CHE453
Bi-Weekly Report - 1

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Objective of the Report:

- **Finalize the process**: Confirm the reaction pathway, method, and feed specifications to be used throughout the project.
- **Develop the block flow diagram**: Prepare and finalize the block diagram of the process and verify overall consistency.
- **Check economic feasibility**: Perform a cost–revenue analysis to evaluate process viability.
- **Select the thermodynamic model**: Determine the most suitable thermodynamic model in Aspen Plus

Project Title: Production of Solketal from Glycol

In this project, our aim was to identify a chemical process that is both technically feasible and economically attractive. After evaluating different alternatives, we focused on processes that could make value-added products from readily available, low-cost feedstocks. Glycerol, a major by-product of biodiesel production, stood out as a promising candidate since it is produced in large quantities but has relatively low market value.

Based on this, we selected the production of Solketal (2,2-dimethyl-1,3-dioxolane-4-methanol). The reaction involves combining glycerol with acetone in the presence of an acid catalyst. This is an equilibrium reaction where one mole of glycerol reacts with one mole of acetone to form one mole of solketal and one mole of water. To improve the conversion, the process usually uses either excess acetone or removes the water formed. Both liquid acids (like sulfuric acid or p-toluenesulfonic acid) and solid acid catalysts (such as Amberlyst resins or zeolites) can be used.

We chose this process because solketal has a wide range of industrial applications, especially as a fuel additive. It can improve gasoline properties by increasing octane number, enhancing cold-flow behavior, and reducing engine deposits. From an economic point of view, the conversion is also attractive: while crude glycerol sells at only about $210–390 per ton, solketal can be sold at around $2,500–3,000 per ton. This large difference makes the process promising both technically and commercially.

Specifications for product and feed streams

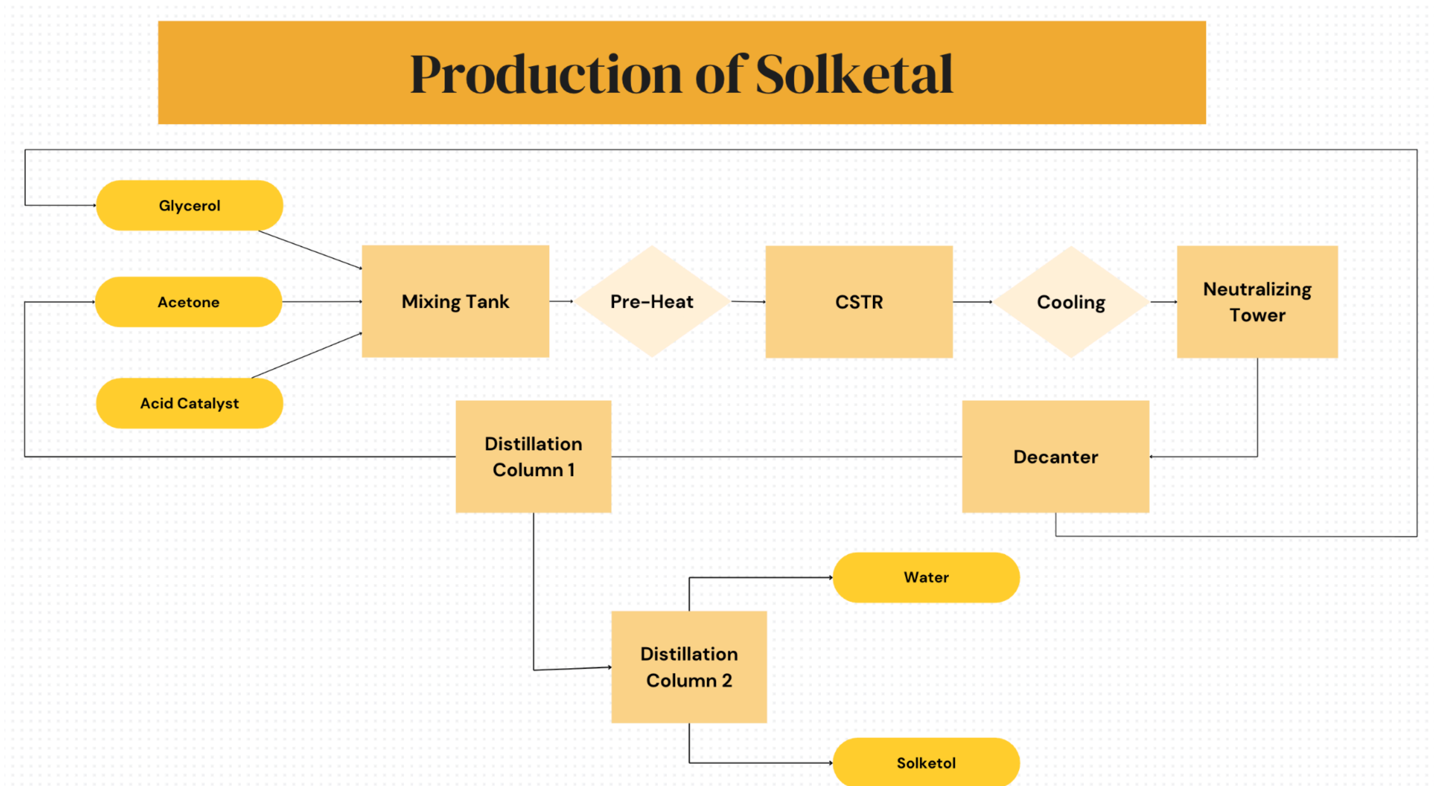
Molar Ratio: A slight excess (molar ratio 3-9:1 acetone:glycerol) can be used to drive the equilibrium.

