PROCESS - GLYCEROL TO PROLEYENE GLYCOL

TEAM -1

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Contents

SECTION - 1

Rationale & Feasibility

Product Choice & Specs

Pharmaceuticals

Solvent, carrier, hydrating agent, preservative in creams, shampoos, toothpaste, and drug formulations

Chemical Intermediates / Polymers

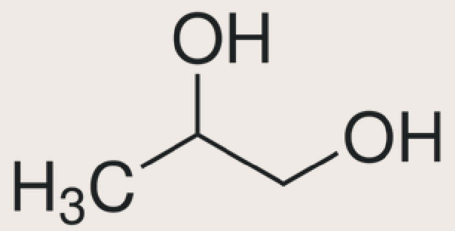
Reactant for polyester resins, polyurethanes, and dipropylene glycol production

Food & Beverage

Humectant (E1520), stabilizer, solvent in flavors, fragrances, and food-contact

Industrial Applications

Used in antifreeze, heat transfer fluids, de-icing, coatings, and detergents



Global Market size:

USD 4.8–5.0 billion in 2024

8.43% expected growth rate over 2025-30

Product Purity Specification - 99%

Regulatory & Safety Compliance

Food, pharma and cosmetic applications demand strict adherence to USP/EP/Food Grade standards

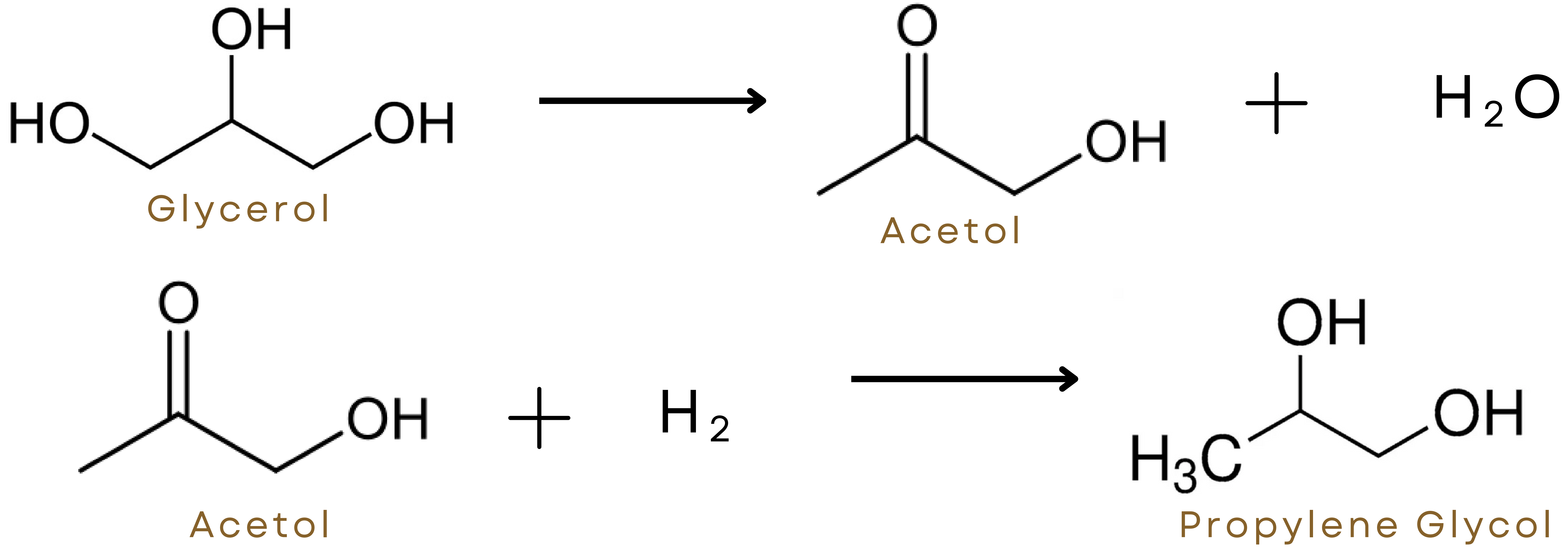
Quality & Performance

Even trace impurities can alter colour, odor, taste, stability, or reactivity, which is unacceptable in sensitive formulations (drugs, food flavors, cosmetics).

Market Access & Value

Higher purity opens access to premium markets (pharma, food, personal care) and ensures global acceptability, whereas lower grades are restricted to industrial uses.

Reaction Pathway



Feedstock Quality

1. Availability of Glycerol

India's biodiesel / oleochemical industries generate glycerol as by-product. If supply is stable and cost is low, that gives a feedstock advantage and improves sustainability.

Feed	Composition	Conditions
Crude Glycerol ($C_3H_8O_3$)	80% glycerol 20% water (w/w)	1 bar, 298K
Hydrogen (H_2)	100%	20 bar
Copper Chromite ($Cu_2Cr_2O_5$)	100%	-

2. Sustainability / Bio-based Product Demand

Increasing regulatory push and consumer preference for green / bio-based chemicals. Using glycerol gives a lower carbon footprint vs propylene oxide (petrochemical)

3. Value Addition in Glycerol Chain

Instead of selling crude glycerol (often low value), converting it to a higher value product like PG increases margin.

Products Purity

Products	Molar Mass (g/mol)	Purity (%)
Acetol* ($C_3H_6O_2$)	74.079	99%
Propylene glycol ($C_3H_8O_2$)	76.095	99%

Acetol* is a by-product used in production for Propylene Glycol

Economic Feasibility

Target (per 1.000 kg PG)
Moles of PG required: 1000 g/76.095 g/mol = 13.1415 mol
Because **overall stoichiometry is 1:1:1:1**, the same moles apply to **glycerol, acetol (intermediate), H_2,** and **H_2O** where relevant.

Stepwise balances

Step 1: Dehydration
Input:
Glycerol = 13.1415 mol → 1.2103 kg
Output:
Acetol = 13.1415 mol (intermediate) → 0.9735 kg
Water = 13.1415 mol → 0.2367 kg

Step 2: Hydrogenation
Input:
Acetol = 13.1415 mol (from Step 1) → 0.9735 kg
H_2 = 13.1415 mol → 0.02649 kg
Output:
Propylene glycol = 13.1415 mol → 1.000 kg

Overall mass balance (per 1 kg PG)

Inputs
Glycerol: 1.2103 kg
H_2: 0.02649 kg
Total in = 1.23674 kg

Outputs
Propylene glycol: 1.000 kg
Water (by-product): 0.23674 kg
Total out = 1.23674 kg

Total mass in = total mass out

Required glycerol feed = 1.2103 kg
Catalyst (5% of glycerol feed): 0.05 ×1.2103 = 0.0605kg

Catalyst can be regenerated 10 times
catalyst per 1kg PG = 60 g / 10 = 6 g

Economic Feasibiliy

Glycerol required (pure basis):
1.21kg pure per 1kg Propylene Glycol

Crude glycerol required:
1.21/0.8 =1.51kg crude per 1kg Propylene Glycol

Compound	**Price** (Rs/Kg)	**Amount to be used** (in Kg)	**Cost of Raw material** (in Rs)
Crude Glycerol	30	1.510	45.39
Hydrogen	397	0.0265	10.52
Copper Chromite	1050	0.006	6.3

