Bi-Weekly Report 2

Team number: 1

Team members:

Anas Ali (220137)

Ansh Sethi (220167)

Aryan Jadon (220223)

Jatin Madan (220475)

Lokesh Yadav (220594)

Madhav Lata (220597)

Pratyush Gupta (220813)

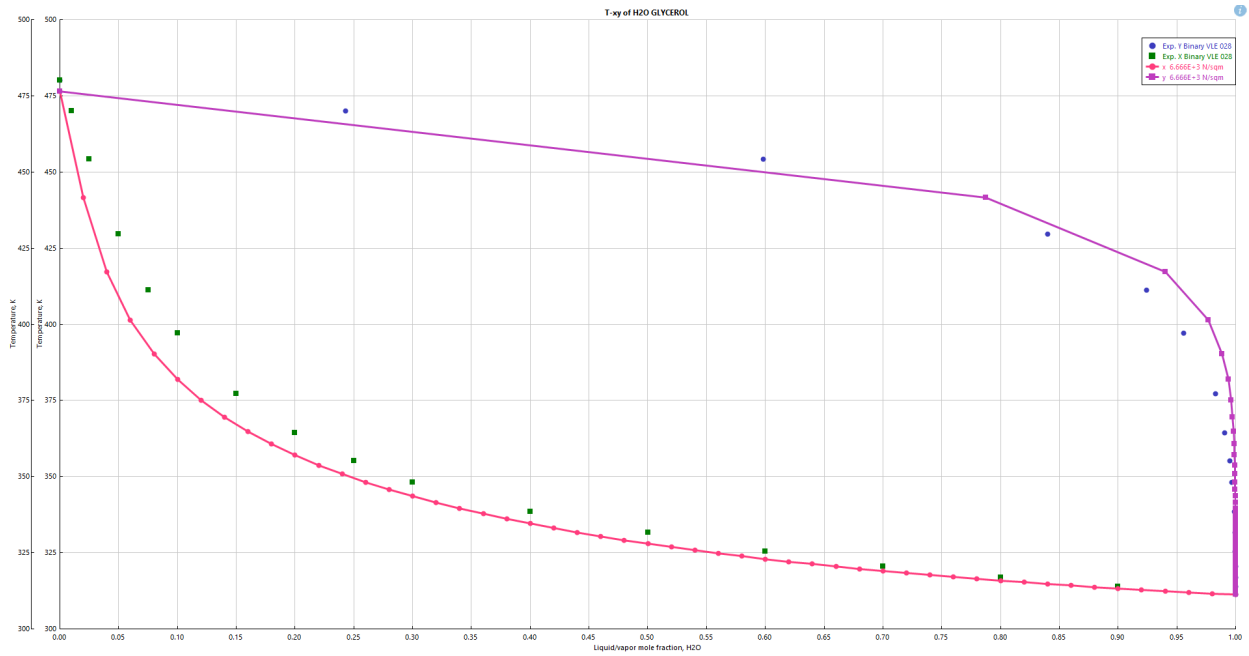
Punam Singh (220835)

Objectives

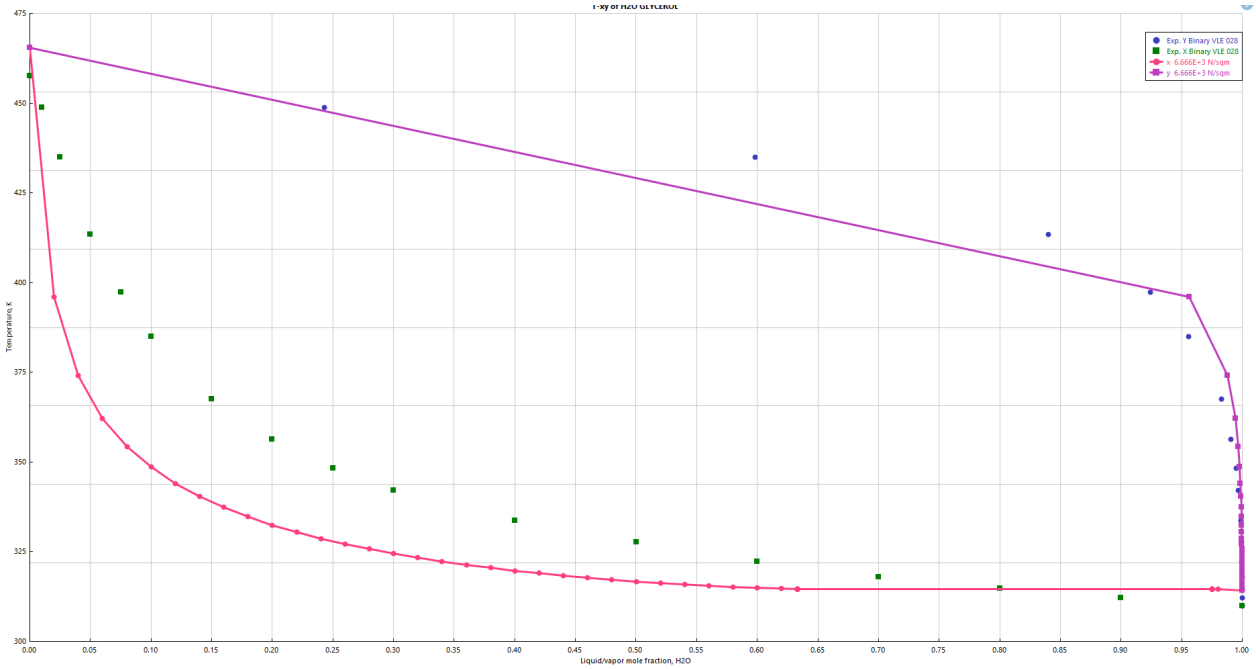
This report focuses on analyzing thermodynamic and physical properties to determine operating conditions. It also aims to synthesize the process and develop a process flow diagram. A comprehensive flowsheet simulation is carried out using Aspen Plus, incorporating material and energy balances to evaluate process performance based on defined specifications. Additionally, improvements have been made by incorporating feedback received on the previous lab report.