Flow rates (basis): Literature examples use scales like 100,000 t/yr glycerol (≈11.4 t/h) . For a preliminary Aspen model, any consistent basis can be chosen 10 t/h glycerol).

- **Glycerol feed (biodiesel-derived):** Use a "crude glycerol" stream (e.g. 85–90 wt% glycerol with methanol, fatty acids, salts, etc. impurities) . We can consider **~90% glycerol and 10% inert** (water/methanol/ash) by weight
- **Acetone feed:** Industrial acetone (~95–99% purity) is assumed. No major impurities are expected. We can consider **~95% glycerol and 5% inert**
- **Catalyst:** Fixed load of H_2SO_4 or Amberlyst resin.

- **Solketal product:** Aim for ~95–98 wt% solketal in the purified stream. Laboratory/bench processes report up to ~99% purity , but setting a 95% target helps convergence. We can target a **purity of 97%**

Block Diagram



Input-output cost analysis & preliminary economic feasibility

Using current commodity prices, we estimate material costs and product value to gauge feasibility:

- **Raw material costs:**
  - Crude glycerol $210–390/ton **($0.25/kg)**
  - Acetone $1,200/ton ($1.20/kg)
- **Product value:**
  - Solketal $2,500–3,000/ton **($2.50–$3.00/kg)** (note: this is bulk price)

- **Simple mass balance (per 1 tonne glycerol basis):**
  - 1 t glycerol (10,870 mol, MW 92) + 1 t glycerol yields theoretical 1.43 t solketal (at 100% conv) plus ~0.16 t water.
  - Assuming an **85% conversion** (realistic), yield ≈1.22 t solketal. Required acetone (1:1 molar) ≈0.63 t.

- **Cost vs. revenue:** For 1 t glycerol: glycerol cost ≈$300, acetone cost (0.63 t) ≈$750; total raw ≈$1,050. Product sold: 1.22 t × $3,000/t ≈$3,660. Gross margin ≈$2,600 per t glycerol. (Even at 80% yield, margin ~$2,400/t). Hence this process is economically feasible

