Operational Model for C3 Feedstock Optimization on a Polypropylene Production Facility

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

marchet@andrew.cmu.edu

Wiley A. Bucey, Rita A. Majewski
Braskem America

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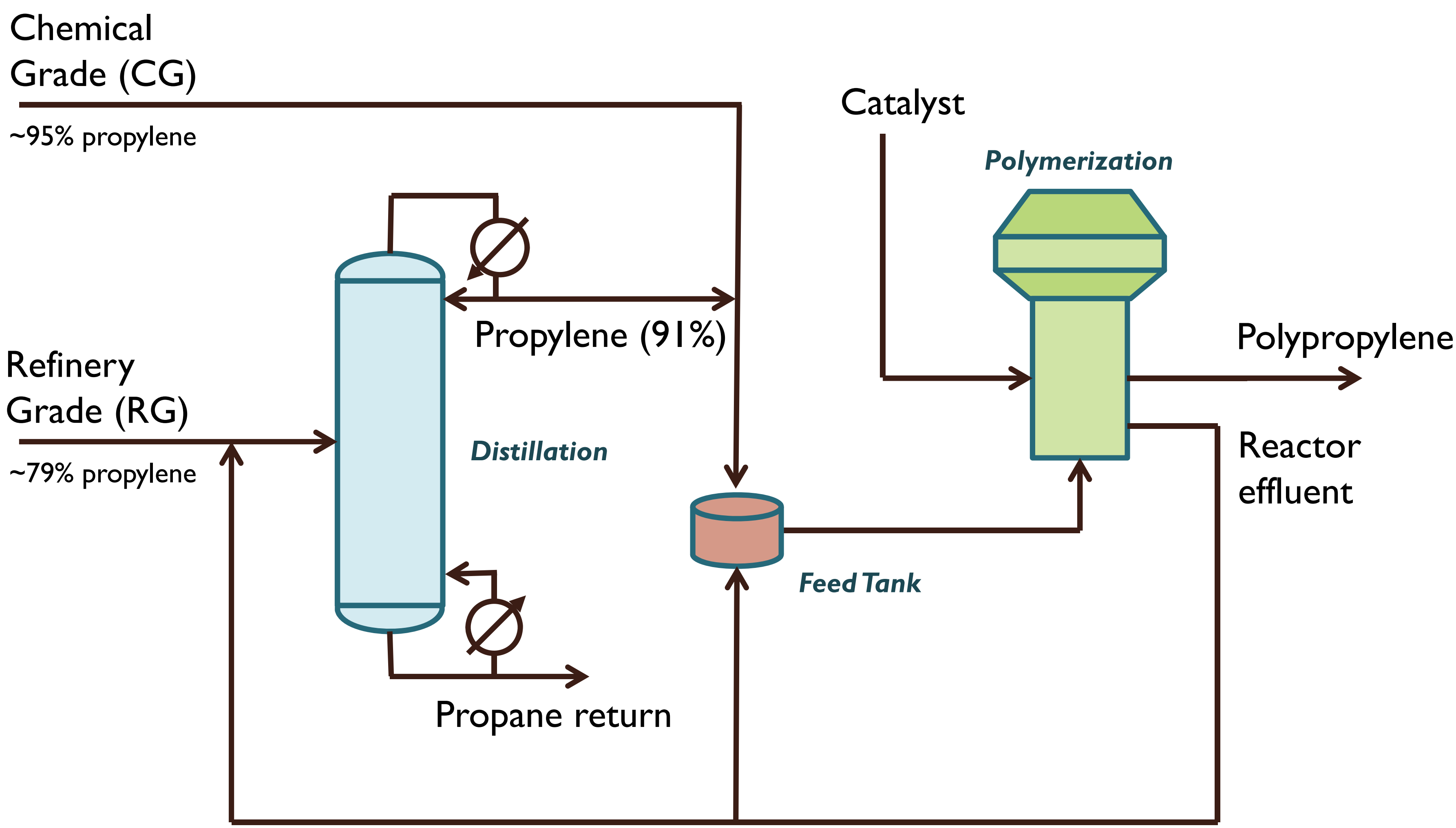
- Objectives:
  - Development of a Non-linear Programming (NLP) model to maximize benefits by obtaining a better balance of RG and CG feedstocks for single or multiple production orders.
  - Determine operation rates for a schedule of multiple production orders within a 3-month timeframe.
  - Implement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

