Course: Capstone Design Project (CHE453)

Submitted by: Punam Singh(220835)

Group No: 1

Our Group's Key Achievements

- Confirmed the process is highly viable by developing a complete **end-to-end process flowsheet** in Aspen Plus. This simulation, validated with the **UNIQUAC** thermodynamic model, models the two-step reaction and a complex three-column distillation train to meet **0.98 mole fraction purity targets**.
- Designed and simulated critical utility systems, including a **cogeneration power plant** for heat and electricity and a **closed-loop cooling water tower** to manage thermal duties.

My Individual Contributions

- **Thermo Model Validation:** I helped validate UNIQUAC as our best model, checking its accuracy against experimental data for the tricky glycerol-water mixture.
- **Process Design (PFD):** I contributed to the foundational process design and PFD, which set up our two-step reaction and three-column distillation train.
- **Aspen Simulation**: I was hands-on in building the complete Aspen simulation, setting up the reactors and columns (C1-C3) and getting the recycle loops to converge for our final balances.
- **Utility System Design:** I also designed and simulated the critical utility systems, preparing the Aspen flowsheets for our cogeneration plant and cooling water loop.

Key Technical Aspects I've Learned

- **Designing a Rigorous Separation**: I learned how to design a complex, multi-column distillation train. We used DSTWU for initial estimates, then applied the rigorous RadFrac model to set our 0.98 mole fraction purity specs and manage the recycle streams.
- **Validating Our Thermo Model:** I learned how important it is to validate models for non-ideal mixtures. We selected UNIQUAC, performed parameter regression with VLE data for accuracy, and ran an azeotrope search to confirm our strategy was feasible.
- **Integrating the Process and Utilities:** I learned how to integrate major utilities with the core process. This meant designing a cogeneration plant for steam/electricity demands and sizing a cooling water loop for condenser loads, focusing on energy efficiency.

Technical Challenges in Our Process

- **Separation of Hydrogen gas:** The C3 column was a major hurdle. The feed contained our product (propylene glycol), acetol, and hydrogen gas. A standard column with a total condenser failed because the hydrogen would build up, blocking the acetol from condensing and killing the reflux. We had to re-engineer the top section, adding a flash drum and a **partial condenser** to vent the hydrogen while still condensing the acetol needed for reflux.
- **Heat Exchanger Network (HEN) Design:** Implementing pinch technology was a significant hurdle. We struggled with how to set up the analysis and, more importantly, how to decide on the final temperature and pressure conditions for the heat exchangers to ensure we were maximizing energy recovery efficiently. It took some discussion and rethinking our approach to finally design the network.