Approximately Price of Raw material for 1Kg Propylene Glycol = **Rs 62.21**

Other costs (labour, utilities, energy, maintenance, etc) for **1 Kg PG Rs 15**

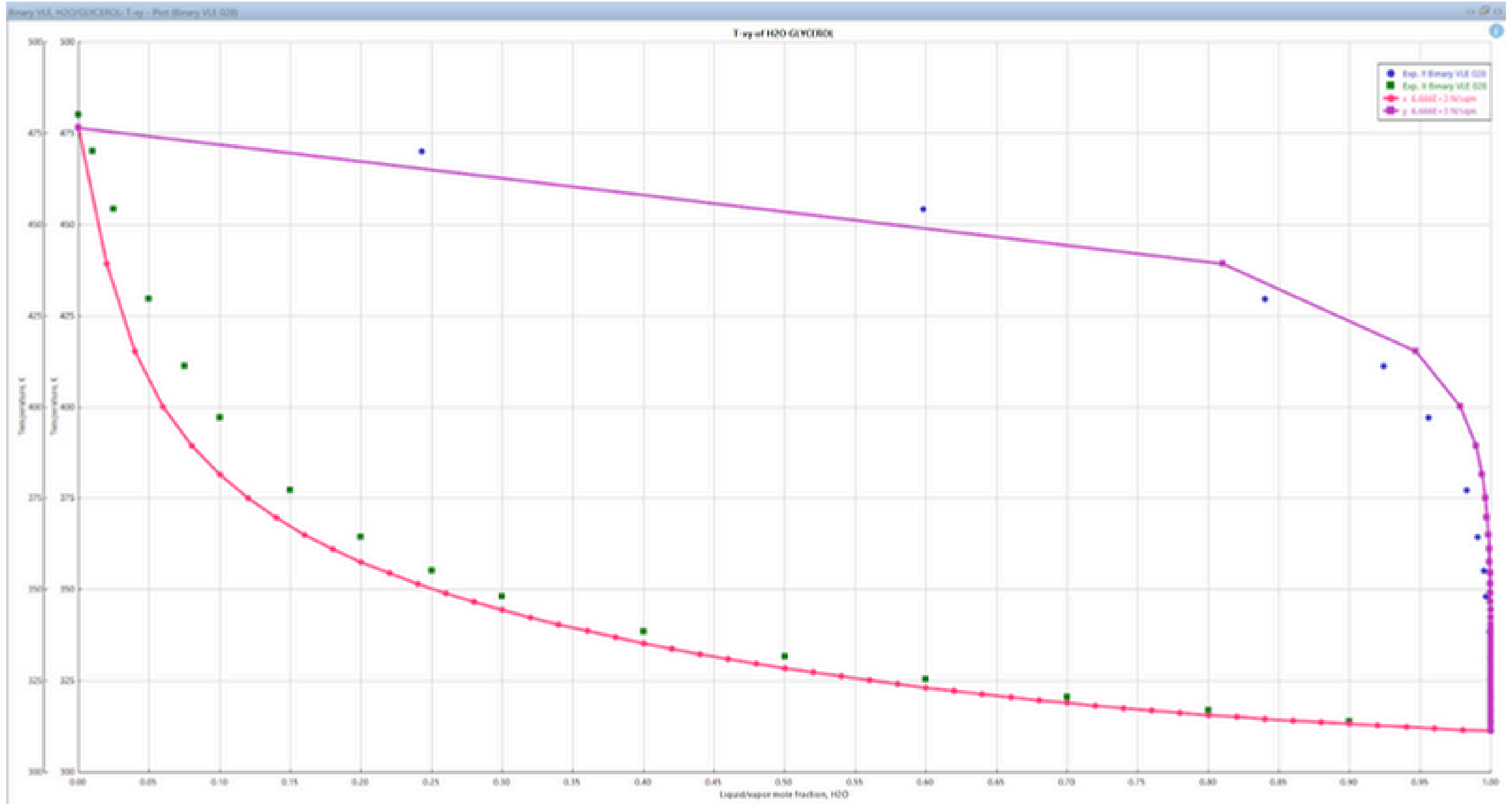
As per data, the **Retail price** of **Propylene Glycol** per Kg = **Rs 135**

Profit = Retail price - Raw material price - Other cost

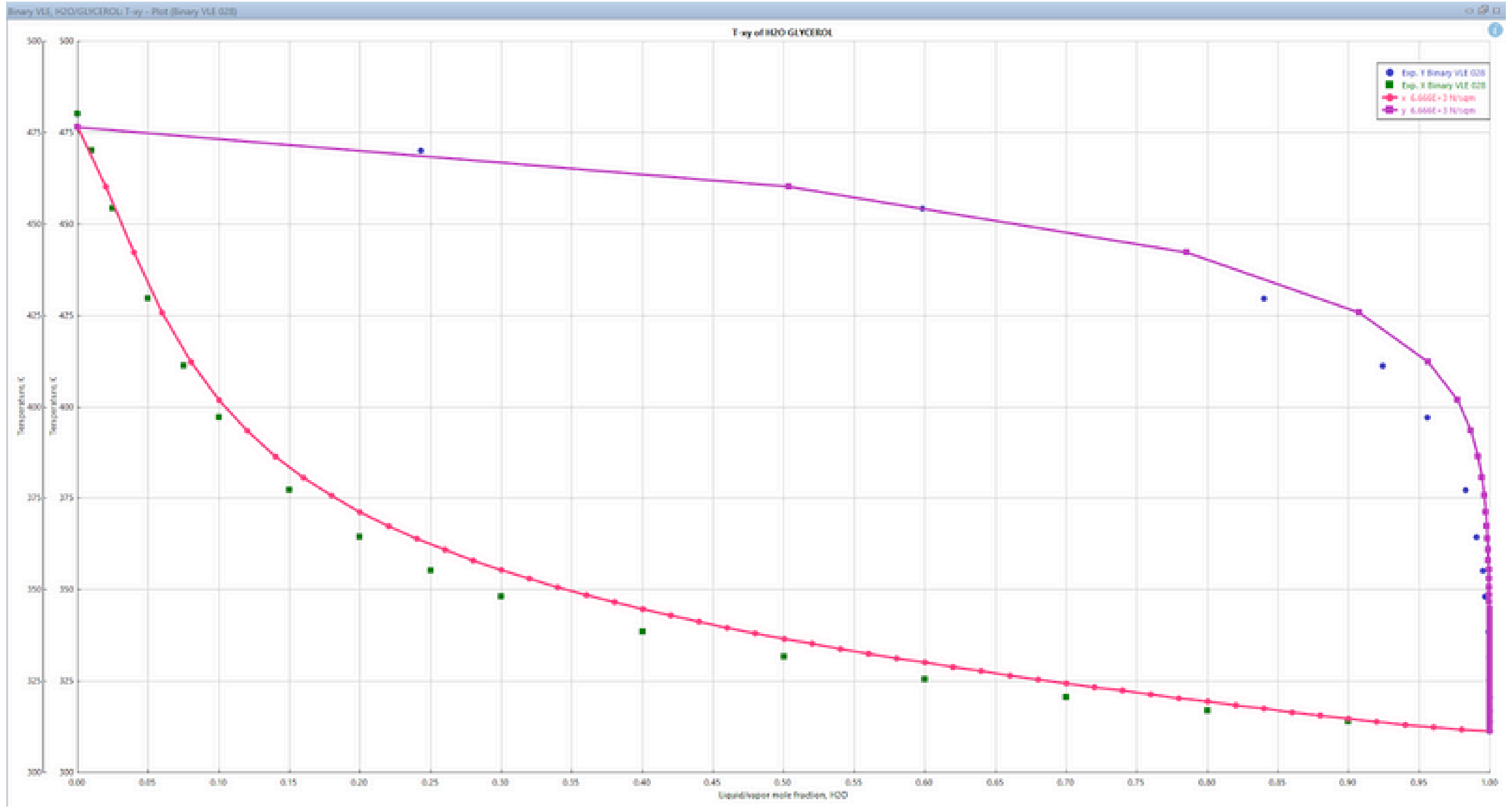
Profit = **57.79 Rs /Kg** (42.8% profit)