Process and Problem Description



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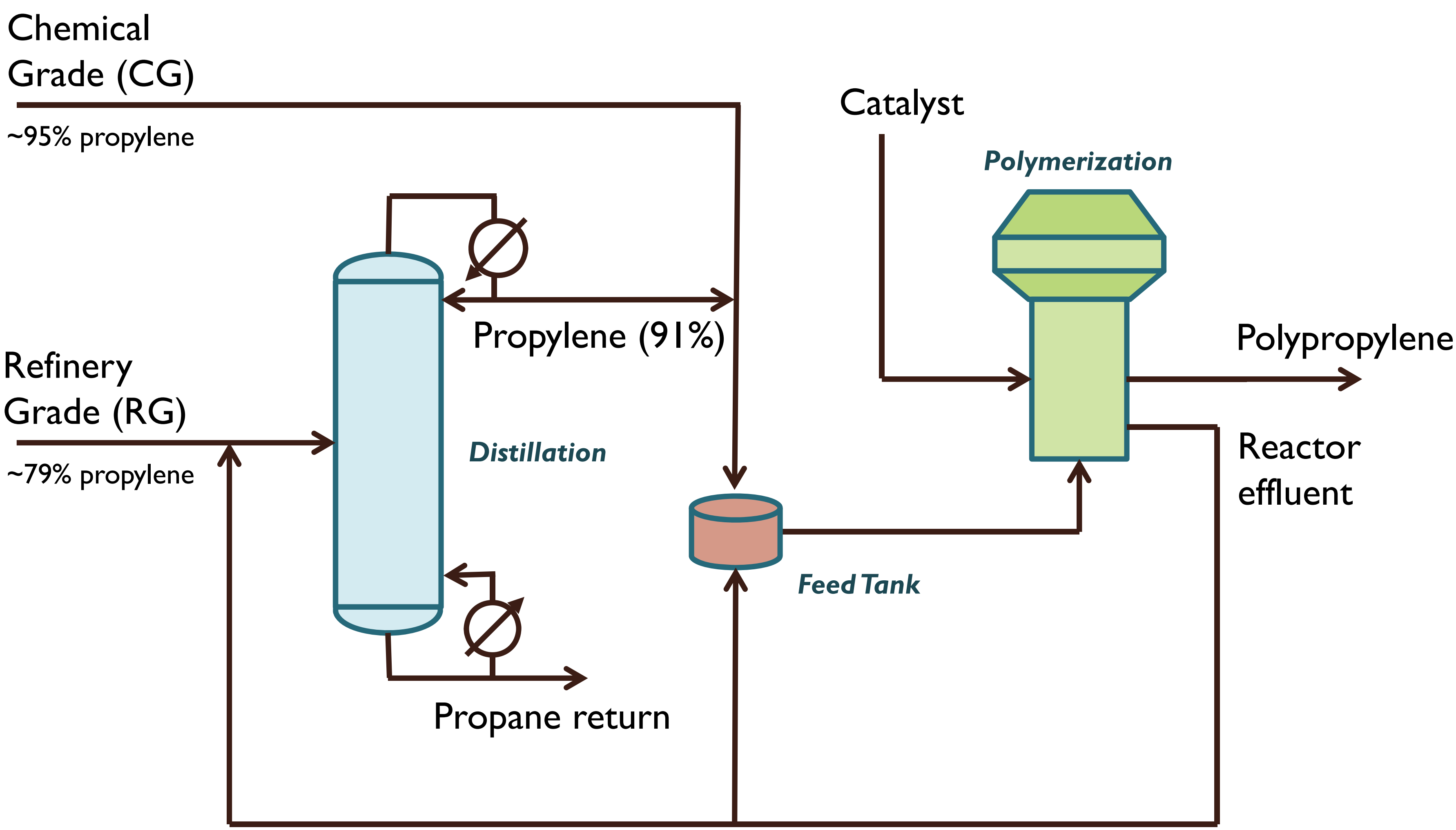