Thermodynamic Model Selection and Regression

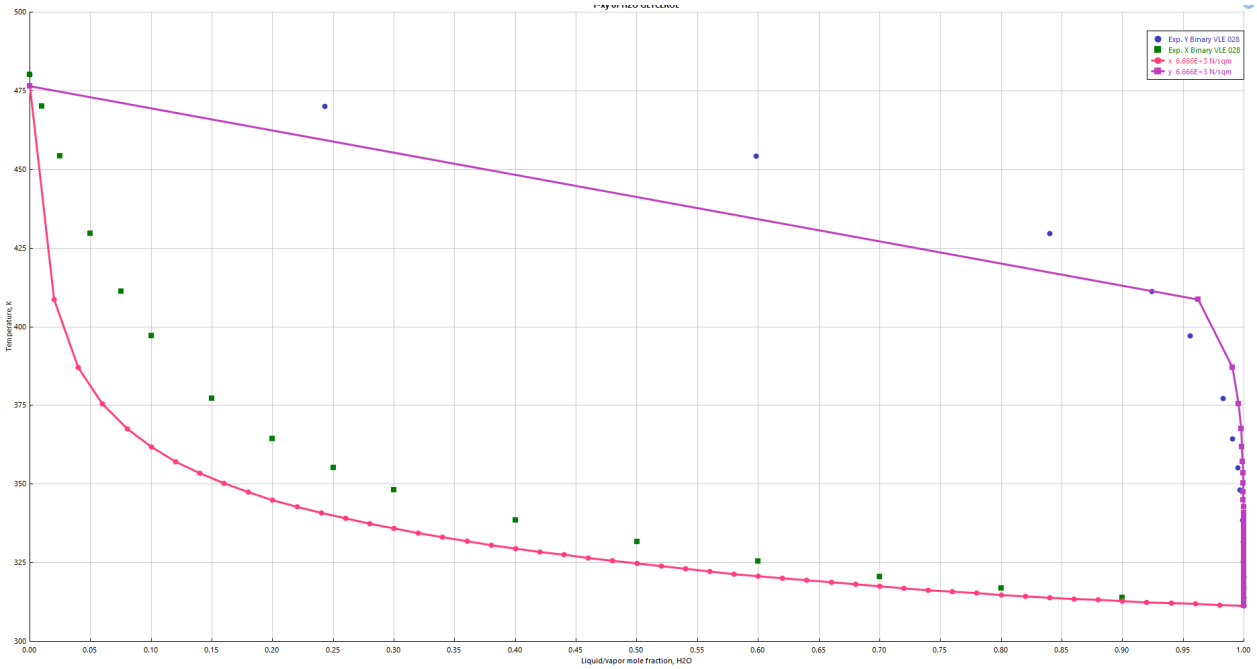
Several thermodynamic models were considered, including NRTL, Peng-Robinson, UNIFAC and UNIQUAC. After evaluation, UNIQUAC was selected for its suitability in handling the highly non-ideal behavior of glycerol–water mixtures. Regression was performed using experimental VLE data to obtain model parameters.