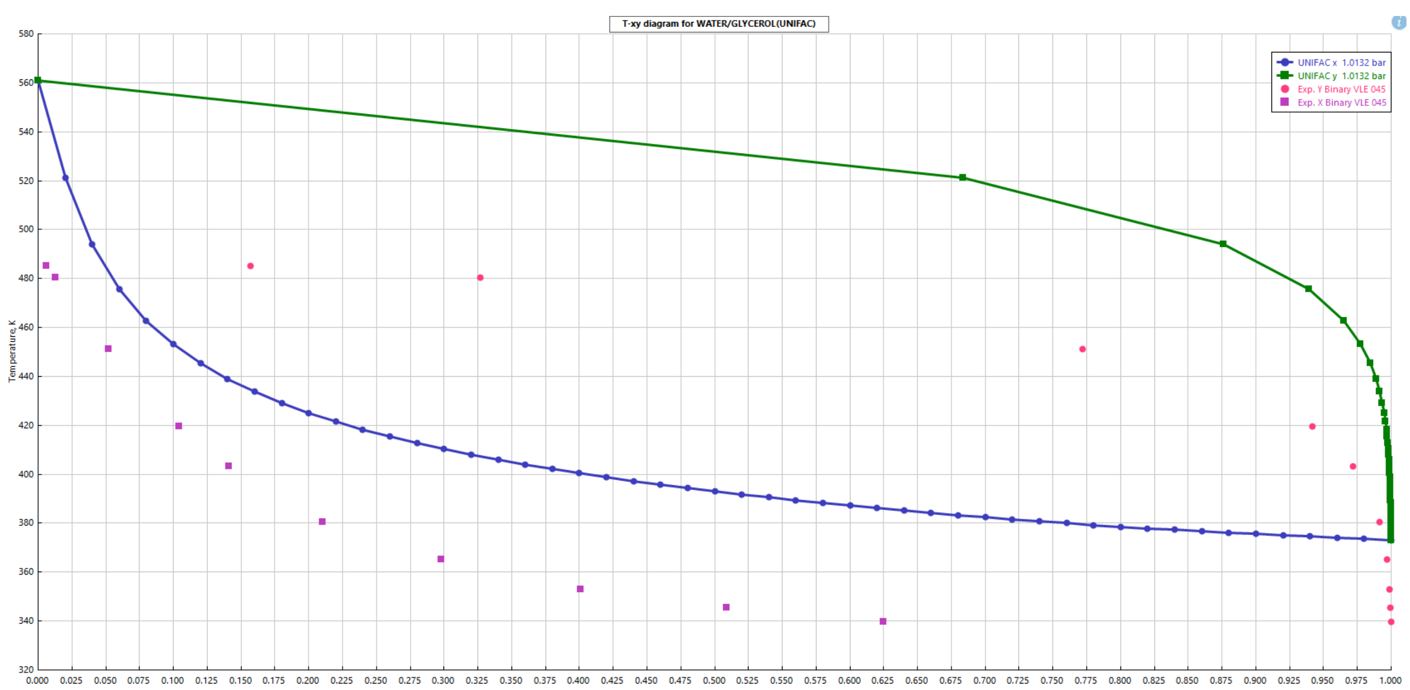
Source for Costs: (i) [Continuous Valorization of Glycerol into Solketal: Recent Advances on Catalysts, Processes, and Industrial Perspectives]() (ii) [Acetone Prices, Trend, Chart, Index, Graph and Forecast]()

(VLE) Modeling of the Glycerol–Water System:

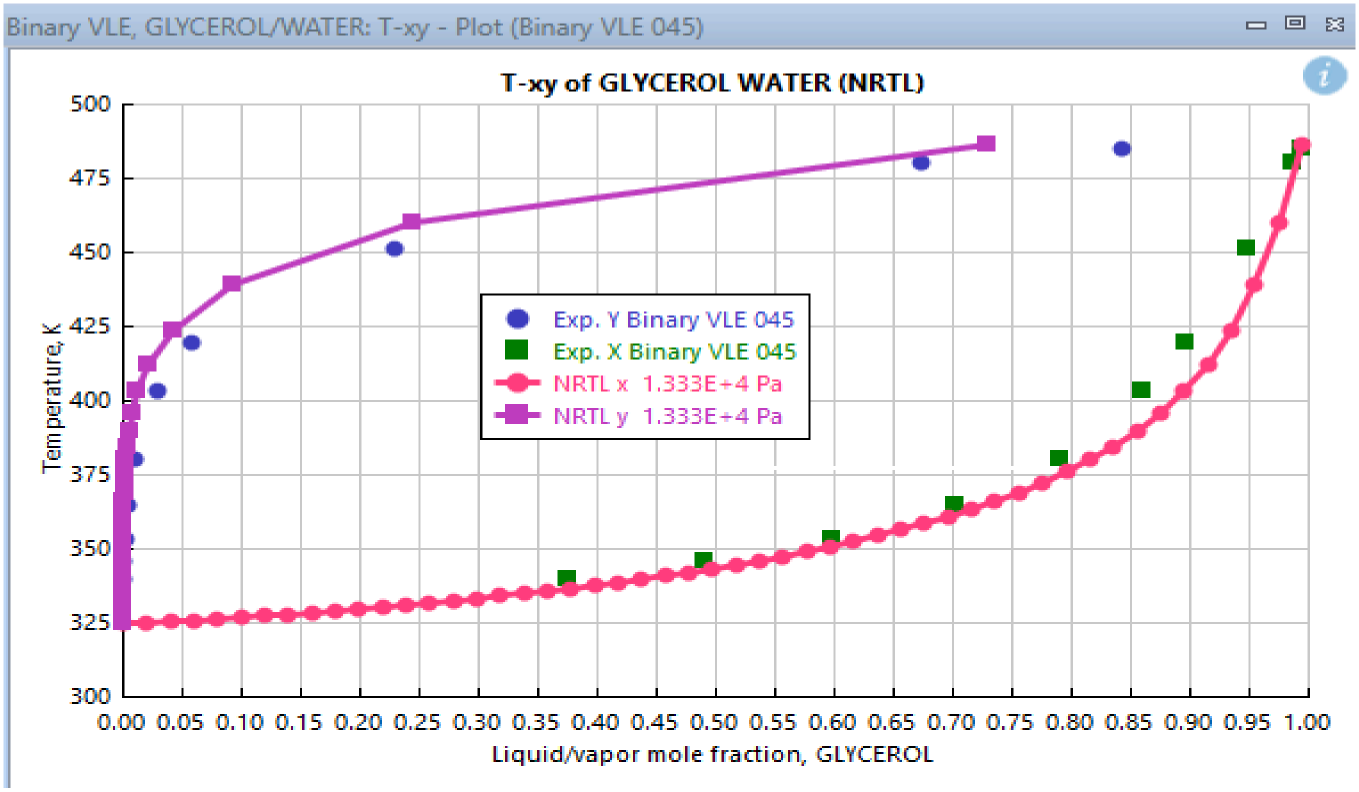
Regressed parameters

Parameter	Component i	Component j	Value (SI units)
NRTL/1	WATER	GLYCEROL	-1.90334
NRTL/1	GLYCEROL	WATER	0.509184
NRTL/2	WATER	GLYCEROL	868.883
NRTL/2	GLYCEROL	WATER	-434.344
NRTL/3	WATER	GLYCEROL	3.3

It presents a temperature–composition diagram comparing experimental vapor–liquid equilibrium data with model predictions for accuracy. The report outlines key deliverables including process identification, cost analysis, and thermodynamic model validation for the study.



The work involves water–glycerol separation analysis, where experimental VLE data is compared with UNIFAC predictions, showing strong non-ideal behavior. The study includes process identification, product specifications, economic feasibility, and thermodynamic model regression to improve accuracy.



The work involves process identification, model selection, and parameter regression for the glycerol–water system. Thermodynamic modeling using NRTL was performed, and regressed parameters were validated against experimental VLE data to ensure accurate prediction of phase behavior.

- The glycerol–water system was modeled using NRTL and UNIFAC thermodynamic models to predict VLE behavior. The NRTL model, which requires regressed parameters, was validated against experimental T–xy data, showing good agreement after parameter tuning. The UNIFAC model, a group contribution method, provided generalized predictions without regression but with less accuracy. Model validation involved comparing predicted curves with experimental points, where closer alignment indicated higher reliability. Regression of NRTL parameters minimized deviations, yielding optimized values with low standard deviation for improved precision. The tuned NRTL model was thus selected for accurate process design and simulation of this system.

Results:

Selected Reaction: Ketalization of glycerol with acetone to produce solketal.
Economic Analysis: Completed feasibility study evaluating cost versus revenue.
Thermodynamic Model: Found NRTL as the best fit for the Aspen Plus simulation using academic references.
Source: In a study of the liquid-liquid equilibrium of an acetone, solketal, and glycerol mixture, researchers made experimental measurements at temperatures of 303.2, 313.2, and 323.2 K and a pressure of 101.3 kPa. The data was then correlated using the Nonrandom Two Liquid (NRTL) model. The model's predictions showed a good agreement with the experimental findings. This research is relevant to the synthesis of solketal from glycerol and acetone.

Block Diagram: Finalized process flow including mixing of glycerol, acetone, and acid catalyst, CSTR for reaction, cooling and neutralization, followed by phase separation in decanter and two-stage distillation for water and solketal recovery.

Challenges:

Non - availability of proper data for analysis of thermodynamic model best for our process.

Time Spent on Project Work:

Approximately 8 - 10 hours.

Contributions:

- **Process Identification and Specifications:** Manas & Akshat
- **Report and Economic Analysis:** Mohit & Ankit
- **Aspen Related Work**: Saurabh & Divya
- **Others**: Supriya & Kishore