Maximizing the amount of RG may not be the best economic option

Mathematical Model (NLP)

- 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

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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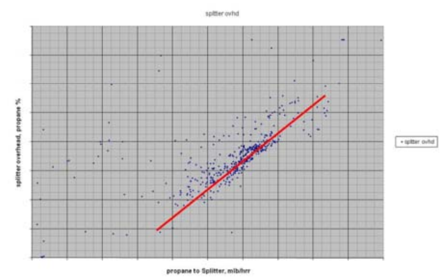
Models Implemented with GAMS

Improvements on Distillation Model

Current model is based on a linear correlation obtained from plant data, relating the overhead composition of propane with flowrate of propane feed to the splitter.



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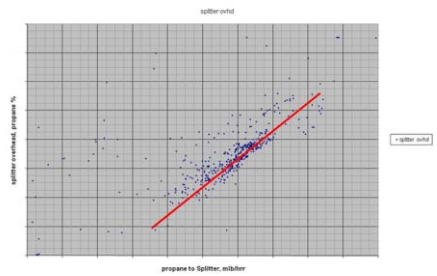

Goal

- **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 (Aspen)**

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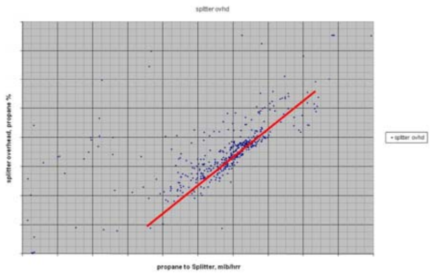

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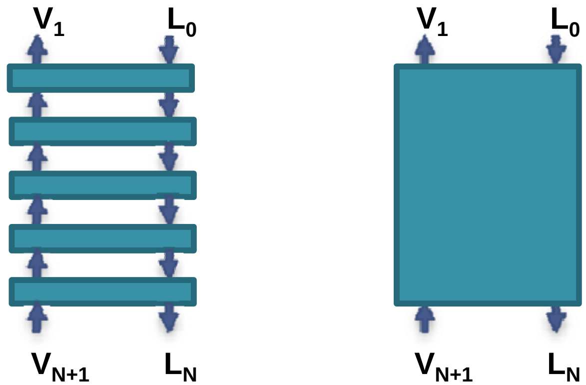
Aggregated group-method of Kamath et al. (2010)

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



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

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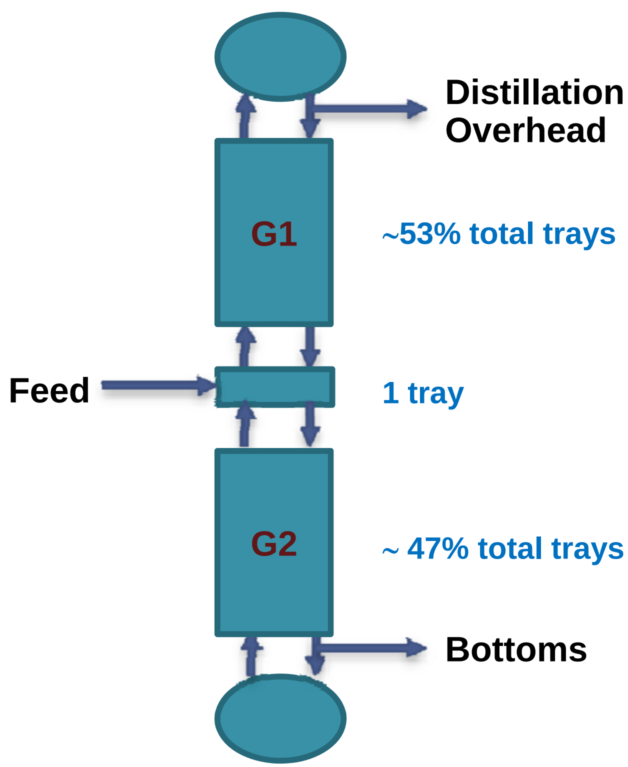
C3 Splitter modeled with Group-Method