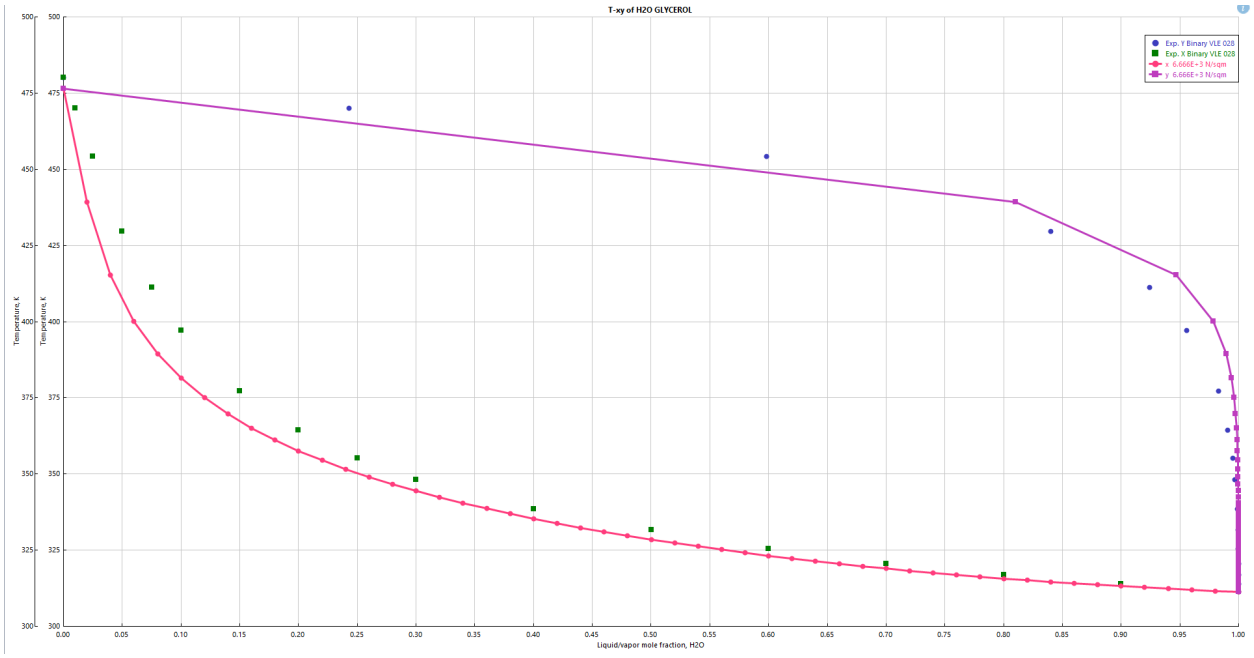
T-xy of H_2O, Glycerol using NRTL



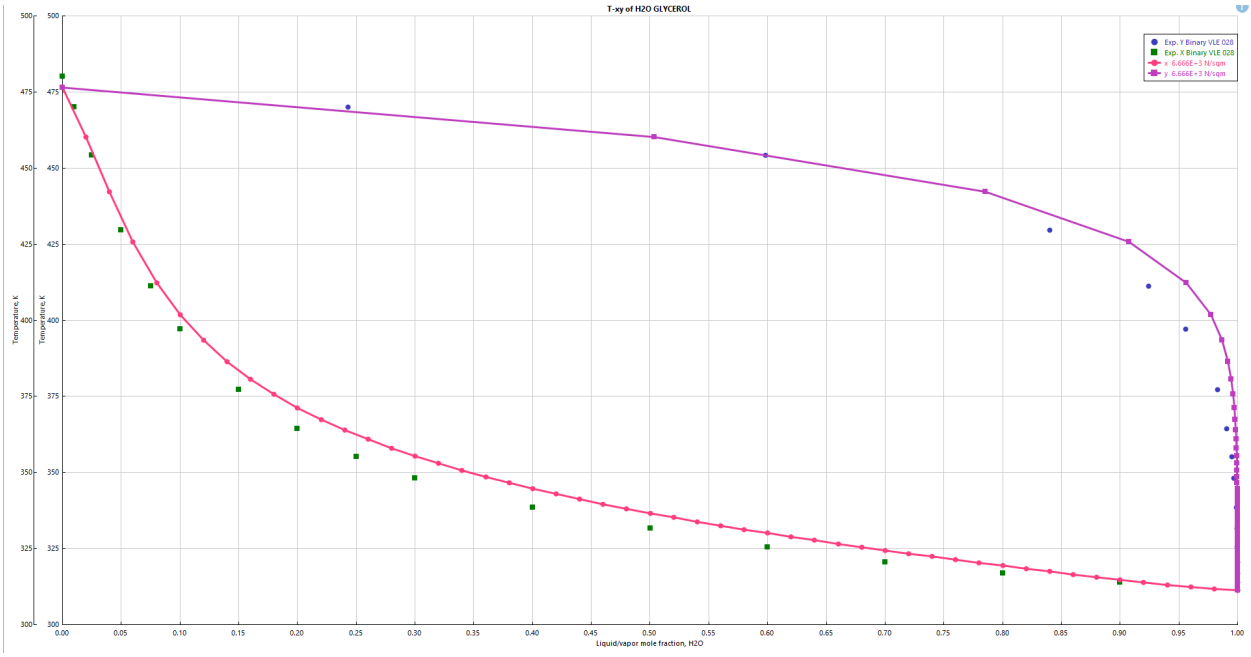
T-xy of H_2O, Glycerol using PENG-ROB



T-xy of H_2O, Glycerol using UNIFAC



T-xy of H_2O, Glycerol using UNIQUAC



T-xy of H_2O, Glycerol using UNIQUAC (After regression)

Parameter UNIQ | Help | Data set 1 | Swap | Enter Dechema Format | Estimate using UNIFAC | View Regression Information | Search | BIP Completeness

Default temp. unit C

Temperature-dependent binary parameters

Component i	Component j	Source	Temp. Units	AIJ	AJI	BIJ	BJI	CIJ	CJI	DIJ	DJI	TLOWER	TUPPER	EIJ	EJI
H2O	GLYCEROL	R-DR-1	C	2.02979	2.8699	-1064.53	-487.411	0	0	0	0	-273.15	726.85	0	0
H2O	PROPDIOL	APV140 VLE-IG	C	0	0	-268.338	248.883	0	0	0	0	15	100	0	0
GLYCEROL	PROPDIOL	APV140 VLE-IG	C	0.4348	-0.2234	-8.7211	-73.4455	0	0	0	0	88.6	180.9	0	0

Update parameters result for regression

Case ID	Parameter	Component i	Component j	New Value (SI units)	Old Value	Old Value Temp. Unit	Old Value Prop. Unit
DR-1	UNIQ/1	H2O	GLYCEROL	2.02979	0.9755	C	
DR-1	UNIQ/1	GLYCEROL	H2O	2.8699	0.2609	C	
DR-1	UNIQ/2	H2O	GLYCEROL	-1064.53	-188.494	C	
DR-1	UNIQ/2	GLYCEROL	H2O	-487.411	-45.9076	C	