Thermodynamic model validation

T-xy of H_2O, Glycerol using UNIQUAC



Before regression



After regression

Model Parameters

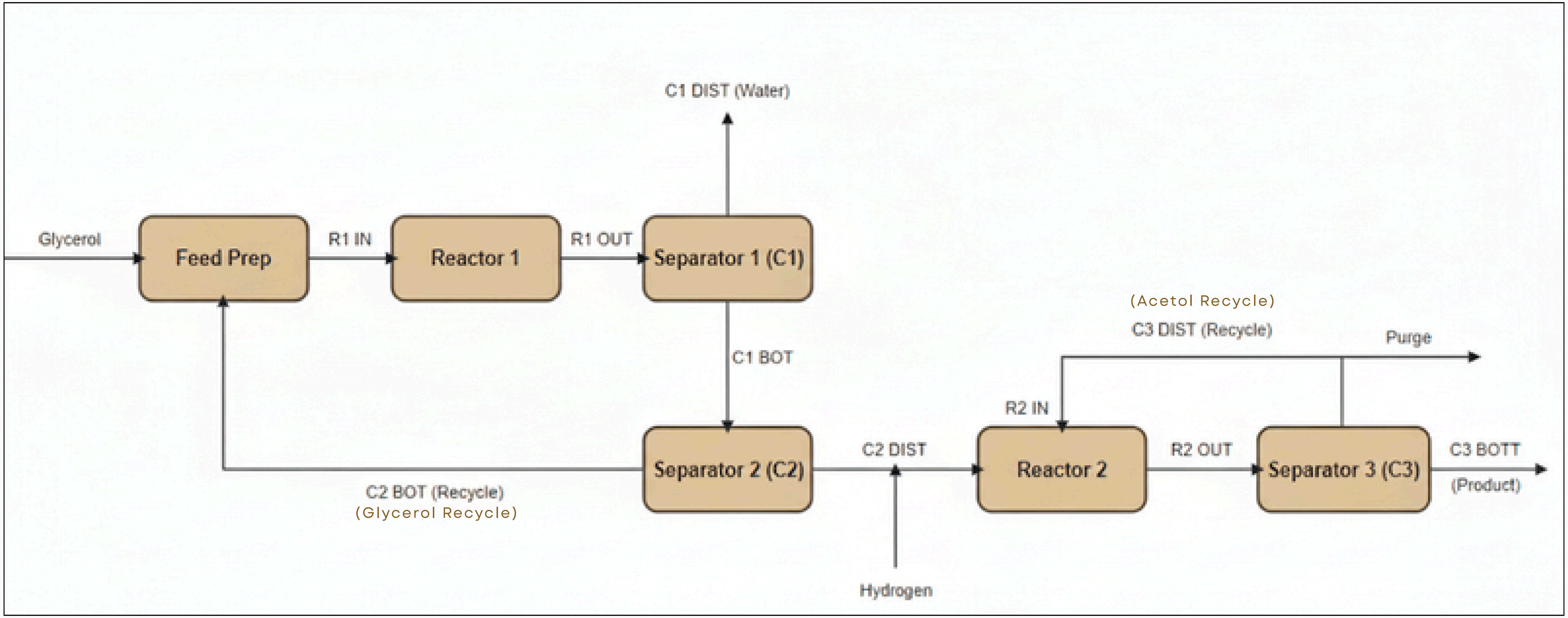
System (i–j)	Aij	Aji	Bij	Bji	Temp. Range (°C)
H_2O – Glycerol	2.03	2.87	-1064.5	-487.4	-273 - 726
H_2O – Propanediol	0	0	-268.3	248.9	15 - 100
Glycerol – Propanediol	0.4348	-0.2234	-8.72	-73.4	88.6 - 180.9

Parameter	Component i	Component j	Old Value	New Value
UNIQ/1	H_2O	Glycerol	0.976	2.03
UNIQ/1	Glycerol	H_2O	0.261	2.87
UNIQ/2	H_2O	Glycerol	-188.5	-1064.5
UNIQ/2	Glycerol	H_2O	-45.9	-487.4

