs vs production rates** (depending on available time).

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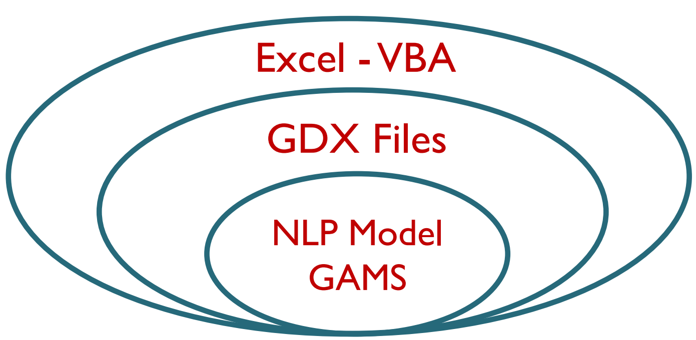
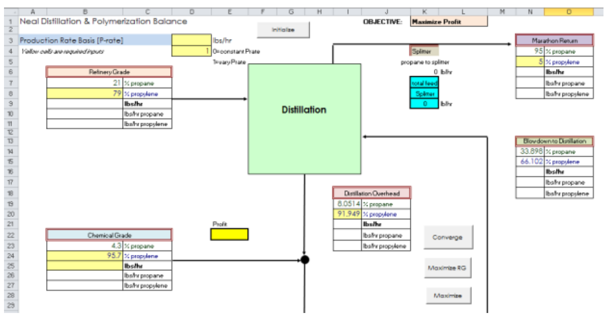
Models implemented with GAMS

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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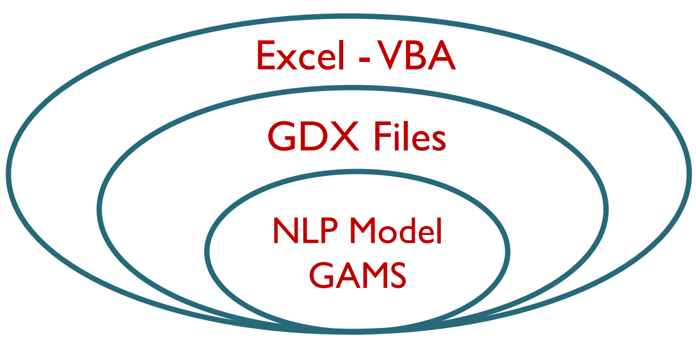
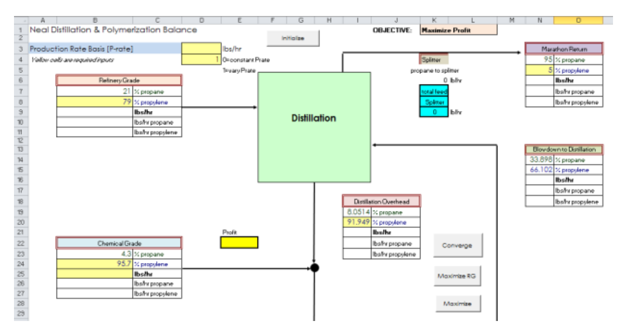
Specific parameters for testing gain/loss scenarios:

- Time horizon
- Addition of slack product (yes/no)