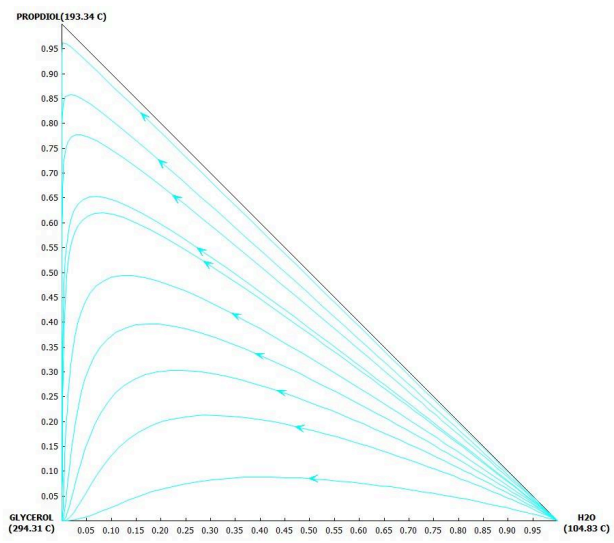
Updated parameters after regression

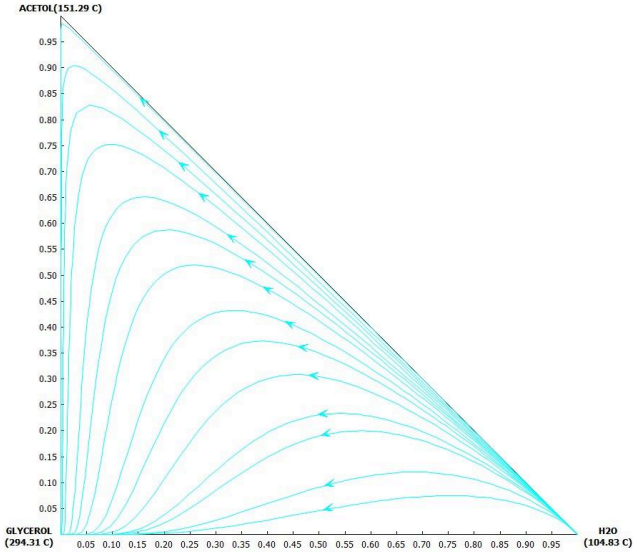
Azeotrope Search

Azeotrope formation was investigated using the UNIQUAC model for:

- Glycerol–water–propylene glycol
- Glycerol–water–acetol

No azeotropes were detected, confirming that distillation-based separation is possible.





AZEOTROPE SEARCH REPORT

Physical Property Model:UNIQUAC **Valid Phase:**VAP-LIQ

Mixture Investigated For Azeotropes At A Pressure Of 1.2 BAR

Comp ID	Component Name	Classification	Temperature
H2O	WATER	Unstable node	104.83 C
GLYCEROL	GLYCEROL	Stable node	294.31 C
ACETOL	ACETOL	Saddle	151.29 C

No Azeotropes Were Found

Feed Material Properties and Operating Conditions [1]

The two-step reaction process described in the study for converting glycerol to propylene glycol involves distinct feed materials and operating conditions for each step:

1st Reaction (Formation of Acetol Intermediate)

- Feed: Crude glycerol (80mol%) was used as the starting material.
- Operating Conditions:
    - Temperature: 200 °C
    - Pressure: Atmospheric pressure

2nd Reaction (Hydrogenation of Acetol to Propylene Glycol)

- Feed: Acetol (99mol%) isolated from step 1
- Operating Conditions:
    - Temperature: 200 °C
    - Pressure: 200 psi hydrogen pressure

The operating conditions of the reactors and distillation columns will be further optimized in future analysis.

Process Synthesis and Flow Diagram

The overall process for propylene glycol production from glycerol proceeds in two main steps:

1. **Dehydration of Glycerol**: Glycerol undergoes catalytic dehydration in a plug-flow reactor (PFR) to produce acetol and water.

2. **Hydrogenation of Acetol**: The acetol formed is subsequently hydrogenated in a second plug-flow reactor, in the presence of hydrogen (200 psi), to yield propylene glycol.

Both the reactions were simulated through a PFR. At this stage, the plug-flow reactor dimensions (length and diameter) were chosen arbitrarily and will be optimized in future.

Following the reactor sections, a sequence of distillation columns is used for product purification and recycling of unreacted species:

- **C1 Column (RadFrac)**: Separates water as the **C1 distillate** (target purity = 0.99 mole fraction), while the **C1 bottoms** contain glycerol and acetol.

- **C2 Column (RadFrac)**: Splits the C1 bottoms stream into **acetol-rich distillate** (0.99 mole purity, fed to the hydrogenation reactor) and **glycerol-rich bottoms** (0.99 mole purity, recycled back to the dehydration reactor).

- **C3 Column (RadFrac)**: Separates the hydrogenation reactor outlet into **acetol (C3 distillate)** and **propylene glycol (C3 bottoms, 0.99 mole purity)** as the final product.

For initial column setup, the **DSTWU shortcut model** was applied to estimate design parameters, and these results were refined using RadFrac.

