Plant Design and Profitability Analysis for the Production of Ethyl Acetate from Renewable Ethanol Feedstock

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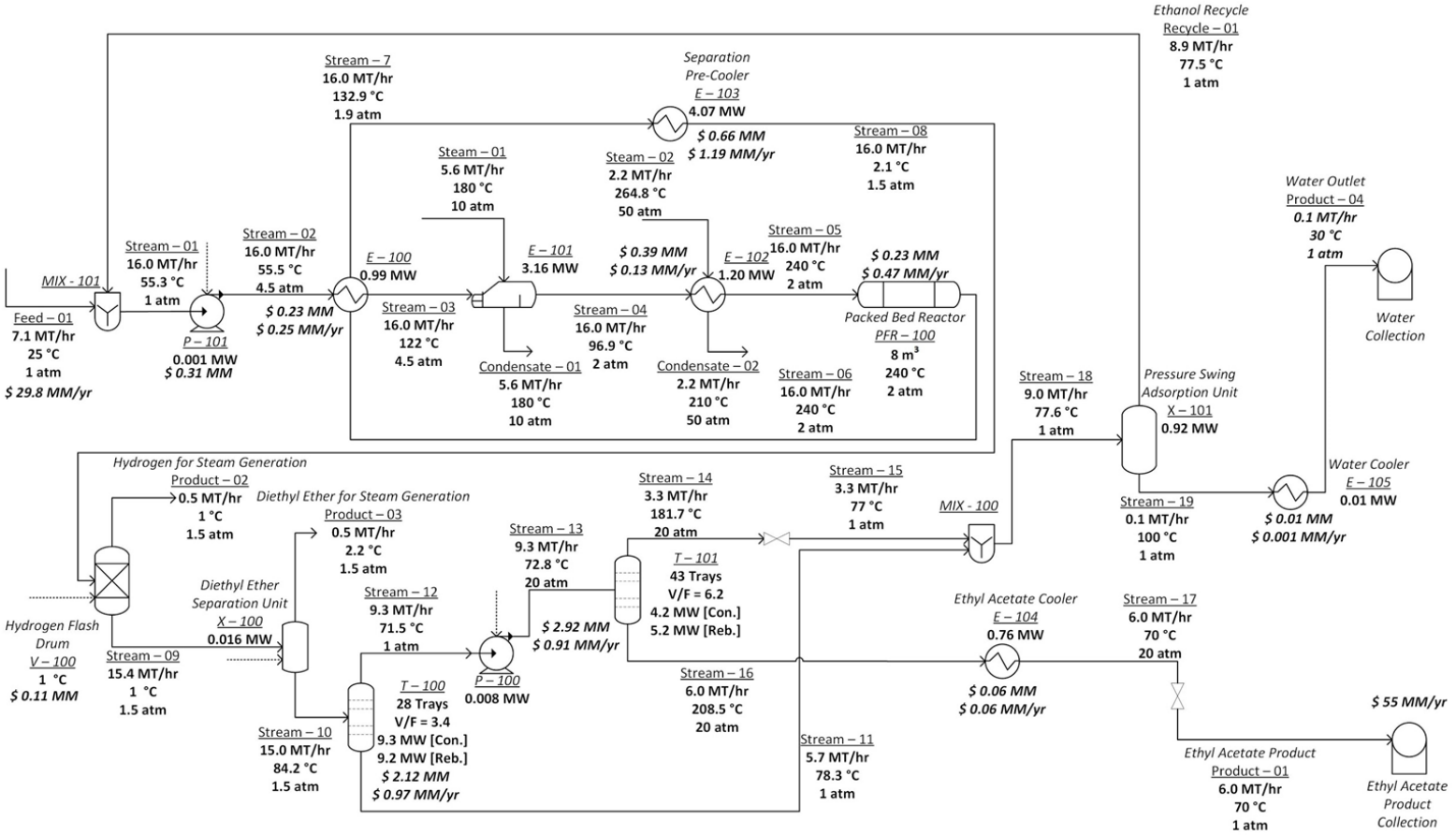
Introduction