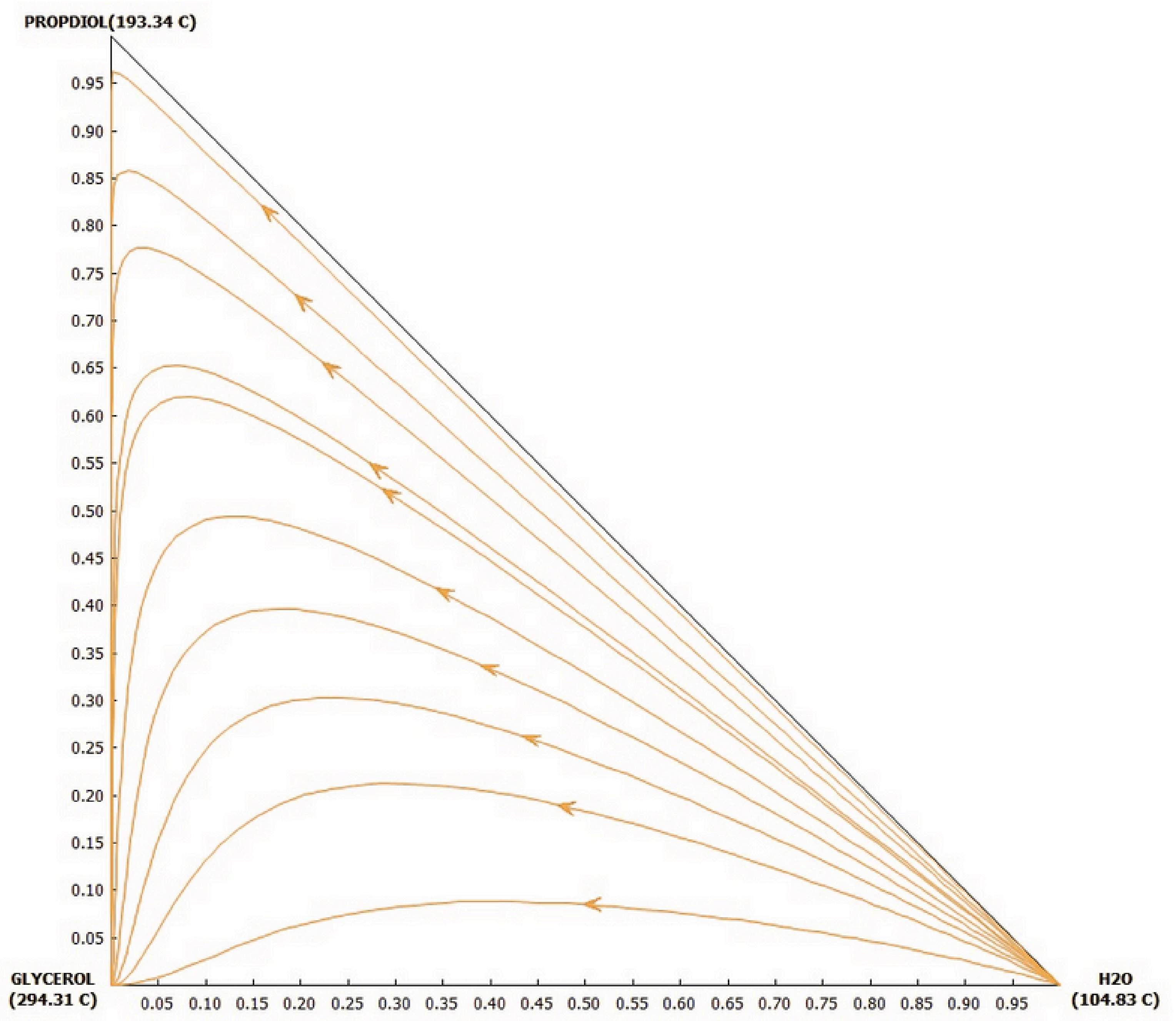
SECTION - 2

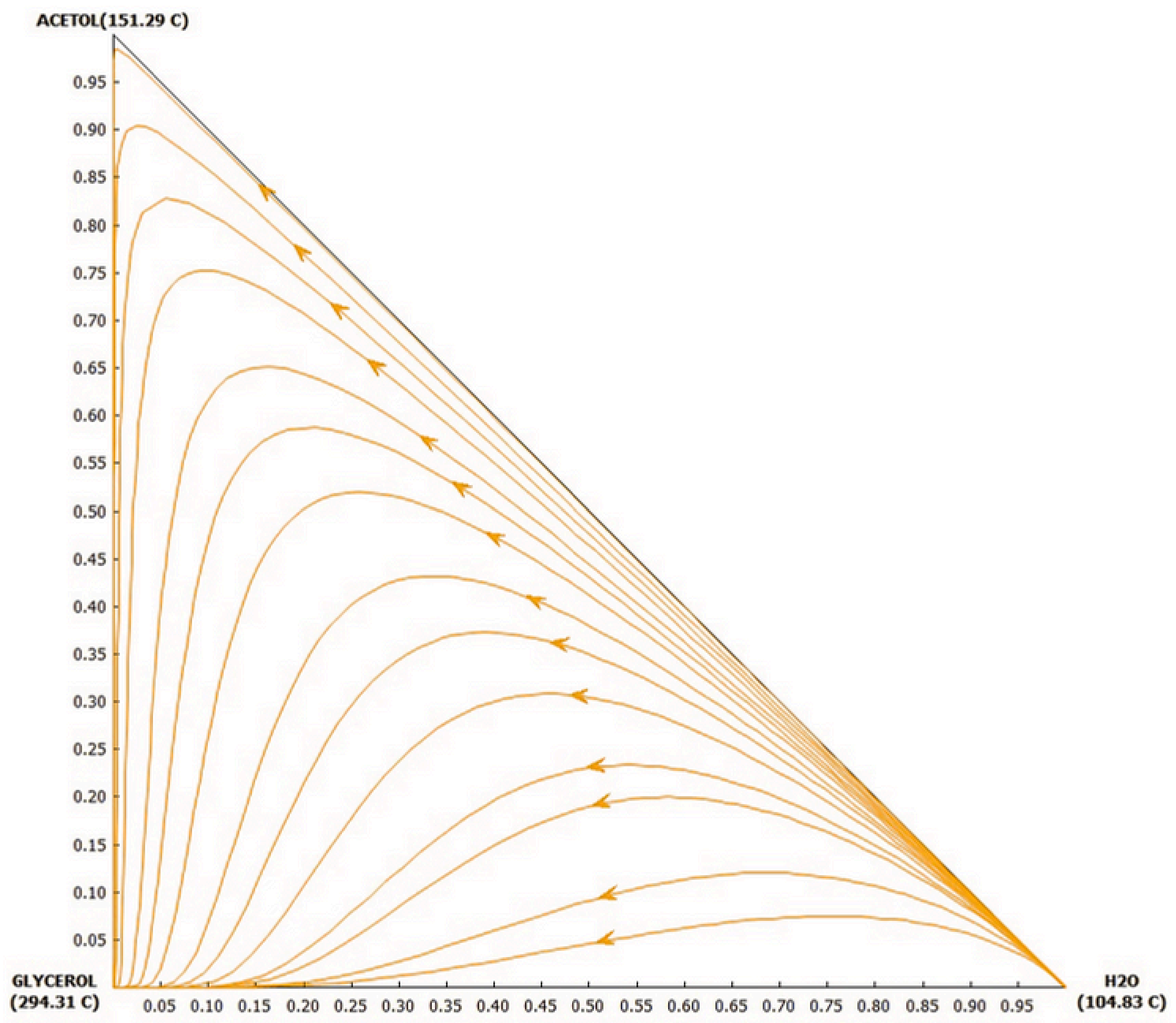
Process Synthesis & Material Balance

Block Diagram



Azeotrope Search





Process Design

Rationale for Process Design: Feed & Product Stages

- Separator 1 (C1): Removes the water produced during the dehydration reaction. Separating the water first simplifies the downstream separation of glycerol and acetol and reduces the energy load on subsequent columns.

- Separator 2 (C2): Isolates unreacted glycerol from the acetol intermediate. This provides a high-purity acetol stream for the second reactor and allows for the valuable unreacted glycerol to be recycled.

- Separator 3 (C3): As the final purification unit, this separator is critical for meeting market specifications (>99% purity). It removes unreacted acetol and hydrogen (if remaining), which are then recycled to enhance efficiency.

Process Design

Rationale for Process Design: Recycles & Purge

Glycerol Recycle (C2 Bottoms):

- What: Unreacted glycerol from Separator 2 is recycled back to the feed preparation stage.
- Why: This significantly improves the overall process economy by minimizing the consumption of fresh glycerol, thereby increasing the total conversion of raw material to product.