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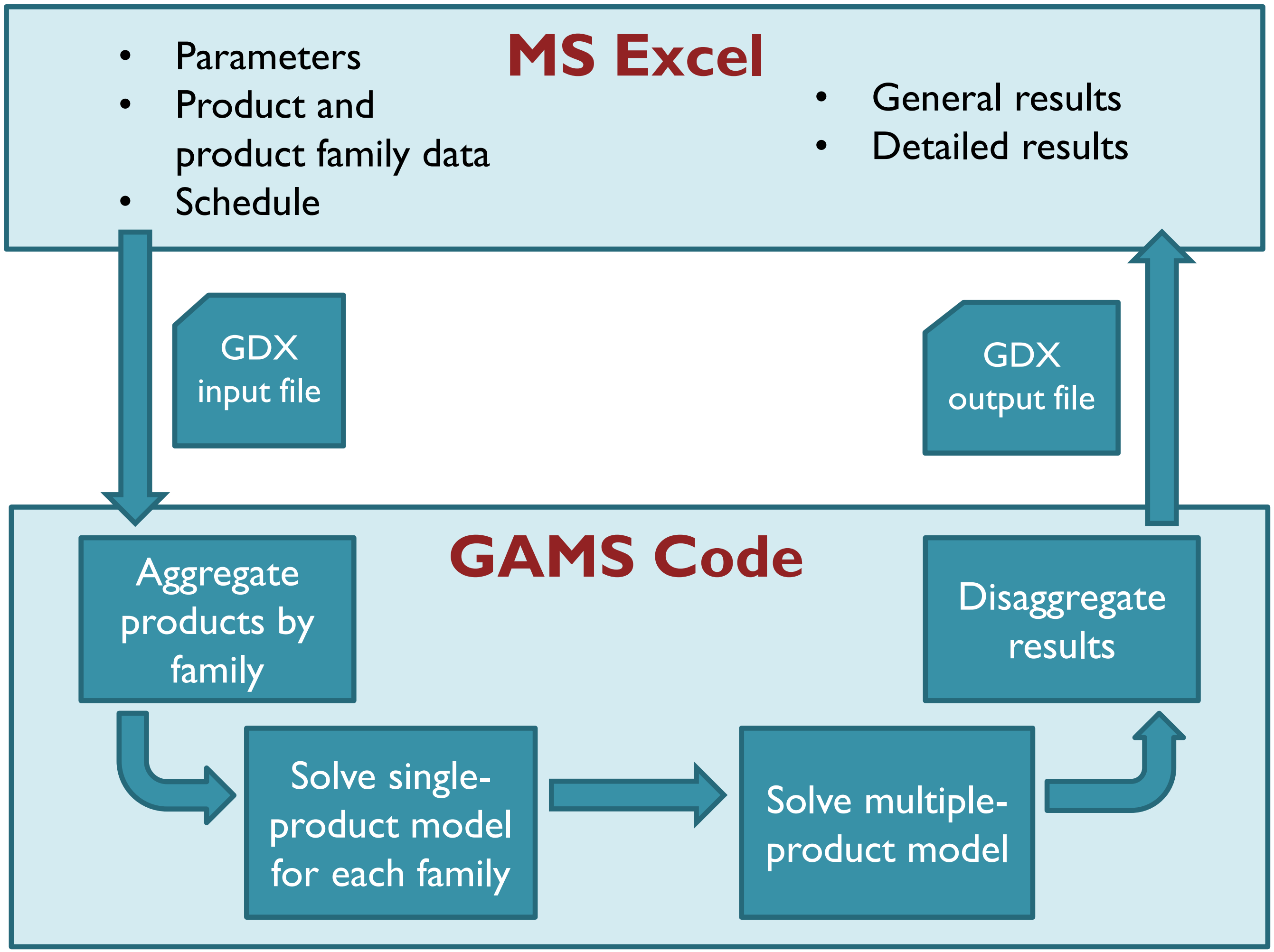
Overview of GAMS/Excel integration



