Bi-Weekly Report 1

Team number: 1

Team members:

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Project title: Glycerol-to-Propylene Glycol Process

Objectives for this report: This report aims to identify the process, define feed and product specifications, and represent it through a block diagram. It also aims to assess preliminary economic feasibility and validate a suitable thermodynamic model with parameter tuning

Results with short discussion:

We were able to successfully prepare the block diagram for the glycerol-to-propylene glycol process. It represents two main steps of reaction mechanism - first, dehydration of glycerol to acetol which is followed by hydrogenation to produce propylene glycol.

From the economic feasibility analysis, we found that producing 1 kg of propylene glycol requires around requires approximately **1.805 kg** of crude glycerol feed (80% purity basis) along with **0.0284 kg** of fresh hydrogen When we add catalyst usage as well to it, cost is **Rs 88.02 per kg of product**. Factoring in additional expenses such as labor, utilities, and maintenance (about **Rs 15 per kg**), total cost is still much lower than market selling price of product which is **Rs 135 per kg**. This gives a profit margin of roughly **Rs 46.98 per kg**, indicating the process to be economically feasible at this stage of analysis.

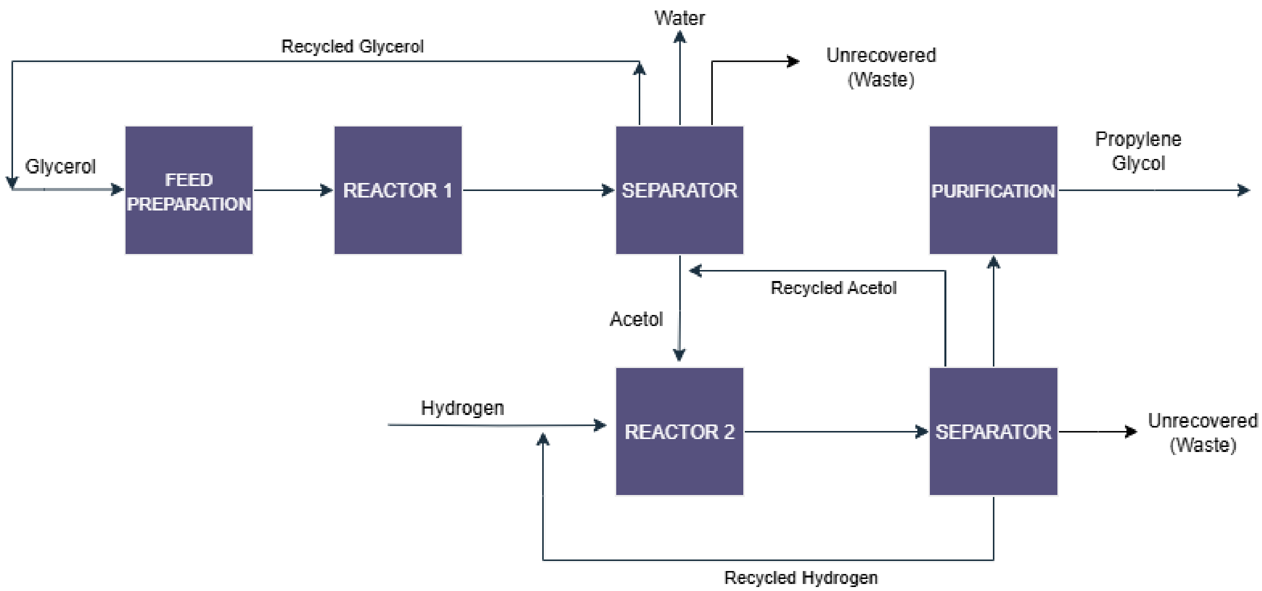
For the thermodynamic model, we tested parameters before selecting **UNIQUAC** as the most suitable option. The Txy plot for the water-glycerol mixture at 1 atm showed good convergence with experimental data.

Objectives which could not be accomplished with reasons: All of the objectives are completed for the Bi-weekly report 1.

Any other challenges: The License of the Aspen had expired when we visited the lab, but it was resolved later.

<u>Number of hours spent on Capstone project during this period</u>: 7-8 hours

<u>Block Diagram</u> :



<u>Economic Feasibility:</u>

We have determined the material requirements, mass balances, and approximate economic feasibility of producing 1.000 kg of propylene glycol (Propylene Glycol) via the two-step process starting from glycerol.