Acetol/Hydrogen Recycle (C3 Distillate):

- What: Unreacted acetol and hydrogen (if remaining) from the final separator are recycled back to the inlet of Reactor 2.
- Why: Hydrogen is a costly utility, and recycling it drastically reduces operating costs. Recycling the acetol intermediate ensures it gets another pass through the reactor, maximizing its conversion to the final product.

Purge Stream:

- What: A small fraction of the C3 distillate recycle stream is continuously removed.
- Why: To prevent the buildup of non-reactive impurities or trace byproducts within the recycle loop. Without a purge, these components would accumulate over time, reducing the efficiency of Reactor 2.

Material Balance

Stream ID	Description	Glycerol	Water	Acetol	Propylene Glycol	Total
R1 IN	Feed to Reactor 1	83.71	16.28	0.02	0	100
R1 OUT	Effluent from Reactor 1	18.67	81.31	65.06	0	165.03
C1 DIST	Water from Separator 1	0	81.31	0.82	0	82.13
C1 BOT	Bottoms from Separator 1	18.67	0	64.23	0	82.9
C2 DIST	Acetol to Reactor 2	0.06	0	64.21	0	64.28
C2 BOT	Glycerol Recycle	18.61	0	0.02	0	18.63
R2 IN	Feed to Reactor 2	0.06	0	64.21	0	127.78
R2 OUT	Effluent from Reactor 2	0.06	0	0.71	63.5	64.28
C3 DIST	Acetol/H_2 Recycle	0	0	0.53	0.51	1.04
C3 BOTT	Final Product Stream	0.06	0	0.19	62.99	63.24

(in kmol/hr)

SECTION - 3

Operating Conditions and Separation Design

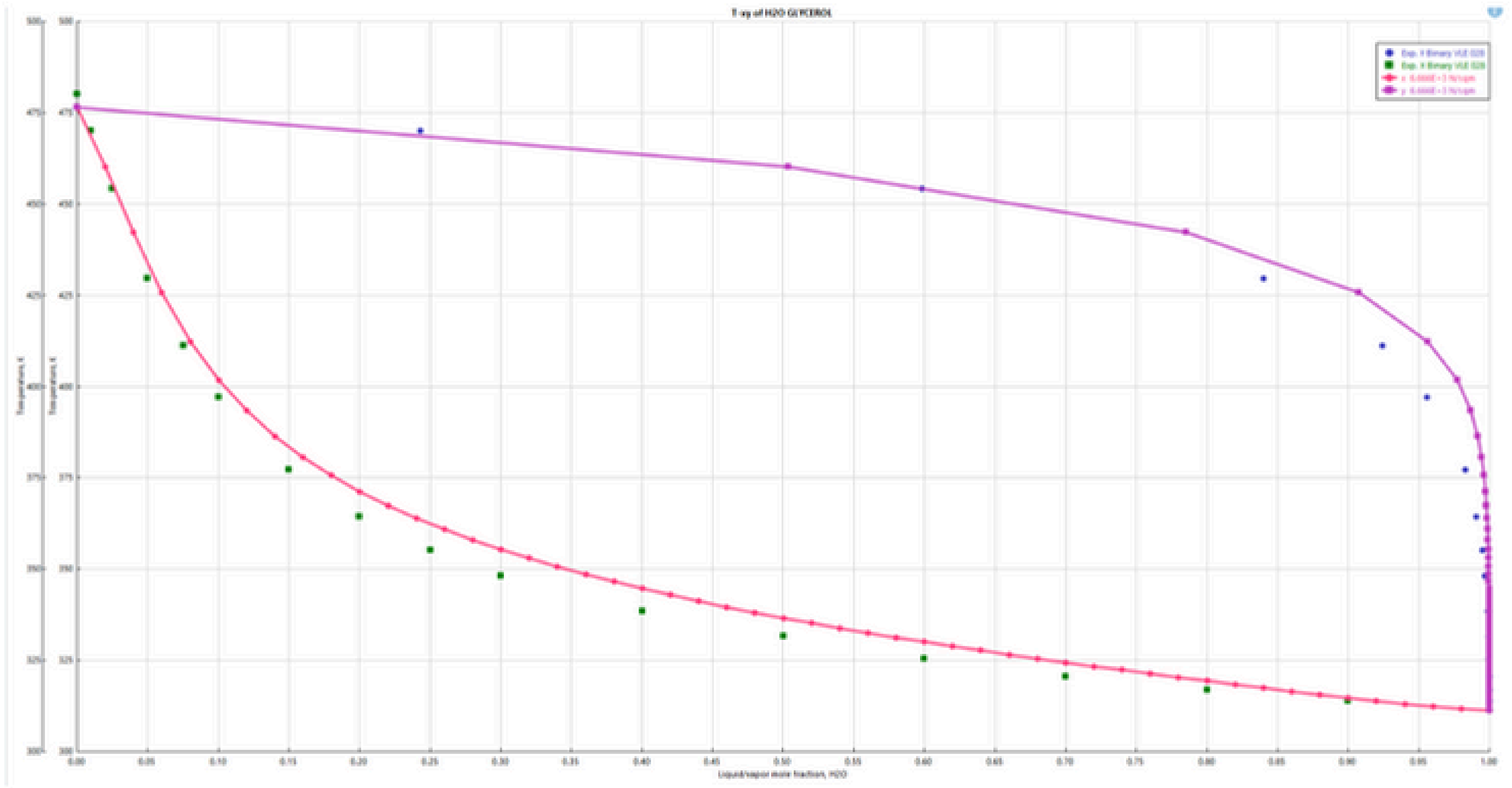
Reactor-1

Reaction Operating Conditions:
Pressure = 15 bar

Stream	Input	Output
Temperature (C)	201.673949424539	200
Pressure (bar)	15	15
Phase	Liquid	Liquid
Glycerol Mole Fraction	0.836085661323677	0.113061613056691
Water Mole Fraction	0.162555414970717	0.492329012587409
Acetol Mole Fraction	0.00135892370560524	0.3946093743559

Reactor-1

Justification Using VLE Data(input) :