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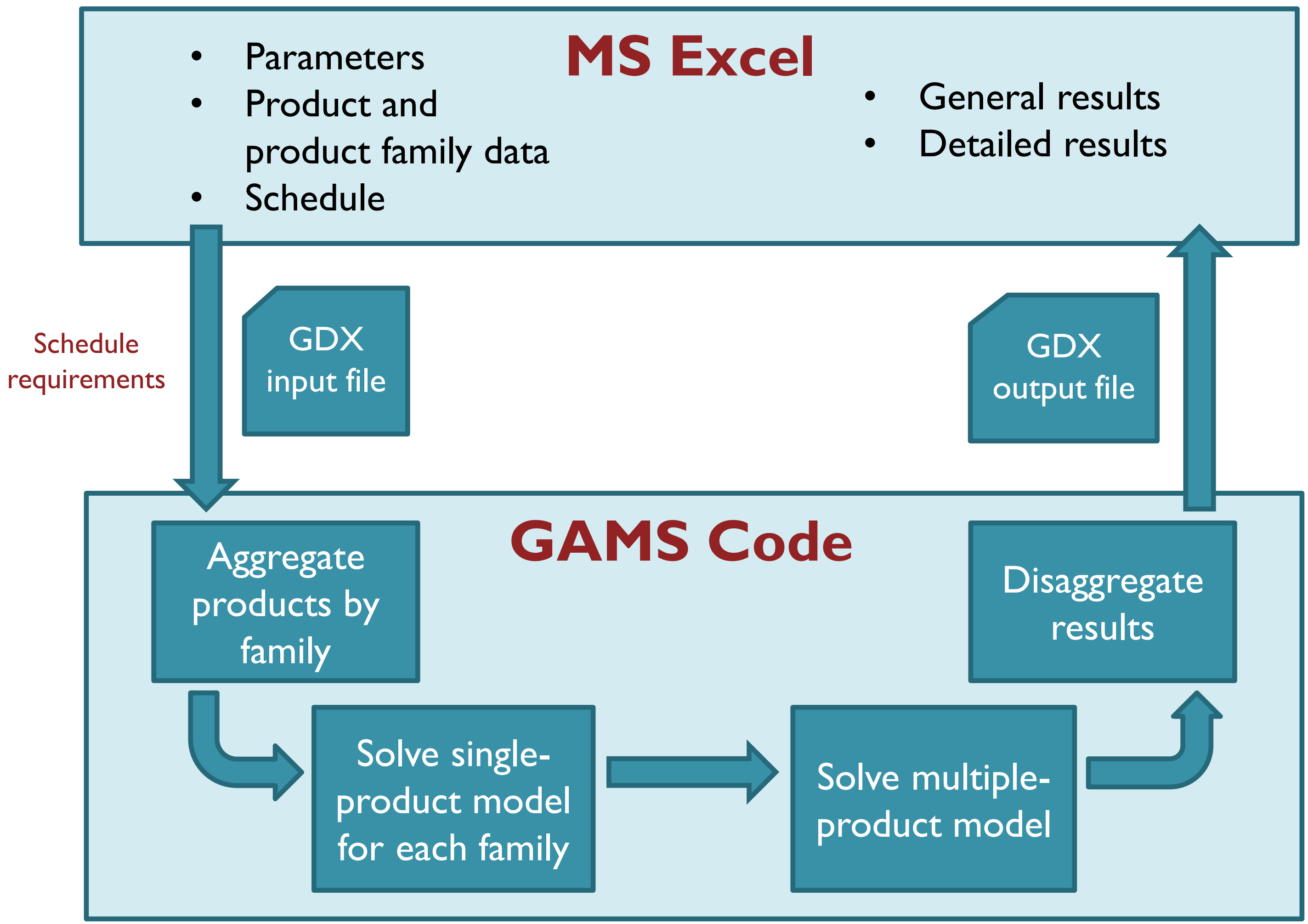

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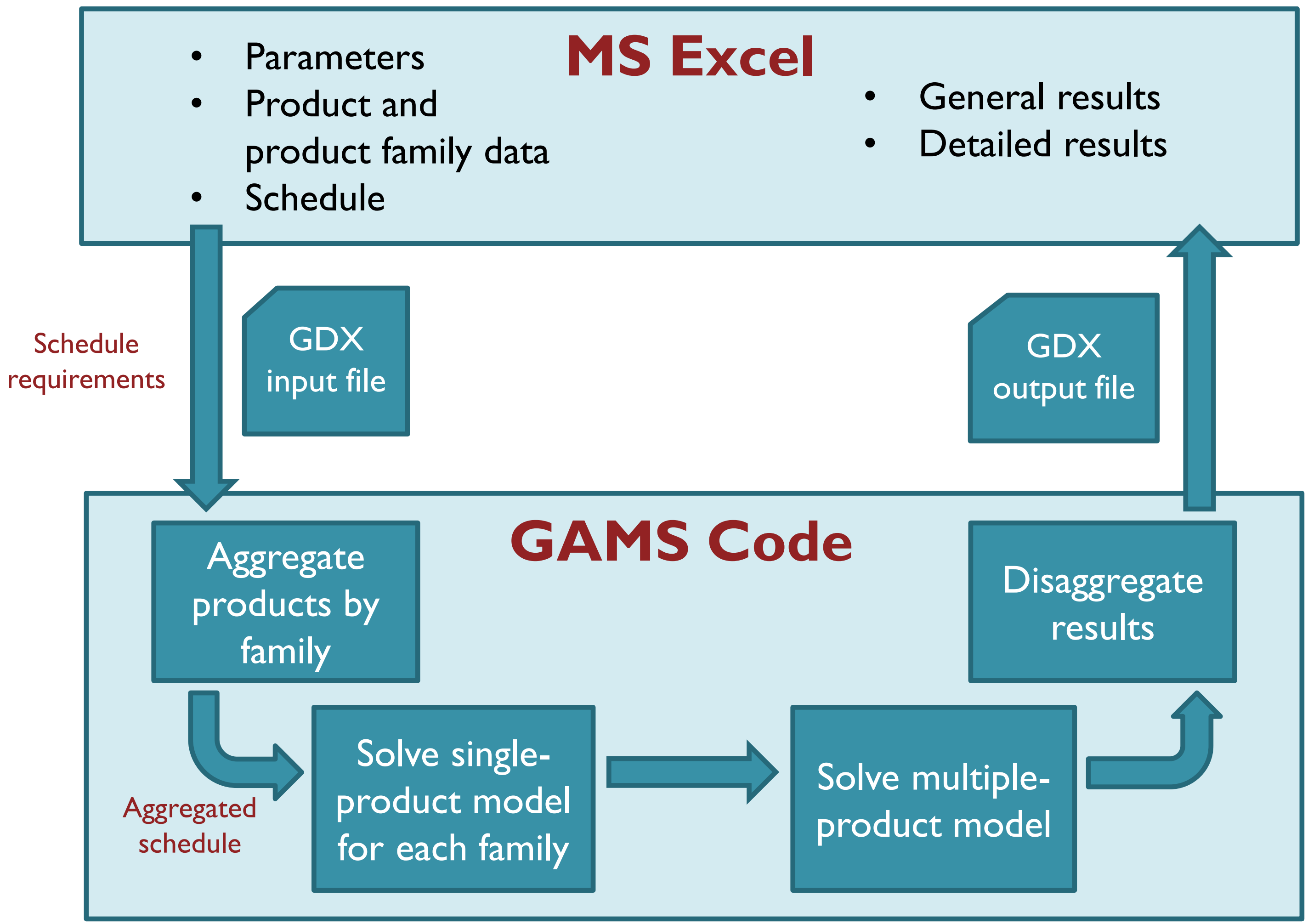