- Global demand of 5 million MT of ethyl acetate per year with a 4.5% projected growth through 2025[1]
- Using oxygenated solvents derived from plant materials reduces CO_2 footprint of paints, inks, pharmaceuticals, and cosmetics

[1] *Ethyl Acetate Market Research 2019, Forecast, Trend, Growth,* Beroe Inc. (2019). https://www.beroeinc.com/category-intelligence/ethyl-acetate-market

- Produce 50 kta of ethyl acetate with a $35 MM total capital investment
- Corn-derived ethanol feedstock reacts over CuO, CoO, Cr_2O_3 catalyst
- $600/MT spread yields $14 MM profit before tax

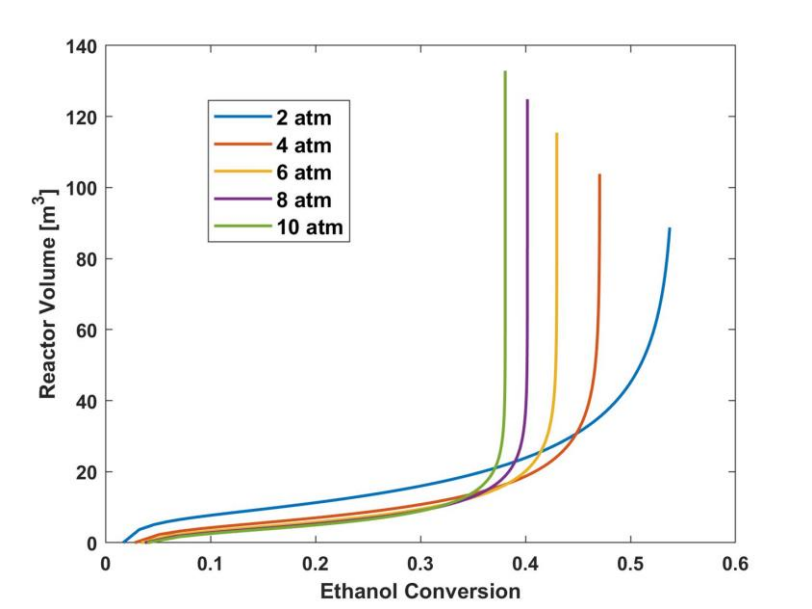
Substance	Price
Ethanol	$500/MT
Ethyl Acetate	$1,100/MT
Diethyl Ether	Fuel Value only
Hydrogen	Fuel Value only
Fuel	$2.50/MM BTU
Catalyst	$10,000/MT
CO2 Charge	$40/MT