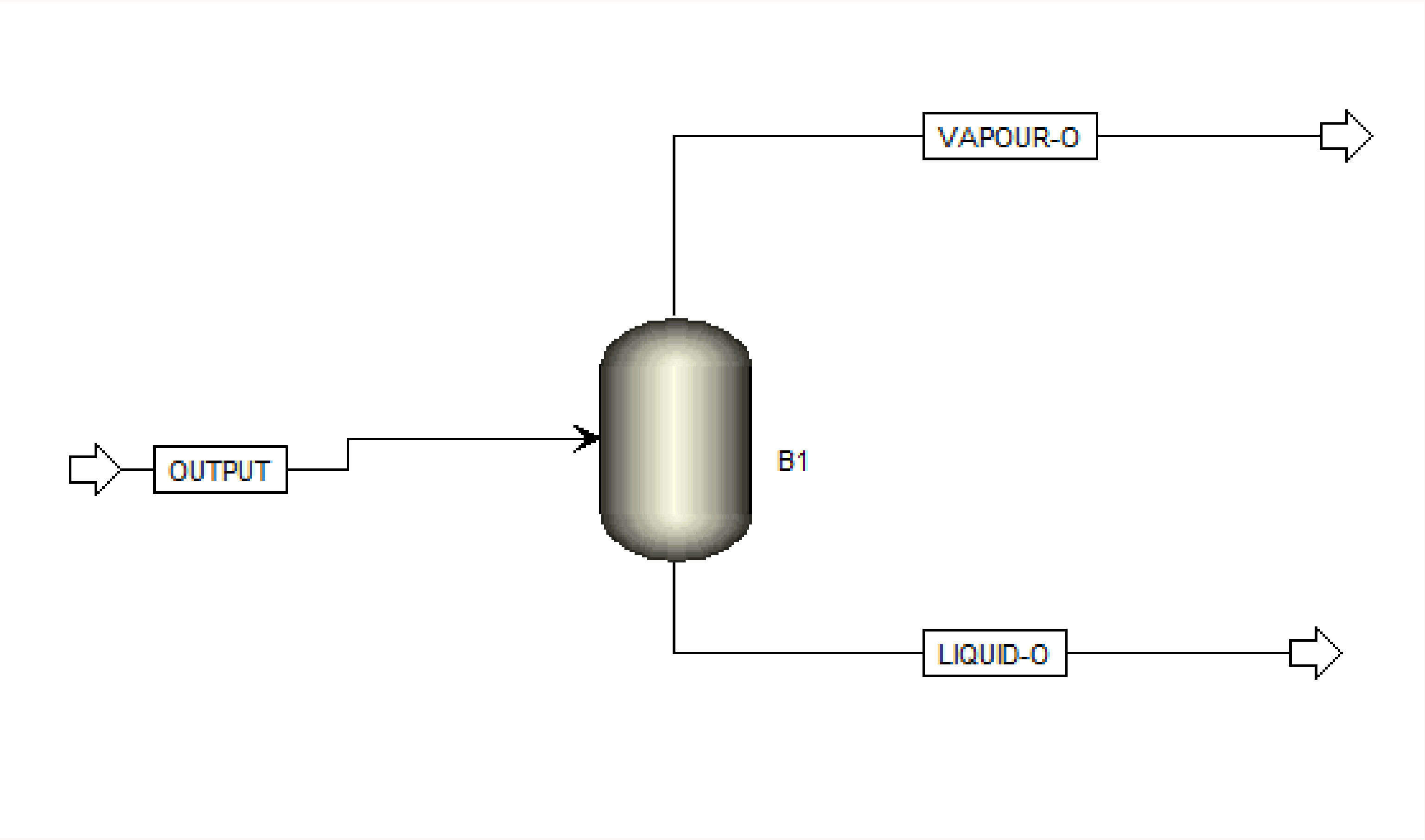


T-xy of H_2O, Glycerol using UNIQUAC (After regression)

The reactor feed consists of a water–glycerol mixture. To ensure the reactor operates in the liquid phase, a T-xy diagram at 1 atm was used to determine the bubble point temperature of the mixture. At the stream composition, the bubble point was found to be above 200 °C. Therefore, at the reactor operating temperature of 200 °C and 15 bar, the mixture is confirmed to be fully in the liquid phase. This validates the use of a liquid-phase reactor model.

Reactor-1

Justification using Flash Column (output):



Stream	Vapour-O	**LIQUID-O**
Temperature(C)	200	200
Pressure(bar)	15	15
Phase	Vapour	Liquid
Glycerol Mole Fraction	0	0.113061613056691
Water Mole Fraction	0	0.492329012587409
Acetol Mole Fraction	0	0.3946093743559

Reactor-2

Reaction Operating Conditions:

Pressure = 20 bar

Stream	Input	Output
Temperature (C)	200	200
Pressure (bar)	20	20
Phase	Vapor-Liquid	Liquid
Glycerol Mole Fraction	0.000501412926172339	0.000997343315126379
Propdiol Mole Fraction	0	0.989070594688051
Acetol Mole Fraction	0.502245822124614	0.00992940531194927

Reactor-2

Justification using Flash Column (input):

Stream	Input	Vapour-O	**LIQUID-O**
Temperature(C)	200	200	200
Pressure(bar)	20	20	20
Phase	Liquid-Vapor	Vapour	Liquid
Glycerol Molar Flows	0.0501413589718075	0.000246531021889377	0.0498948279499184
Acetol Molar Flows	50.2246492950551	13.597868551046	36.6267807440093
Hydroden Molar Flows	49.7252093459731	49.6304861617616	0.0947231842117026

Through flash results, it is evident that the reactor 2 input stream is in Liquid - Vapor phase

Reactor-2

Justification Using Flash Column(output):

Stream	Output	Vapour-O	**LIQUID-O**
Temperature(C)	200	200	200
Pressure(bar)	20	20	20
Phase	Liquid	Vapour	Liquid
Propane Diol Molar Flows	98.9073221622893	0	98.9073221622893
Glycerol Molar Flows	0.0997345744386312	0	0.0997345744386312
Acetol Molar Flows	0.992943263272049	0	0.992943263272049

Through flash results, it is evident that the reactor 2 output stream is in Liquid phase

Columns

Justification for the choice of operating conditions of columns

Properties\Column	Column 1	Column 2	Column 3
Condenser Temperature (C)	99.756424	145.196884	162.47135
Dew Point Temperature (C)	100.3	147	165
Reboiler Temperature (C)	161.021193	287.130735	191.426388
Bubble Point of Heavy Key(C)	145	148	175
Pressure (bar)	1.2	1.1	2

Conditions: The condenser temperature should be lower than dew point temperature of light key and the reboiler temperature should be higher than boiling point of Heavy key.

Column-1

Results Obtained through DSTW

Minimum Reflux ratio	**2.0149**
Actual Reflux ratio	**3.33262**
Minimum number of Stages	**15.3417**
Number of actual Stages	**24**
Feed Stage	**14.8865**
Reboiler Duty(Watt)	**3.56e+06**

Design Specifications and Optimal Reflux Ratio,Reboiler duty

Distillate: water purity ≥ 0.99 mole fraction
Optimal Reflux Ratio=3.342
Condenser Heat Duty= -4037kW
Reboiler Duty= 3560 kW

Column-2

Results Obtained through DSTW

Minimum Reflux ratio	**0.001281**
Actual Reflux ratio	**0.0151086**
Minimum number of Stages	**2.10021**
Number of actual Stages	**20**
Feed Stage	**9.31369**
Reboiler Duty(Watt)	**847526**

Design Specifications and Optimal Reflux Ratio,Reboiler duty

Distillate: acetol purity ≥ 0.99 mole fraction
Bottoms: glycerol purity ≥ 0.99 mole fraction
Optimal Reflux Ratio= 0.0177
Condenser Heat Duty= -795 kW
Reboiler Duty= 921kW