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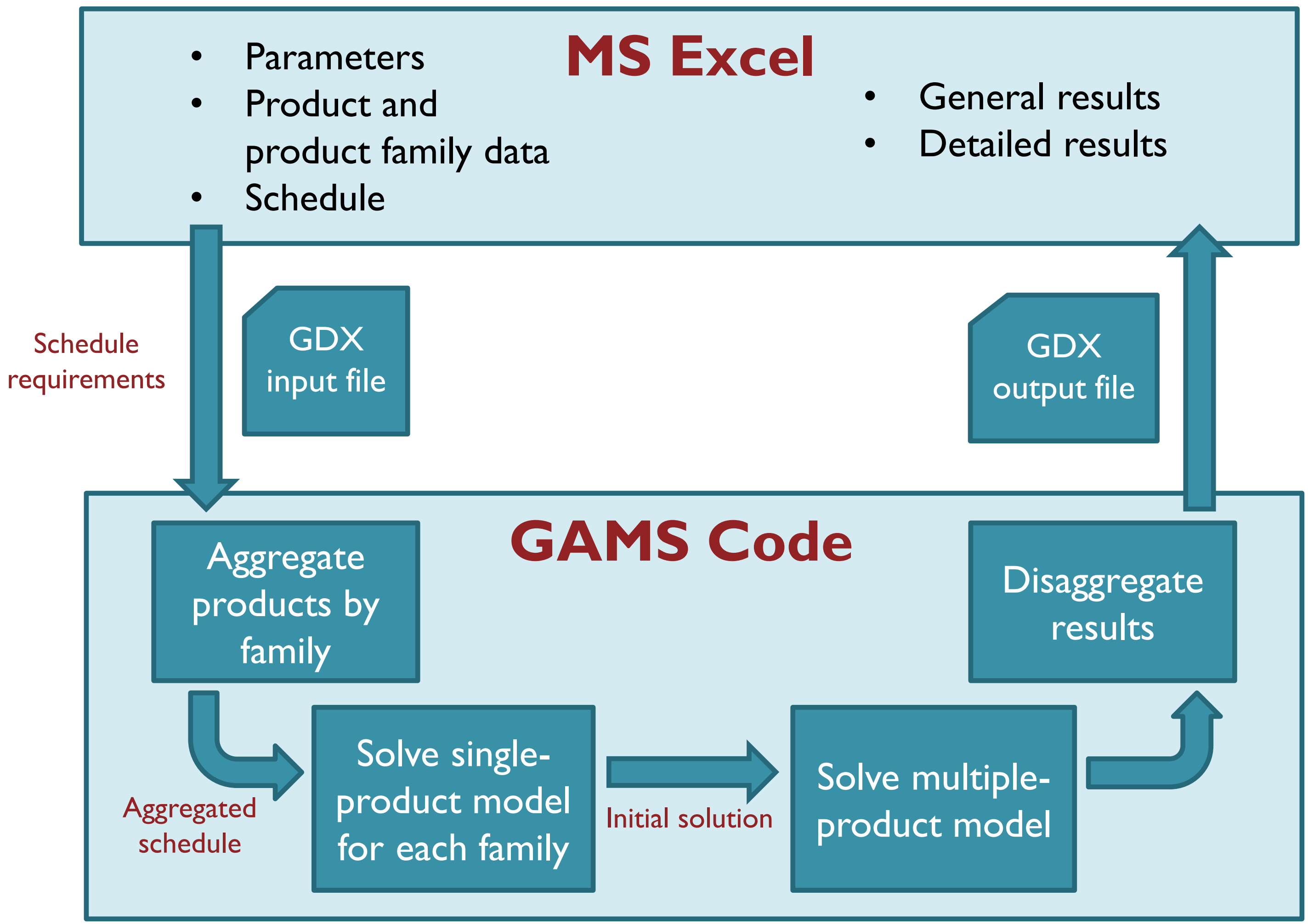