Molar Masses (g/mol):

- Glycerol ($C_3H_8O_3$): 92.094
- Acetol ($C_3H_6O_2$): 74.079
- Propylene glycol ($C_3H_8O_2$): 76.095
- Water (H_2O): 18.015
- Hydrogen (H_2): 2.016

Overall Stoichiometry

- **Step 1 (Dehydration):**
  Glycerol → Acetol + H_2O

- **Step 2 (Hydrogenation):**
  Acetol + H_2 → Propylene Glycol (1,2 Propane diol)

Assumptions

1. **Reaction conversions:**
    - Step 1: 99% glycerol converted
    - Step 2: 99% acetol converted
2. **Recovery efficiencies:**
    - **Step 1:**
        - Water: 99% recovered (1% lost as waste)
        - Acetol: 90% of formed acetol sent forward, 10% lost as waste
        - Unreacted glycerol: 99% recycled, 1% waste
    - **Step 2:**
        - Hydrogen: 99% recycled, 1% lost
        - Acetol: 90% recycled, 10% lost
        - Propylene glycol (Propylene Glycol): 95% recovered (product), 5% lost
3. **Catalyst usage:** Copper chromite, 5% of glycerol feed; reusable 10 cycles.
4. **Crude glycerol has 80% purity.**
5. **Target product purity:** Propylene Glycol recovered after Step 2 = final saleable product.

Stepwise Mass Balances

Step 0: Propylene Glycol Requirement

Moles Propylene Glycol target =

$$\frac{1000}{76.095} = 13.1415 \text{ mol}$$

Step 2 First (Back-calculation):

Propylene Glycol recovery = 95%
So acetol moles entering Step 2 must be:

$$\frac{13.1415}{0.95} = 13.833 \text{ mol}$$

Since Step 2 conversion = 99%; required acetol feed (from Step 1 to Step 2):

$$\frac{13.833}{0.99} = 13.972 \text{ mol}$$

Thus Step 2 acetol input = **13.972 mol = 1.035 kg**

Hydrogen requirement (stoichiometric): equal moles = 13.972 mol = **0.0282 kg H_2**

But only 1% lost, 99% recycled; Net fresh H_2 needed = **0.000282 kg**

Step 1: Acetol Supply

To get 13.972 mol acetol into Step 2, and knowing only 90% recovery of produced acetol
Acetol produced in Step 1 must be:

$$\frac{13.972}{0.90} = 15.524 \text{ mol}$$

With 99% conversion of glycerol; glycerol consumed = 15.524 mol
So glycerol fed =

$$\frac{15.524}{0.99} = 15.676 \text{ mol}$$

$$15.676 \text{ mol glycerol} = 1.444 \text{ kg}$$

Water Balance (Step 1)

Stoichiometric water formed = 15.524 mol = 0.280 kg
99% recovery; 0.277 kg recovered, 0.003 kg waste

Net Mass Balances (per 1 kg Propylene Glycol)

- **Glycerol feed (pure):** 1.444 kg

- **Crude glycerol (80%):**

$$\frac{1.444}{0.80} = 1.805 \text{ kg}$$

- **Hydrogen fresh feed:** 0.0282 kg + 0.000282 kg (after every kg of PG)

- **Catalyst (5% of glycerol feed / 10 reuse):**

$$0.05 \times 1.444 = 0.0722 \text{ kg batch}$$

  Effective per run (divided by 10): 0.0072 kg

- **Main by-product:** Water recovered ≈ 0.277 kg

Cost Calculation (per 1 kg Propylene Glycol)

Raw Material	Rate (Rs/kg)	Amount	Cost (Rs)
Crude Glycerol	30	1.805 kg	54.15
Hydrogen	397	0.02848 kg	11.31
Copper Chromite	1050/Kg	0.0072 kg	7.56

Total Raw Material Cost = **Rs 73.02**

Other costs (labour, utilities, energy, maintenance): **Rs 15/kg Propylene Glycol**