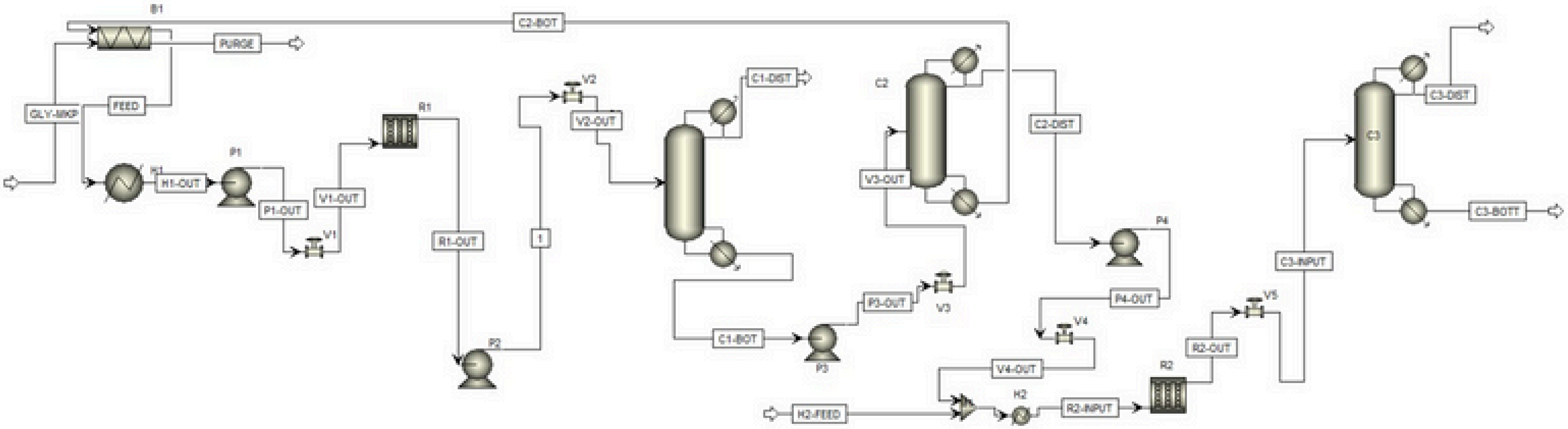
Column-3

Results Obtained through DSTW

Minimum Reflux ratio	**0.62318**
Actual Reflux ratio	**0.7556**
Minimum number of Stages	**10.7345**
Number of actual Stages	**25**
Feed Stage	**12.7499**
Reboiler Duty(Watt)	**6811617**

Design Specifications and Optimal Reflux Ratio,Reboiler duty

Bottoms: propylene glycol purity ≥ 0.99 mole fraction
Optimal Reflux Ratio= 25.4172
Condenser Heat Duty= -381.486 kW
Reboiler Duty= 341.49 kW


B1
C2-BOT
PURGE
GLY-MKP
FEED
H1-OUT
P1
P1-OUT
V1
V1-OUT
R1
R1-OUT
P2
V2
V2-OUT
C1-DIST
C1-BOT
P3
P3-OUT
V3
C2
V3-OUT
C2-DIST
P4
P4-OUT
V4
V4-OUT
H2
H2-FEED
R2-INPUT
R2
R2-OUT
V5
C3-INPUT
C3
C3-DIST
C3-BOTT

SECTION - 4

Cogeneration Power Plant and Cooling Water Loop

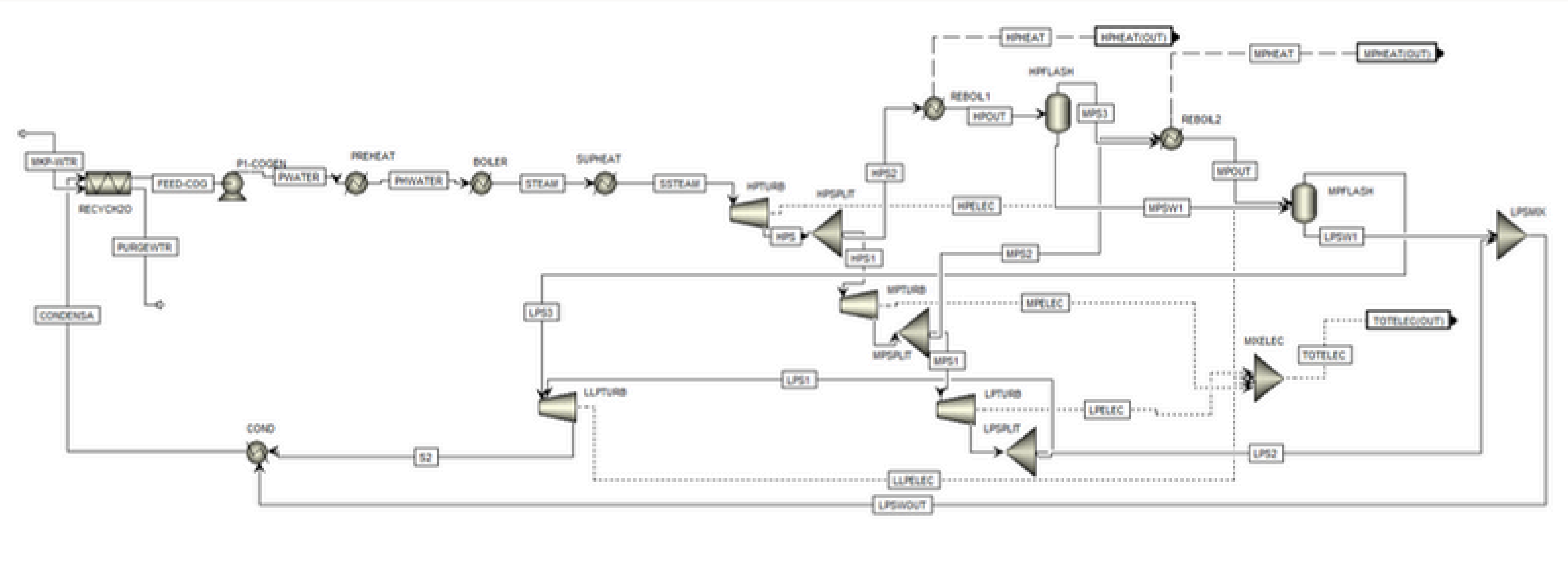
Cogeneration Power Plant

Total Energy Requirements :-

Equipment	Energy Required (Watt)	Temperature (K)	Steam Grade
Heater 1	668814.973	473.15	HP Steam
Heater 2	334530.015	473.15	HP Steam
C1 Reboiler	3560000	434.171193	HP Steam
C2 Reboiler	920299	404.772	MP Steam
C3 Reboiler	341494	464.576387	HP Steam

Total HP Steam Energy Required - **4904.839 KW**
Total MP Steam Energy Required - **920.299 KW**

Cogeneration Power Plant



Co-generation Power Plant Results

FEED-COG - **6 tonnes/hr**
MKP-WTR - **3.6e-10 tonnes/hr**

Feed Temperature - **372.699 K**
Feed Pressure - **1e5 N/sqm**

HPS2 Flow - **4.675 tonnes/hr**
MPS2 Flow - **0.55 tonnes/hr**

Total Electricity Out - **-267.2 kW**
HP Heat Out - **2914.4 kW**
MP Heat Out - **920.7 kW**