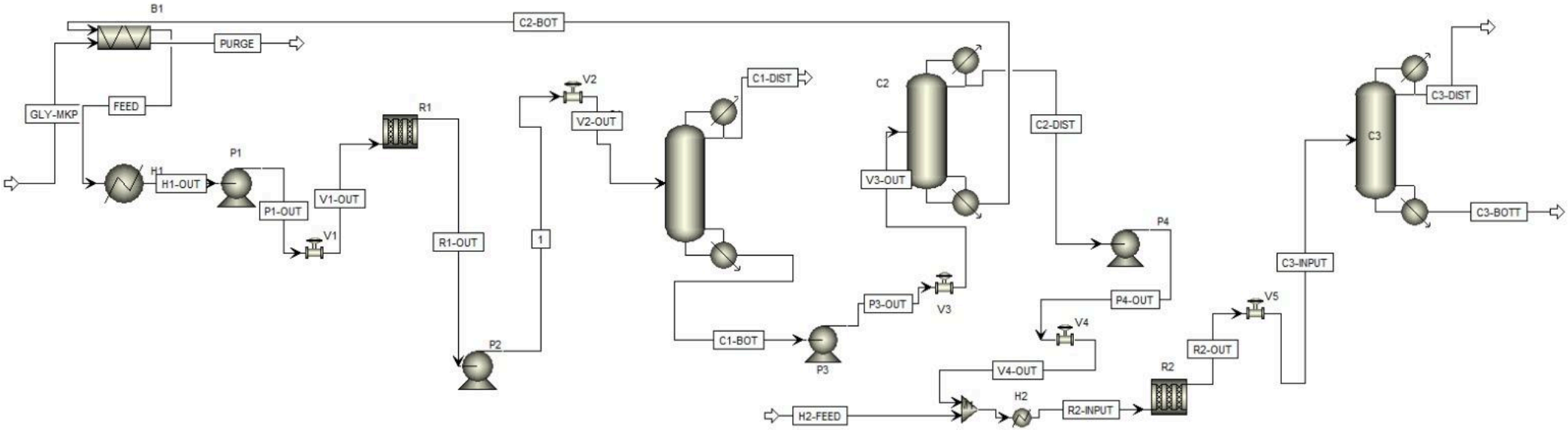
Design specifications on each distillation column:

- C1 distillate: water purity ≥ 0.99 mole fraction

- C2 distillate: acetol purity ≥ 0.99 mole fraction

- C2 bottoms: glycerol purity ≥ 0.99 mole fraction

- C3 bottoms: propylene glycol purity ≥ 0.99 mole fraction



Process Flow Diagram for Glycerol to Propylene glycol process

COMPONENT \ STREAM_NAMES	R1_IN	R1_OUT	C1_IN	C1_DIST	C1_BOT	C2_IN	C2_DIST	C2_BOT	R2_IN	R2_OUT	C3_IN	C3_DIST	C3_OUT
Mole Flows	0.027778	0.045843	0.045843	0.022814391	0.023028893	0.023028893	0.017855	0.005173836	0.035494	0.017855217	0.017855217	0.000288	0.017567009
H2O	0.004521	0.022586	0.022586	0.022586247	4.74E-08	4.74E-08	4.74E-08	2.87E-12	4.74E-08	4.74E-08	4.74E-08	4.74E-08	3.32E-12
H2	0	0	0	0	0	0	0	0	0.017639	0	0	0	0
GLYCEROL	0.023252	0.005186	0.005186	3.04E-62	0.00518631	0.00518631	1.78E-05	0.005168662	1.78E-05	1.78E-05	1.78E-05	7.52E-21	1.78E-05
PROPDIOL	0	0	0	0	0	0	0	0	0	0.017639137	0.017639137	0.000142	0.017496741
ACETOL	5.17E-06	0.018071	0.018071	0.000228144	0.017842536	0.017842536	0.017837	5.17E-06	0.017837	0.000198225	0.000198225	0.000146	5.25E-05
Mole Fractions													
H2O	0.162748	0.492685	0.492685	0.99	2.06E-06	2.06E-06	2.66E-06	5.56E-10	1.34E-06	2.66E-06	2.66E-06	0.000165	1.89E-10
H2	0	0	0	0	0	0	0	0	0.496953	0	0	0	0
GLYCEROL	0.837065	0.113131	0.113131	1.33E-60	0.22520882	0.22520882	0.000997	0.999	0.000502	0.000997343	0.000997343	2.61E-17	0.001013706
PROPDIOL	0	0	0	0	0	0	0	0	0	0.987898226	0.987898226	0.494075	0.995999983
ACETOL	0.000186	0.394184	0.394184	0.01	0.77478912	0.77478912	0.999	0.000999999	0.502544	0.011101774	0.011101774	0.50576	0.002986311
Mass Flows	2.223196	2.223196	2.223196	0.423798331	1.799397652	1.799397652	1.323023	0.476389734	1.358581	1.358581024	1.358581024	0.021635	1.336946352
H2O	0.081443	0.406898	0.406898	0.406897558	8.55E-07	8.55E-07	8.55E-07	5.18E-11	8.55E-07	8.55E-07	8.55E-07	8.55E-07	5.99E-11
H2	0	0	0	0	0	0	0	0	0.035558	0	0	0	0
GLYCEROL	2.141369	0.477632	0.477632	2.80E-60	0.477631749	0.477631749	0.00164	0.47600646	0.00164	0.001640002	0.001640002	6.92E-19	0.001640002
PROPDIOL	0	0	0	0	0	0	0	0	0	1.342255802	1.342255802	0.010836	1.331420102
ACETOL	0.000383	1.338666	1.338666	0.016900773	1.321765048	1.321765048	1.321382	0.000383275	1.321382	0.014684366	0.014684366	0.010798	0.003886249
Mass Fractions													
H2O	0.036633	0.183024	0.183024	0.960120719	4.75E-07	4.75E-07	6.46E-07	1.09E-10	6.29E-07	6.29E-07	6.29E-07	3.95E-05	4.48E-11
H2	0	0	0	0	0	0	0	0	0.026173	0	0	0	0
GLYCEROL	0.963194	0.21484	0.21484	6.61E-60	0.265439798	0.265439798	0.00124	0.99919546	0.001207	0.001207143	0.001207143	3.20E-17	0.001226678
PROPDIOL	0	0	0	0	0	0	0	0	0	0.987983623	0.987983623	0.500849	0.995866513
ACETOL	0.000172	0.602136	0.602136	0.039879281	0.734559727	0.734559727	0.99876	0.00080454	0.972619	0.010808605	0.010808605	0.499112	0.00290681