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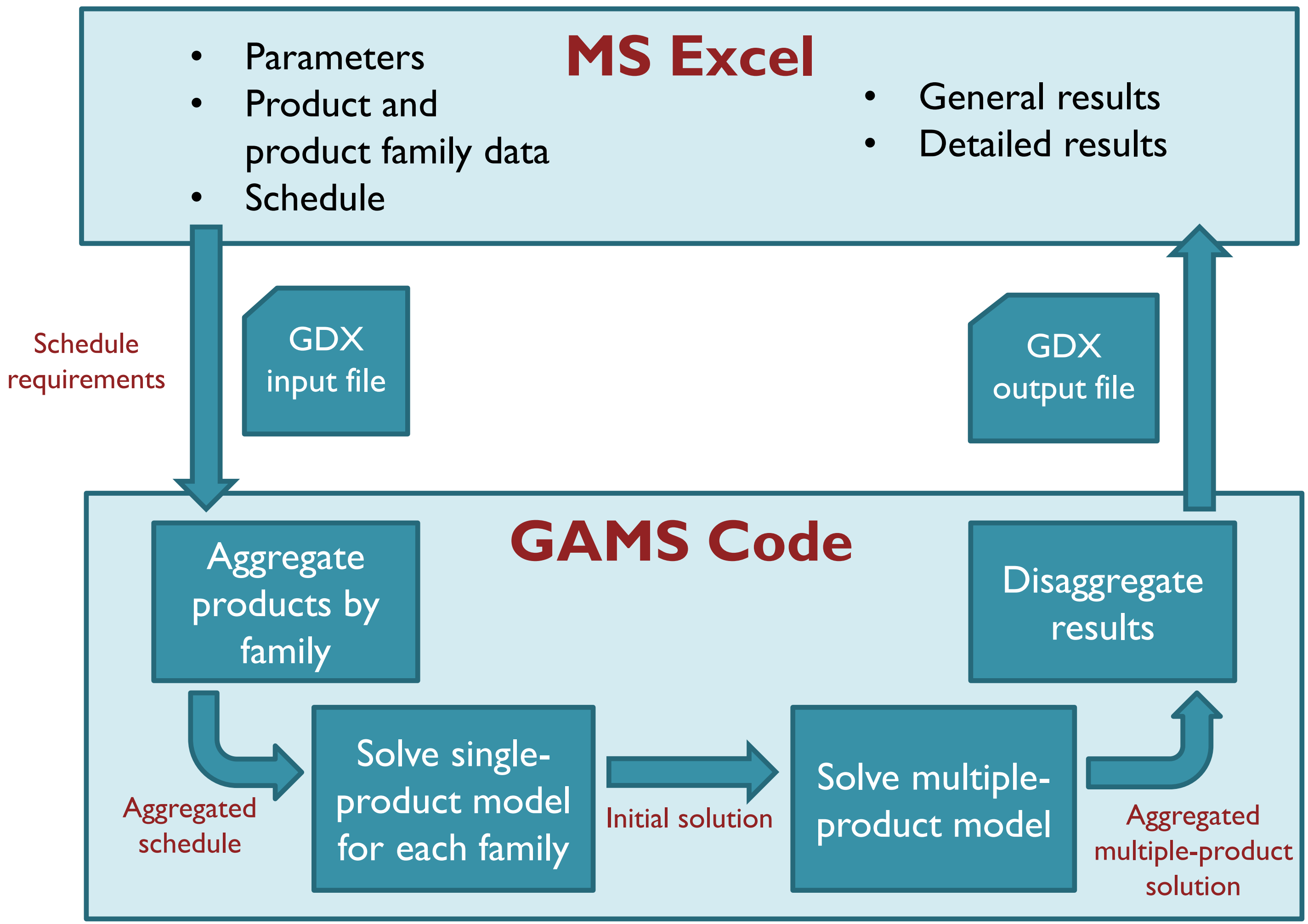