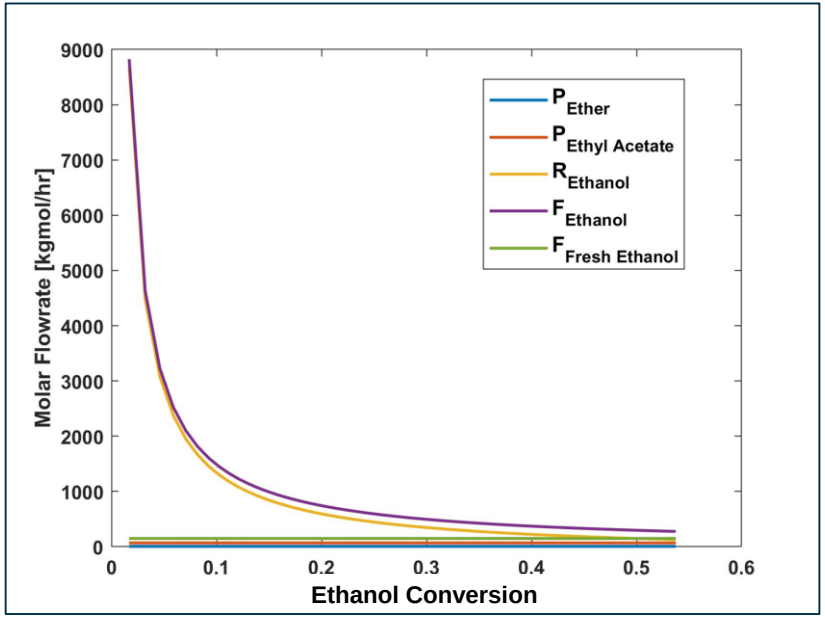
Conceptual Design Process Flow Diagram

Conceptual Design

Reactor Volume vs. Conversion at 240 °C

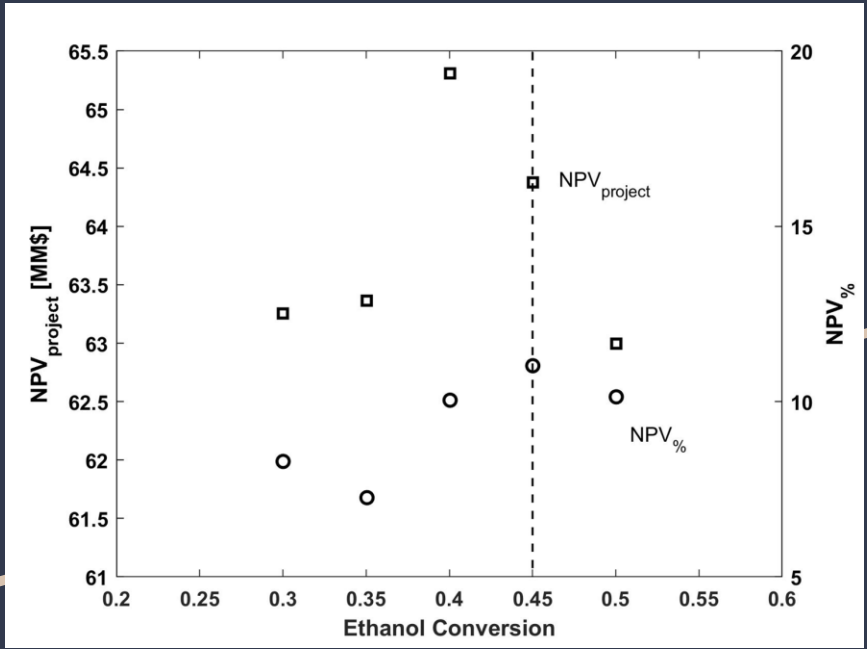


Molar Flow Rates



Conceptual Design

MATLAB simulation and optimization



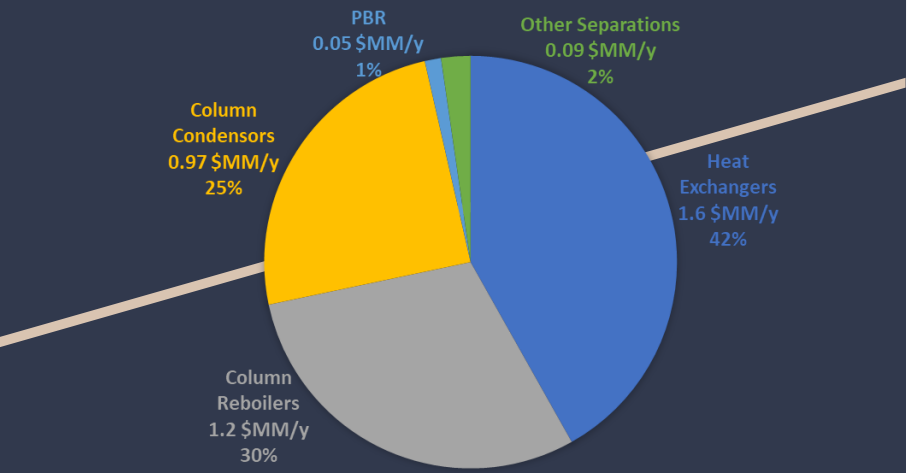
- MATLAB used to simulate and optimize $NPV_{\%}$
- Discrete simulations for 5 values of conversion at the chosen operating conditions
- Parameters Chosen:
  - $X_T = 0.45$
  - T = 240 ℃
  - P = 2 atm
- Economic indicators measured:
  - $NPV_{Project}$, $NPV_{\%}$, ROI_{BT}, IRR