Material Balance

Mole Flow (kmol/sec) Mass Flow (kg/sec)

Energy Balance & other Unit Operations details

Minimum reflux ratio	2.01499408	
Actual reflux ratio	3.33262	
Minimum number of stages	15.3417	
Number of actual stages	24	
Feed stage	14.8865	
Number of actual stages above feed	13.8865	
Reboiler heat duty	3.56603e+06	Watt
Condenser heat duty	-4.06515e+06	Watt
Distillate temperature	372.88	K
Bottom temperature	425.602	K
Distillate to feed fraction	0.507839	
HETP		

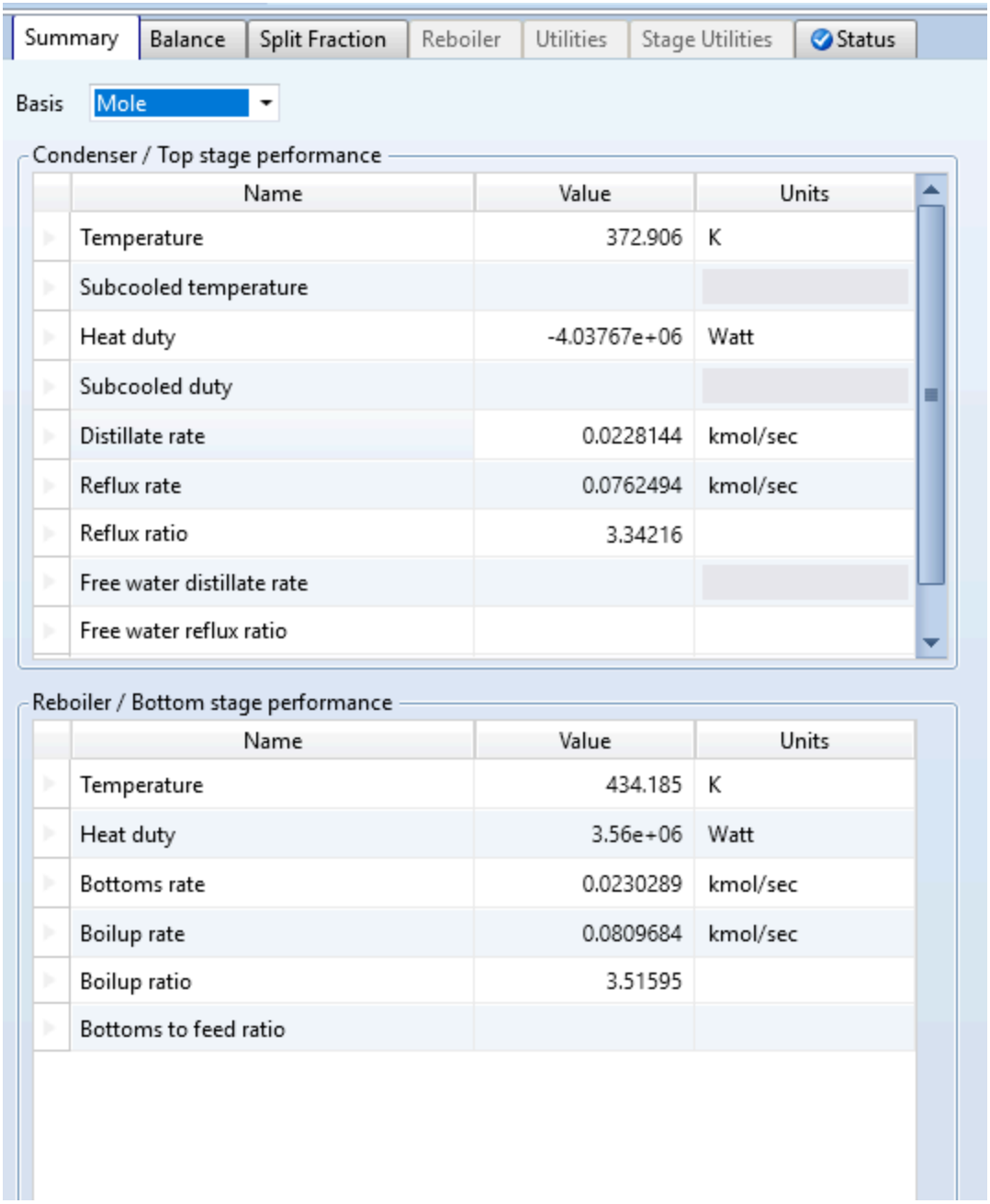
Distillation Column C1 (DSTUW)