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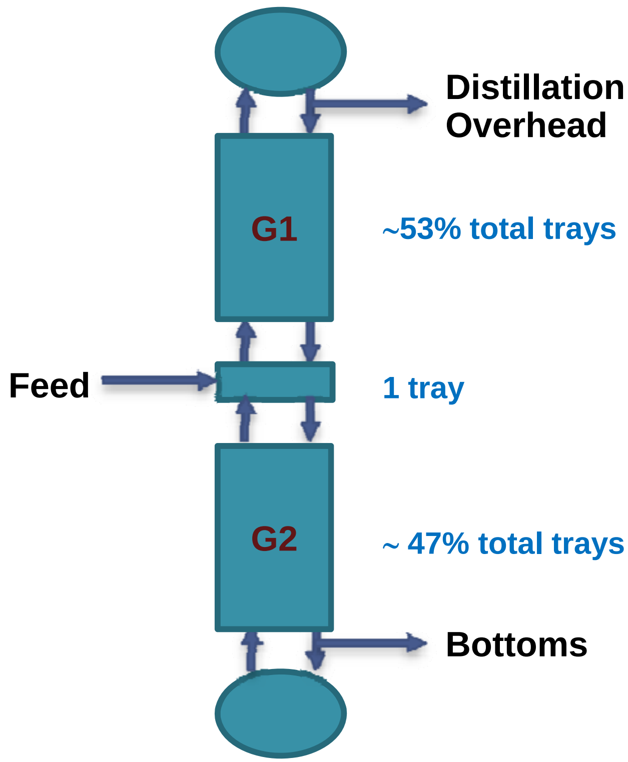

Degrees of freedom:

- **Reflux rate**
- **Bottoms composition**

Additional Assumptions

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

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Parameterization and Validation (Work in Progress)

- Comparison of results obtained by the Aggregated Group-Methods against rigorous tray-to-tray simulations (Aspen) and plant data.

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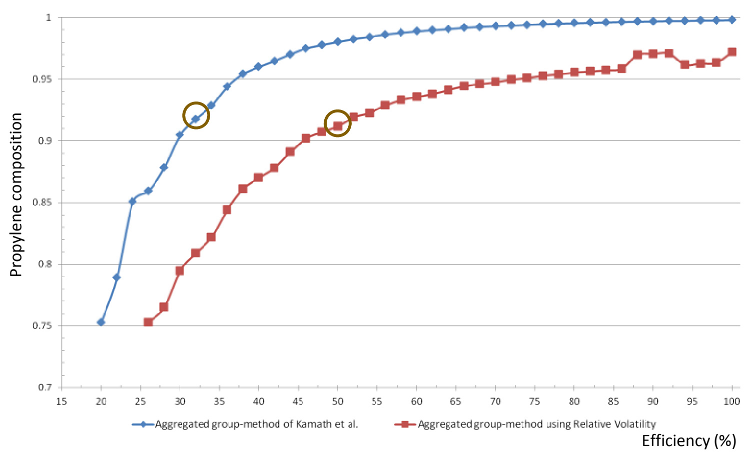
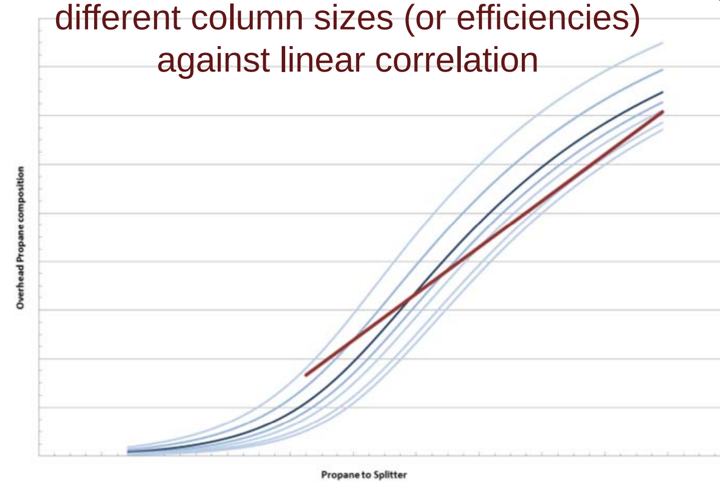
Propylene composition in distillation overhead for different column efficiencies