Base-Case Economic Analysis

Non-Discounted

- ROI_{BT} = 41%
- TCI = $35 MM
- P_{BT} = $14 MM

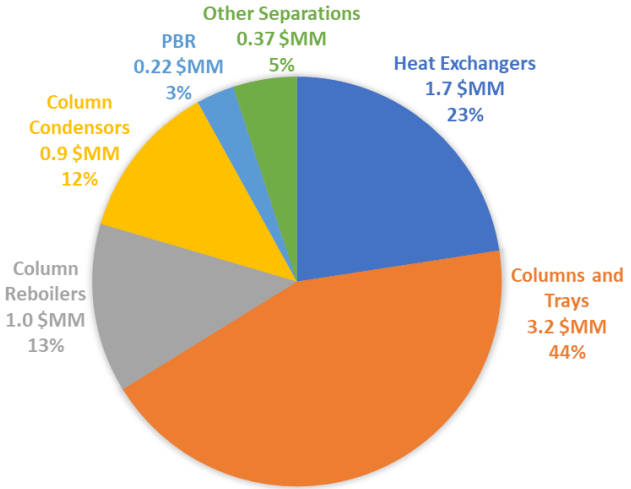
Operating Costs



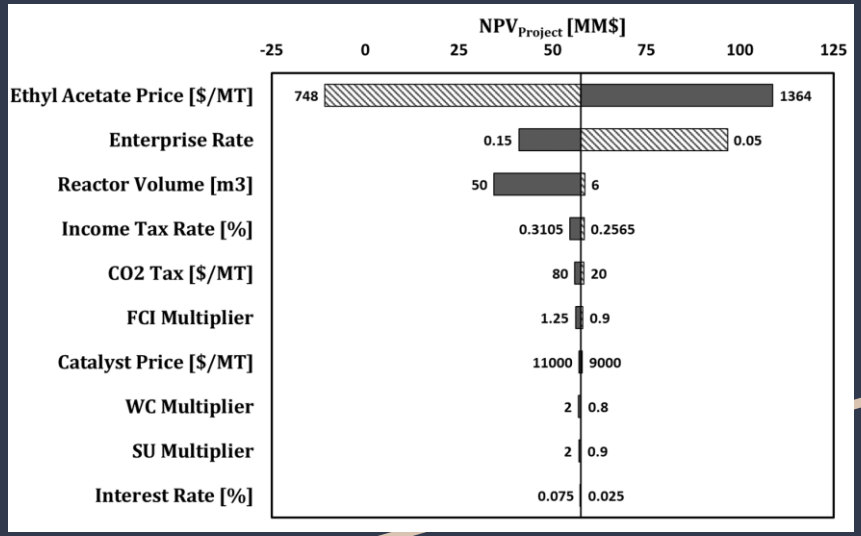
Discounted

- $NPV_{Project}$ = $51 MM
- $NPV_{\%}$ = 9%
- IRR = 23%

Capital Costs



Sensitivity Analysis



- TCI can increase to $97M or ethyl acetate price can decrease to $920/MT and remain profitable
- Plant could be shut down for up to 6 years and still remain profitable
- Monte Carlo simulations show <2% probability of having negative NPV with normal fluctuations

Health, Safety, & Environmental Concerns

- All chemicals except water are highly flammable
- Lowest auto-ignition temperature is 175 °C
- All flash points at or below 13 °C

- Reactor inlet temperature needs an emergency cooling system
- Pressure relief valves should be installed on distillation columns
- Equipment should be made from stainless steel to reduce hydrogen embrittlement and ethanol corrosion