Minimum reflux ratio	0.00128185	
Actual reflux ratio	0.0151086	
Minimum number of stages	2.10021	
Number of actual stages	20	
Feed stage	9.31369	
Number of actual stages above feed	8.31369	
Reboiler heat duty	847526	Watt
Condenser heat duty	-779396	Watt
Distillate temperature	416.728	K
Bottom temperature	532.247	K
Distillate to feed fraction	0.782813	
HETP		

Distillation Column C2 (DSTUW) Results

Minimum reflux ratio	0.623186423	
Actual reflux ratio	0.755629	
Minimum number of stages	10.7345	
Number of actual stages	25	
Feed stage	12.7499	
Number of actual stages above feed	11.7499	
Reboiler heat duty	681617	Watt
Condenser heat duty	-783839	Watt
Distillate temperature	418.327	K
Bottom temperature	460.278	K
Distillate to feed fraction	0.649398	
HETP		

Distillation Column C3 (DSTUW) Results



C1 RadFrac Results

Summary | Balance | Split Fraction | Reboiler | Utilities | Stage Utilities | Status

Basis: Mole

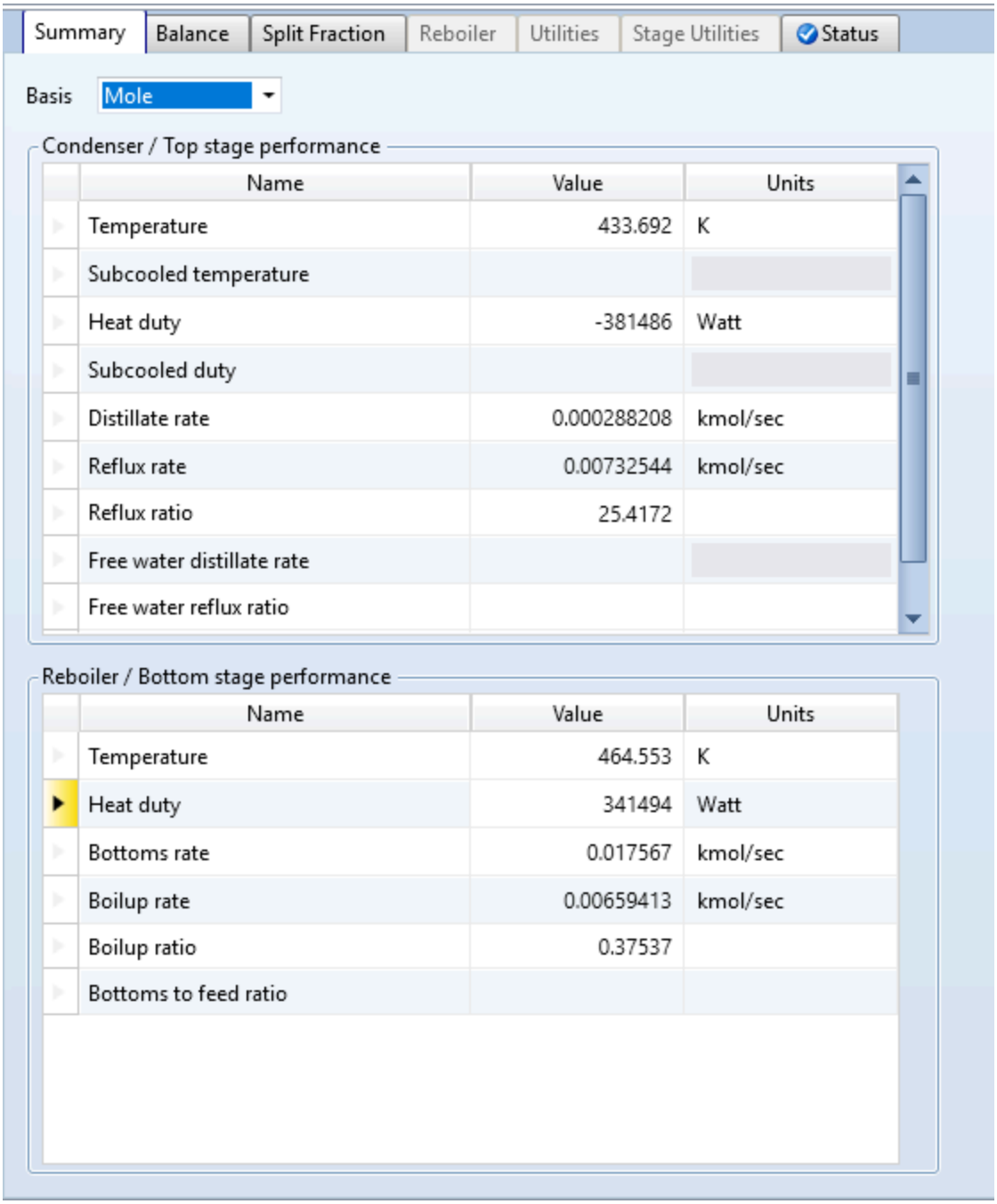
Condenser / Top stage performance

Name	Value	Units
Temperature	418.347	K
Subcooled temperature		
Heat duty	-795114	Watt
Subcooled duty		
Distillate rate	0.0178552	kmol/sec
Reflux rate	0.000316228	kmol/sec
Reflux ratio	0.0177107	
Free water distillate rate		
Free water reflux ratio		