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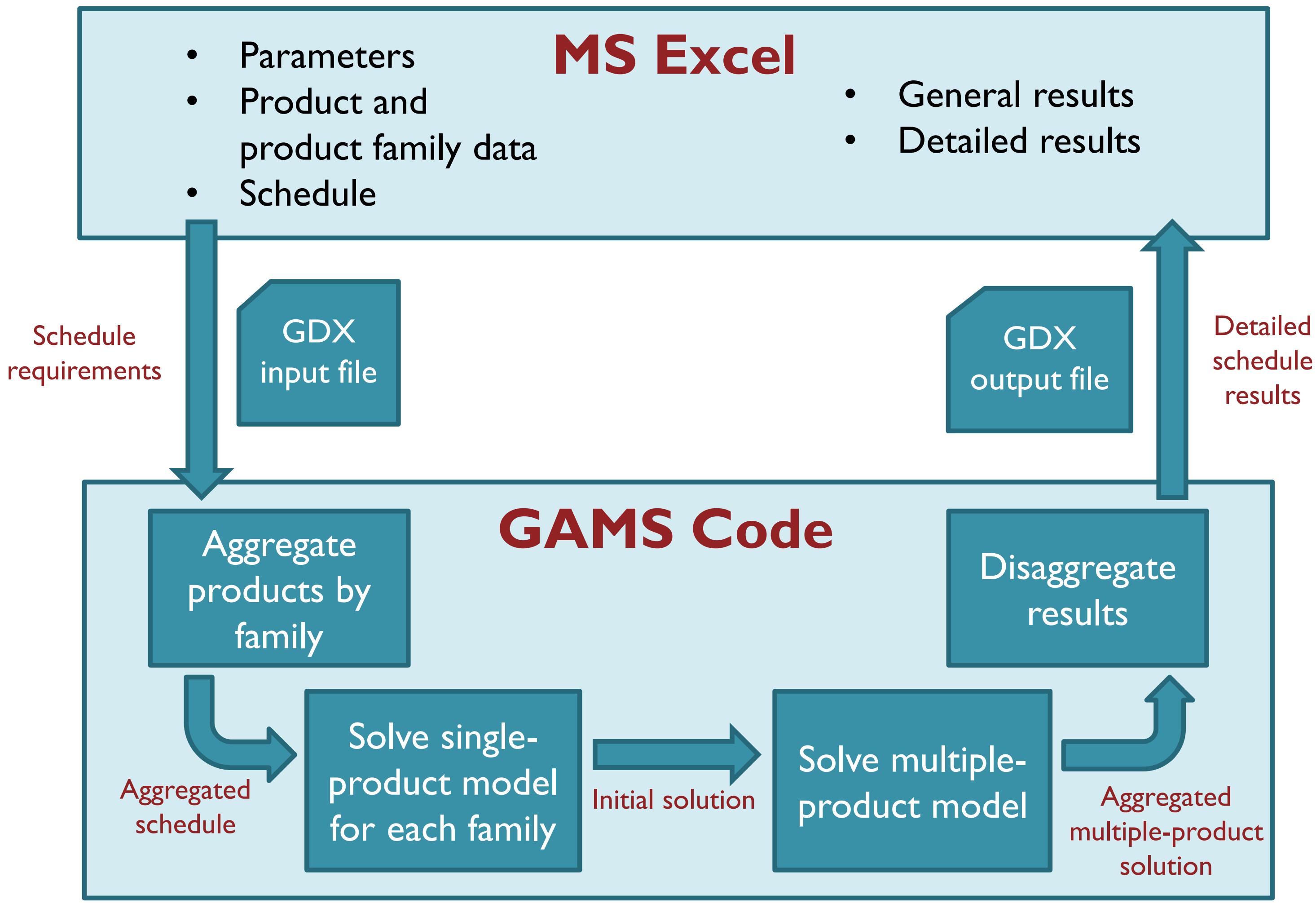