Future Experiments

- Ensure kinetics are accurate at this scale
  - Profitability is very sensitive to reactor size
- Verify fluid models
  - Separations design is very sensitive to the model used

Process Alternatives

- Reactive distillation
  - Can simplify breaking azeotropes/ concentrate ethyl acetate stream sooner
- Diethyl ether extraction
  - liquid-liquid extraction
- Nickel-plated equipment
  - Greater longevity at higher upfront cost

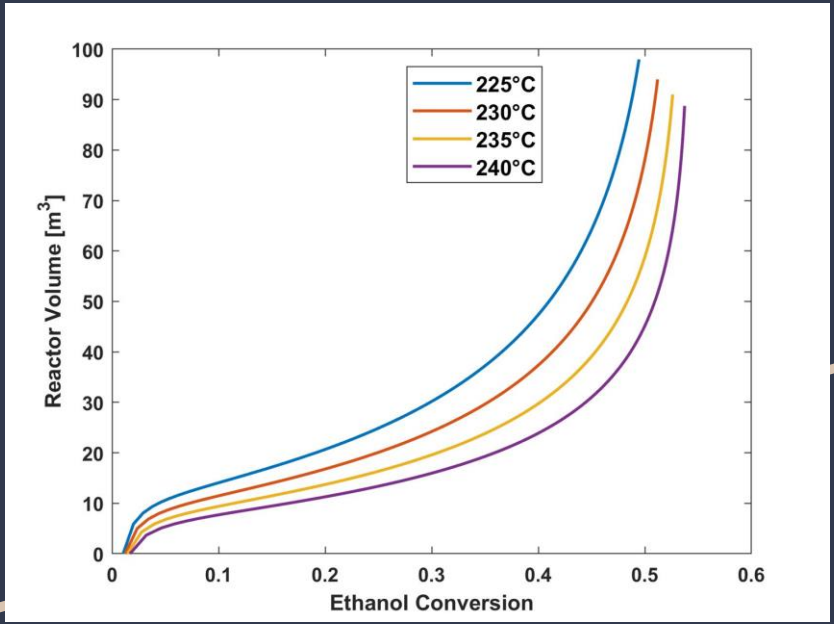
Conclusions

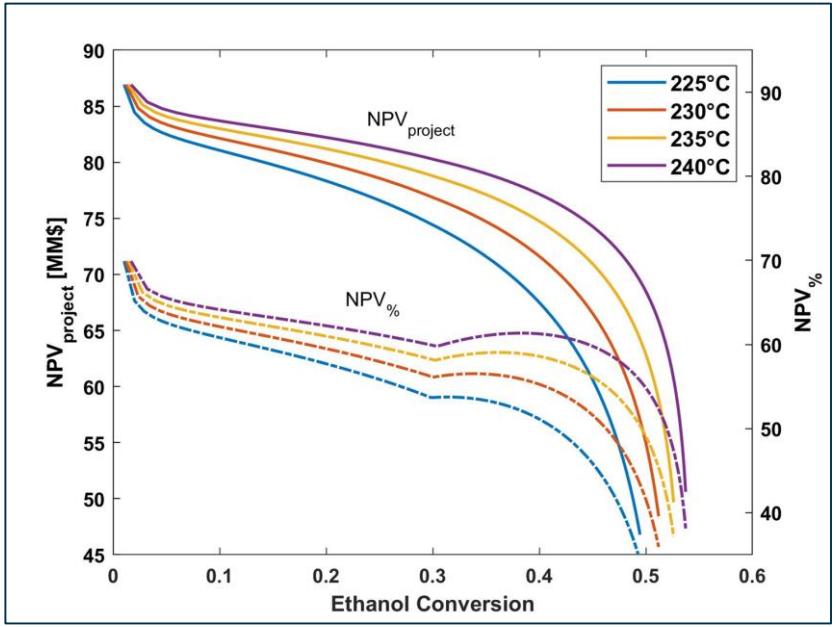
- Design focused on $NPV_{\%}$
- Level 4 plant design is profitable given the high spread between ethanol and ethyl acetate