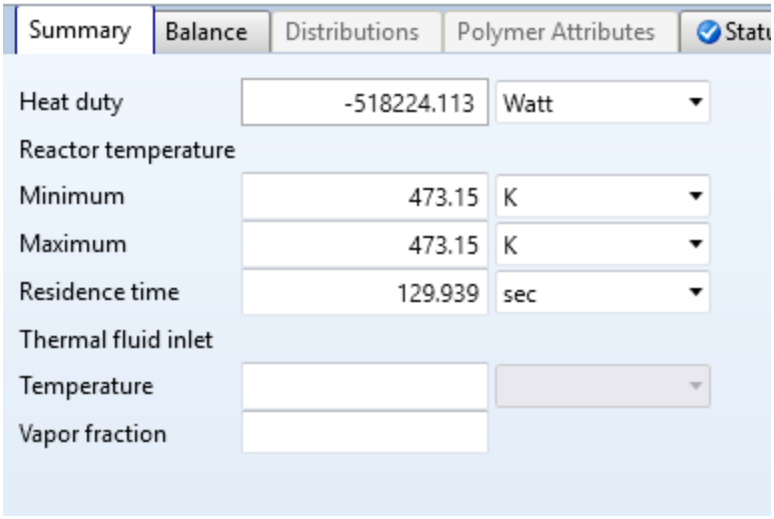
Reboiler / Bottom stage performance

Name	Value	Units
Temperature	566.132	K
Heat duty	920299	Watt
Bottoms rate	0.00517368	kmol/sec
Boilup rate	0.0129221	kmol/sec
Boilup ratio	2.49766	
Bottoms to feed ratio		

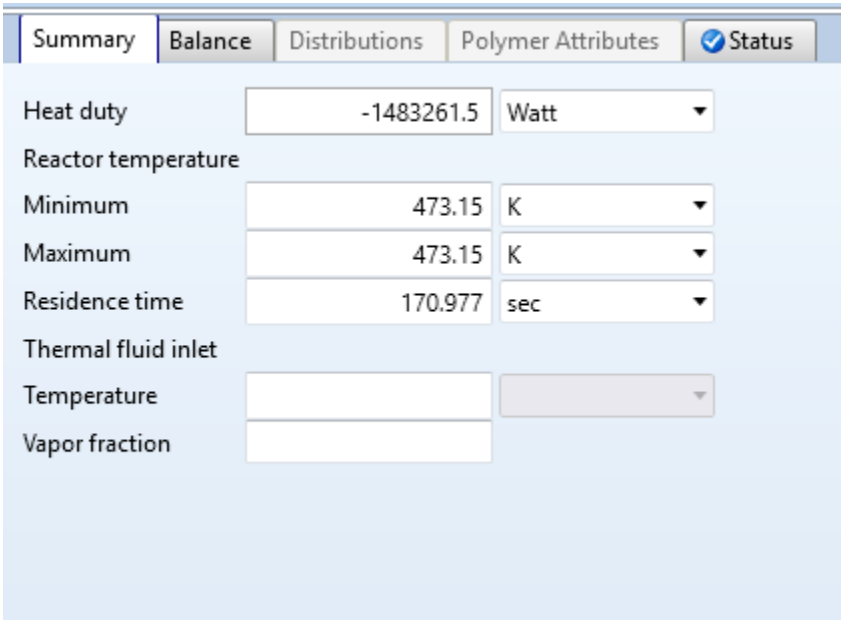
C2 RadFrac Results



C3 RadFrac Results



Heater 1 Results



Heater 2 Results

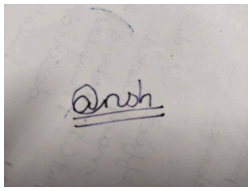
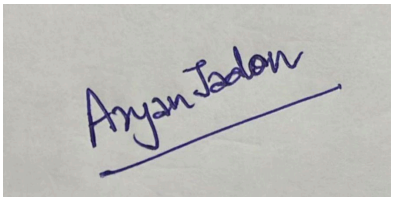
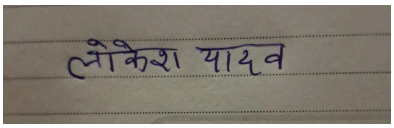
Objectives that could not be accomplished with reasons: - None

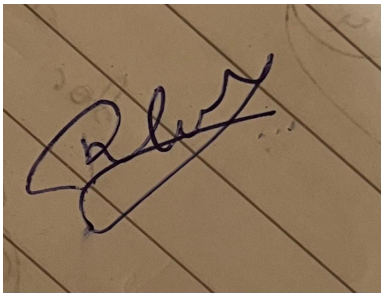
Any other challenges: - None

Number of hours spent on Capstone project during this period: 15 hours

References:

1. **Process Discovery**
2. **Thermodynamic Analysis**

Name (Roll No.)	Contribution	Signature
Anas Ali (220137)	Azeotrope Analysis, Report Compilation Flowsheet Development	
Ansh Sethi (220167)	Material Balance & Energy balance & report compilation	
Aryan Jadon (220223)	Material Balancing, PFD formation & Report Preparation	
Jatin Madan (220475)	Material Balancing, PFD formation & Report Preparation	
Lokesh Yadav (220594)	Model Fitting for Thermodynamics Flowsheet development in Aspen Plus	

Madhav Lata (220597)	Thermodynamic Model Selection and Regression Process synthesis and development of PFD Flowsheet development in Aspen Plus and complete Simulation	
Pratyush Gupta (220813)	Process synthesis and development of PFD Flowsheet development in Aspen Plus and complete Simulation	
Punam Singh (220835)	Process synthesis and development of PFD Flowsheet development in Aspen Plus and complete Simulation