User Interface via Excel Worksheet

Screenshots

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Braskem America - Neal Plant

Feedstock Optimization Model

Schedule Data | Schedule Results | 17-Jun, 08:30 AM

Order	Product	# Cars	Start Time	Duration	Production Rate	Profit
			(date & time)	(hs)	(lbs/hr)	($)
1	#####	10	dd-mmm, hh:mm	##.##	##,###.##	###,###.##
2	######	10	dd-mmm, hh:mm	##.##	##,###.##	###,###.##
3	######	34	dd-mmm, hh:mm	###.##	##,###.##	###,###.##
4	####	2	dd-mmm, hh:mm	#.##	##,###.##	##,###.##
5	#######	8	dd-mmm, hh:mm	##.##	##,###.##	##,###.##
6	####	2	dd-mmm, hh:mm	#.##	##,###.##	##,###.##
7	######	30	dd-mmm, hh:mm	##.##	##,###.##	###,###.##
8	####	2	dd-mmm, hh:mm	#.##	##,###.##	##,###.##
9	#######	14	dd-mmm, hh:mm	##.##	##,###.##	###,###.##
10	######	10	dd-mmm, hh:mm	##.##	##,###.##	###,###.##
11	#######	4	dd-mmm, hh:mm	##.##	##,###.##	##,###.##
12	####	2	dd-mmm, hh:mm	#.##	##,###.##	##,###.##
13	#####	12	dd-mmm, hh:mm	##.##	##,###.##	###,###.##
14	#######	7	dd-mmm, hh:mm	##.##	##,###.##	##,###.##

Time Horizon: 50 days

Add SLACK Product ☑

Run Feedstock Model

Update Results

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2	######	10	dd-mmm, hh:mm	##.##	##,###.##	###,###.##
3	######	34	dd-mmm, hh:mm	###.##	##,###.##	###,###.##
4	####	2	dd-mmm, hh:mm	#.##	##,###.##	##,###.##
5	#######	8	dd-mmm, hh:mm	##.##	##,###.##	##,###.##
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7	######	30	dd-mmm, hh:mm	##.##	##,###.##	###,###.##
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Mutiple-product Feedstock Model - Detailed Results

Time Horizon = 50 days

TIME SLOTS	1	2	3	4	5	6	7
Production Requirements							
Product	######	#######	#######	#####	#######	####	######
Product Family	####	####	####	####	####	####	####
# Cars	10	10	34	2	8	2	30
Results Summary							
Production rate (lb/hr)	##,###	##,###	##,###	##,###	##,###	##,###	##,###
Time (hr)	##.##	##.##	###.##	#.##	##.##	#.##	##.##
Lbs of product	#,###,###	#,###,###	#,###,###	###,###	#,###,###	###,###	#,###,###
Refinery Grade							
% propane	##.####	##.####	##.####	##.####	##.####	##.####	##.####
% propylene	##.####	##.####	##.####	##.####	##.####	##.####	##.####
lbs/hr	##,###	##,###	##,###	##,###	##,###	##,###	##,###
lbs/hr propane	#,###	#,###	#,###	#,###	#,###	#,###	#,###
lbs/hr propylene	##,###	##,###	##,###	##,###	##,###	##,###	##,###
Chemical Grade							
% propane	##.####	##.####	##.####	##.####	##.####	##.####	##.####
% propylene	##.####	##.####	##.####	##.####	##.####	##.####	##.####

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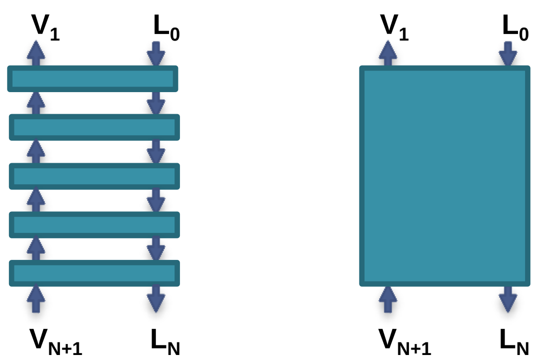
Aggregated group-method of Kamath et al. (2010)