- TCI = $35 MM
- NPV = $51 MM
- $NPV_{\%}$ = 9%

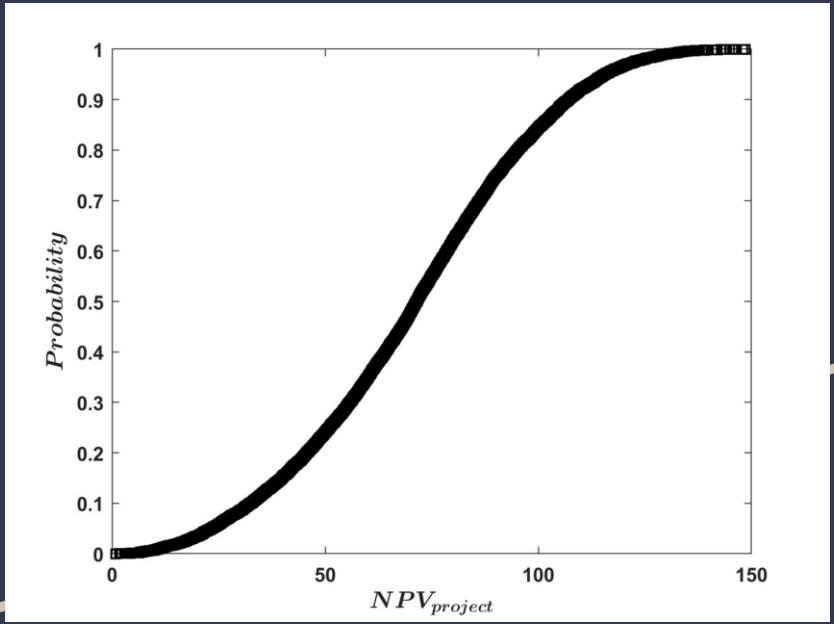
Questions?