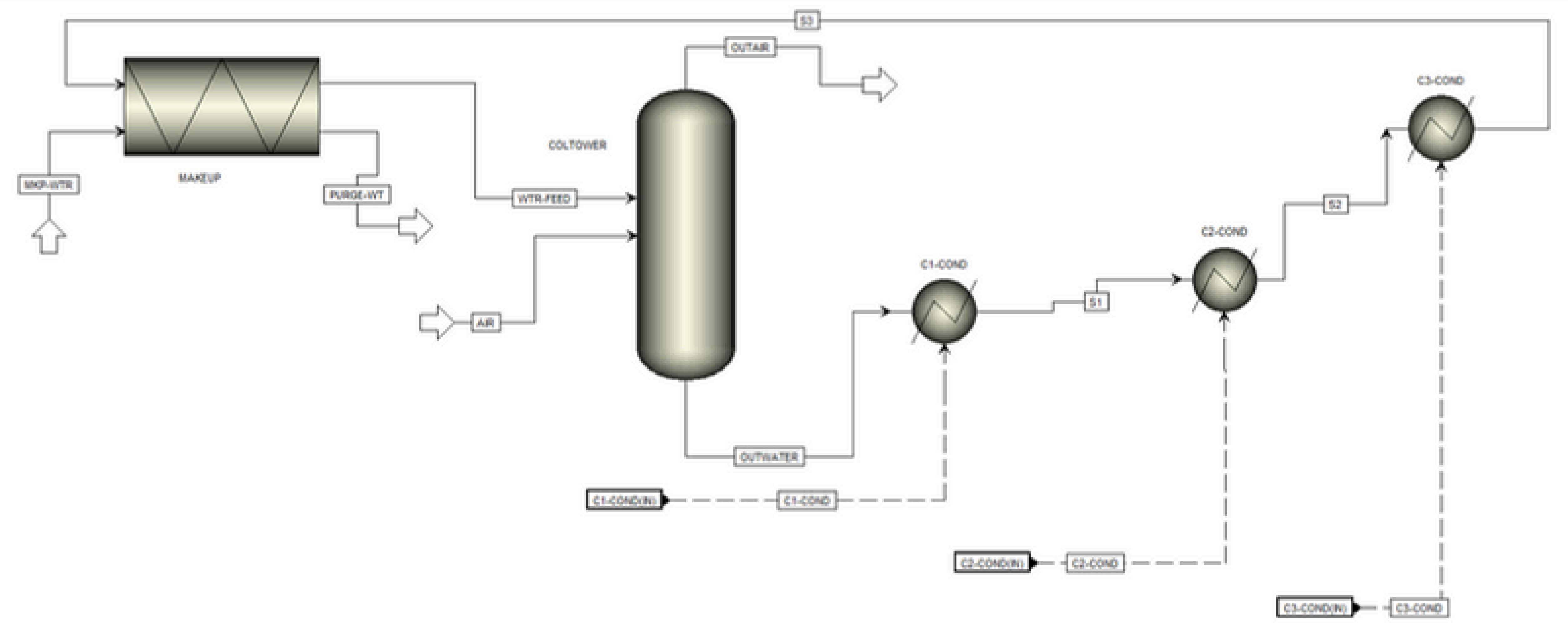
HP Heat from Reactor 1 - **507.5 kW**
HP Heat from Reactor 2 - **1483.2 kW**

Cooling Water Tower

Total Cooling Water Requirements :-

Equipment	Energy Required (Watt)	Temperature Begin (K)	Temperature End (K)
C1 Condenser	4036923.76	373.270495	372.906427
C2 Condenser	793859.642	424.666705	418.346885
C3 Condenser	381270.473	448.151285	435.621374

Cooling Water Tower



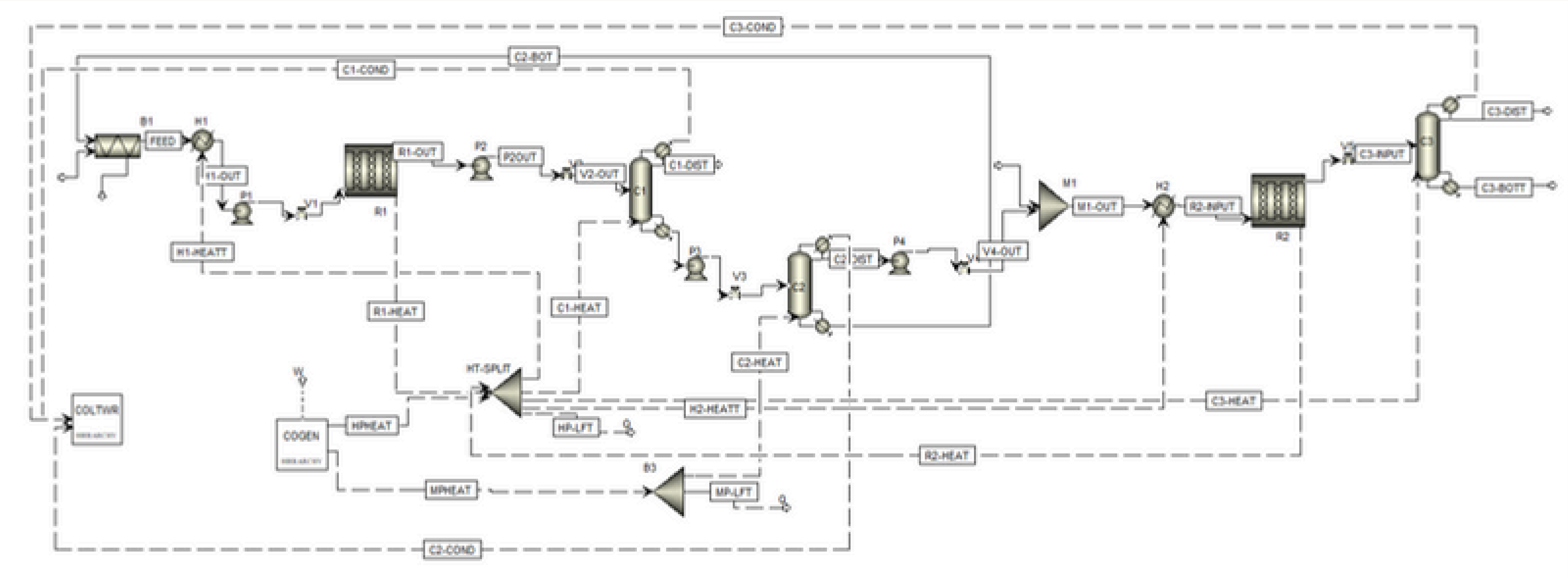
Mass Flow Rates (tonnes/hr)

WTR-FEED - **18.0154**
MKP-WTR - **6.82742**
Recycle - **11.188**

Temperatures (K)

WTR-FEED - **372.798**
OUTWATER - **292.773**
AIR - **297.15**
OUTAIR - **345.5**

Complete Flowsheet



Recycle Stream from C3-DIST to M1 before Reactor 2 is left. We plan to implement this once the reactor design is finalized, based on the detailed kinetics.

Thank You