Retail value of Propylene Glycol: **Rs 135/kg**

Profitability

$$\text{Profit} = 135 - (73.02 + 15) = Rs\ 46.98/\text{kg}$$

Profit margin ≈ **34.8%**

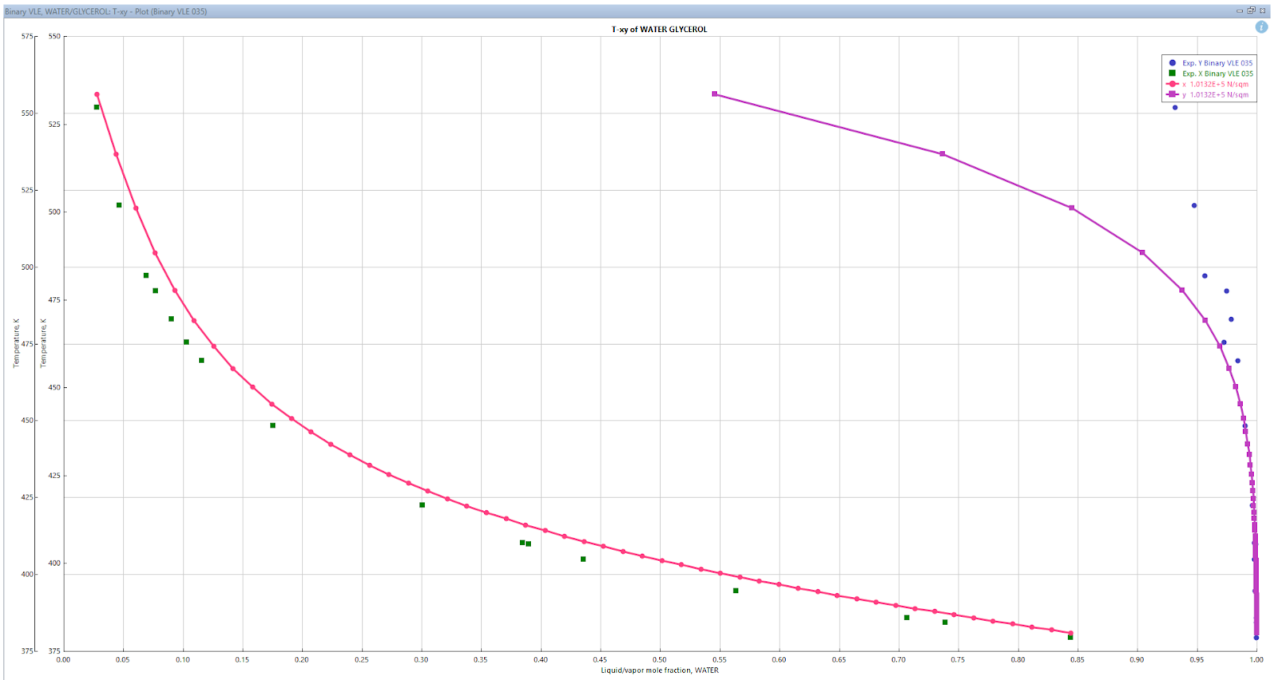
Mass Balance

Stream Name/Label	Components	Mass (kg)	Comments (Conversion, Recovery, Purity)
Glycerol Feed	Glycerol (80%), Impurities (20%)	1.805	Crude glycerol (1.444 kg pure glycerol)
Recycled Glycerol	Glycerol	0.260	99% unreacted glycerol recycled to feed
Reactor 1 Output	Acetol, Water, Glycerol	1.035, 0.280, 0.016	1% glycerol unreacted, 99% acetol conversion
Separator Output (Water)	Water	0.277	99% water recovered
Separator Waste (Water)	Water	0.003	1% water lost
Acetol to Reactor 2	Acetol	1.035	90% acetol sent forward, 10% lost
Recycled Acetol	Acetol	0.115	10% acetol recycled
Reactor 2 Input	Acetol, Hydrogen	1.035, 0.0282	Stoichiometric hydrogen, mostly recycled
Reactor 2 Output	Propylene Glycol, Acetol, Hydrogen	1.050, 0.010, 0.00028	99% acetol conversion, unreacted acetol and H_2
Separator Output (H_2)	Hydrogen	0.028	99% hydrogen recycled
Separator Waste (PG)	Propylene Glycol	0.053	5% unrecovered in purification
Purification Output	Propylene Glycol	1.000	Final saleable product (95% recovery)

Thermodynamic Model Selection :

Model Selected: **UNIQUAC**

T-xy plot of water glycerol binary mixture at 1 atm pressure

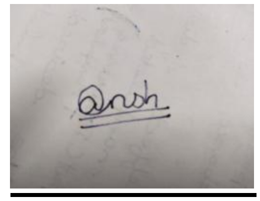
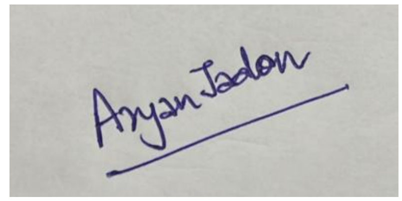
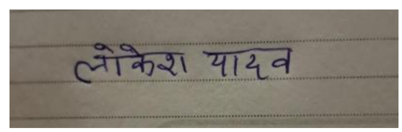
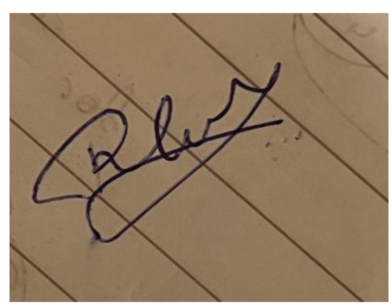


Experimental Data plot and plot as per parameters converged.

References :

https://www.sciencedirect.com/science/article/pii/S0926860X0400941X

Name (Roll No.)	**Contribution**	**Signature**
Anas Ali (220137)	**Block Diagram**	Anas

Ansh Sethi (220167)	**Block Diagram**	
Aryan Jadon (220223)	**Compiling and Report**	
Jatin Madan (220475)	**Economic Feasibility**	
Lokesh Yadav (220594)	**Economic Feasibility**	
Madhav Lata (220597)	**Thermodynamic Model**	
Pratyush Gupta (220813)	**Thermodynamic Model**	

Punam Singh (220835)	**Thermodynamic Model**