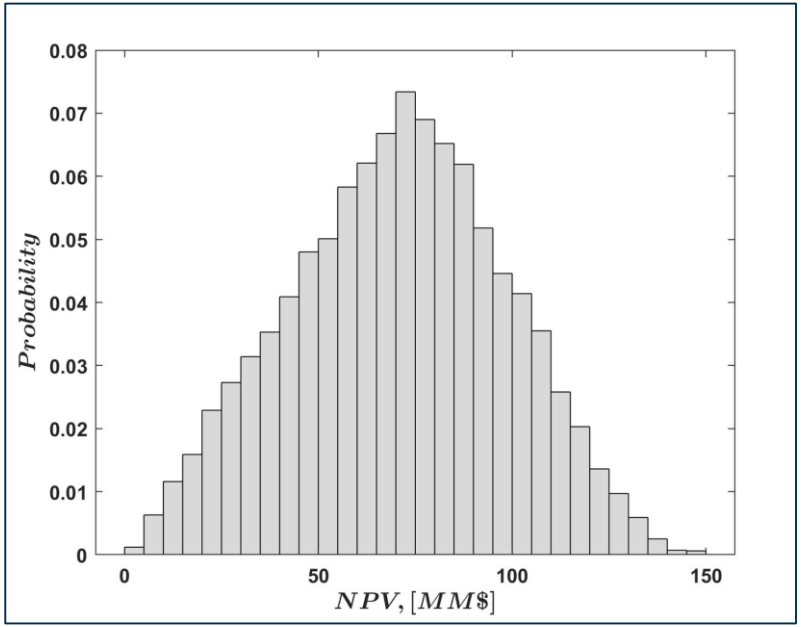
Appendices
Appendix A: Figures





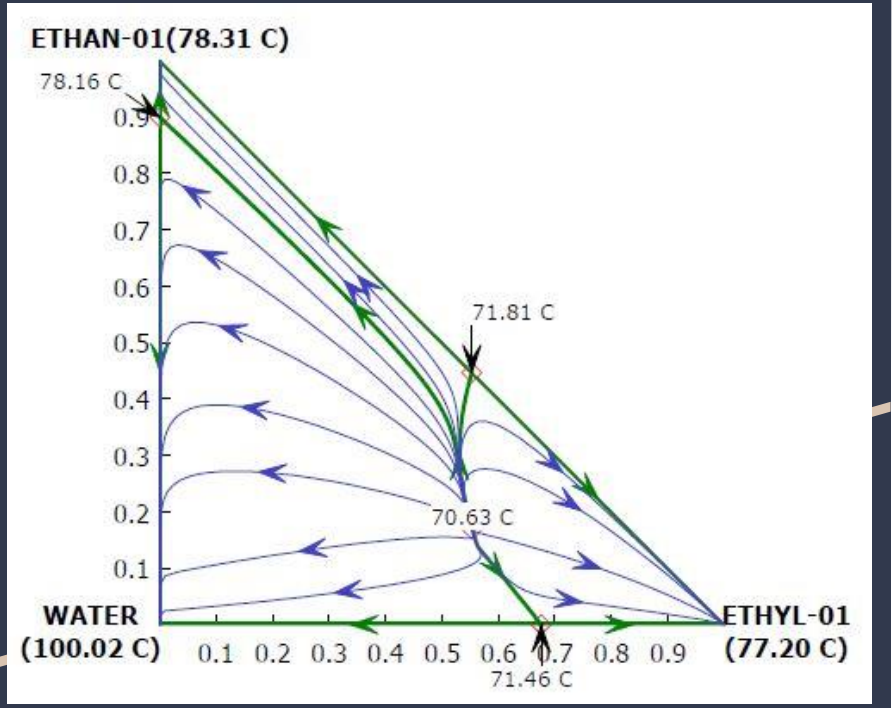
Appendices
Appendix A: Figures



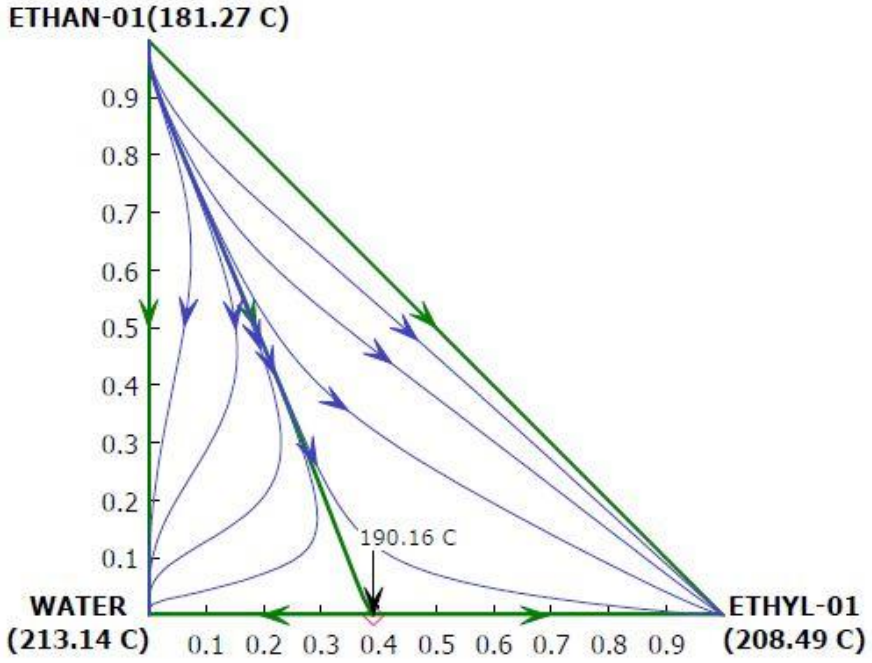


Distillation System

Aspen Plus



1 atm



20 atm

Appendices
Appendix B: Aspen HYSYS Simulation