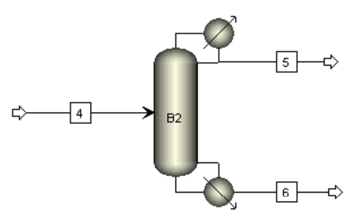


Modified Group-Method - comparison of different column sizes (or efficiencies) against linear correlation

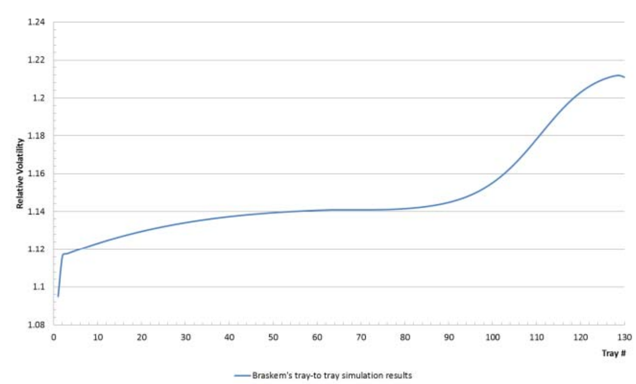
α = 1.1645



Aspen Simulation Results



RadFrac component
Peng-Robinson thermodynamics



Tray-to-tray relative volatilities predicted by rigorous model

Integrated Model and User Interface

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Integration of Group-Method Distillation Model in General Flowsheet Model (Work in progress)

- The new distillation model is being integrated within the single and multiple-product models.
- Initial point for multiple-product model obtained by the solution of several single product models, one for each product.

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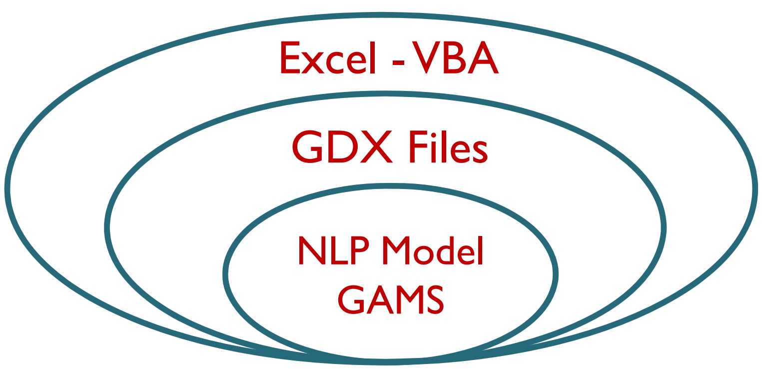
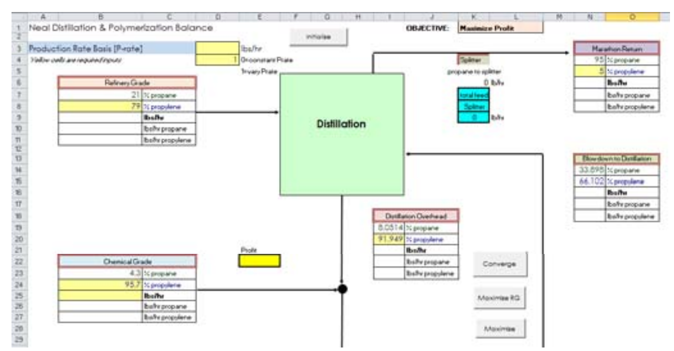
User Interface for GAMS model being developed in Excel

- Excel and VBA as a front-end
- Excel as User Interface (UI) to define input data
- Excel used to display results
- Flexibility to manipulate input data/output results (tables, graphics)





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- Integrated plant formulation developed including distillation and polymerization processes in a single model.
- Single and multiple-product models.
- Distillation model reformulated using aggregated group-methods (based on work of Kamath et al. 2010)
- Comparison with rigorous tray-to-tray simulation results (Aspen) and plant data to parameterize the models.
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FUTURE WORK

- Determine most accurate parameterization of aggregated group-methods to predict distillation column outputs
- Additional tests on larger problem instances
- Deployment of computational tool to assess monthly feedstock purchase decisions