- **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

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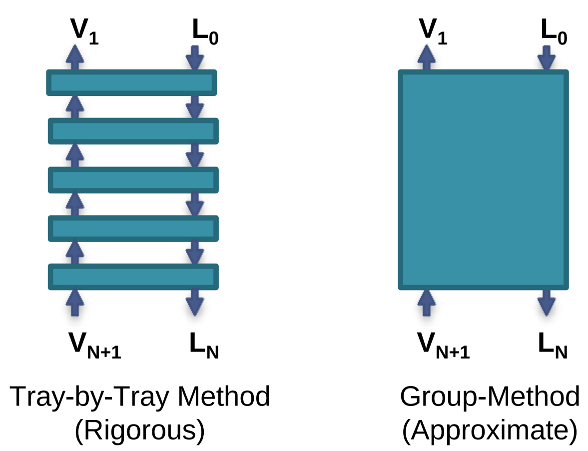
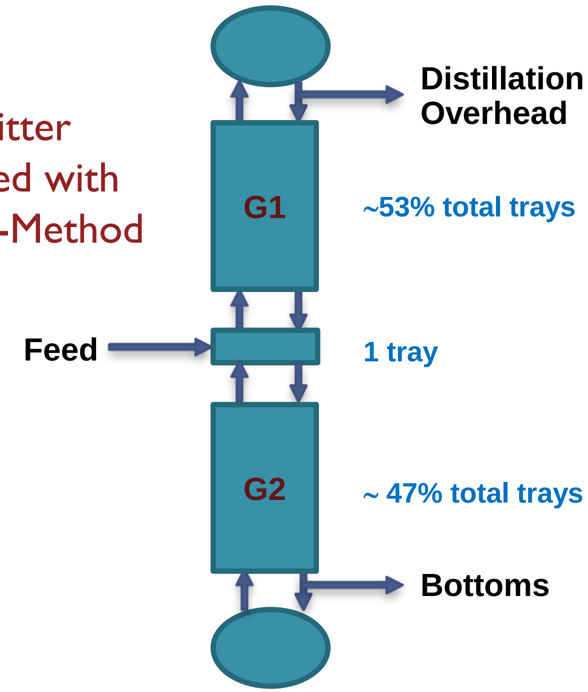


C3 Splitter modeled with Group-Method



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

Additional Assumptions
- **Fixed pressure for the whole column = 9.778 atm**
- **Total condenser (top)**
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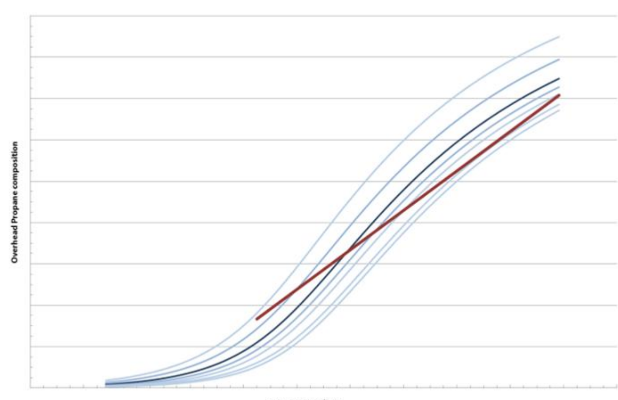
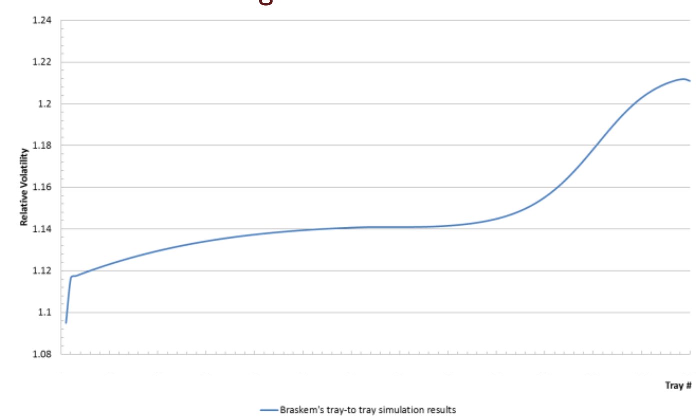
Parameterization and Validation

- 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

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- Single and multiple-product feedstock optimization models including distillation and polymerization processes.
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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.