CHE453: Process Design Capstone Project Report

Team number: 1

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Reaction Kinetics

We used a **power-law kinetic model** to simulate the reaction scheme:

1. **Glycerol → Acetol + Water**

2. **Acetol + Hydrogen → Propylene Glycol**

Reactor	Pre-exponential Factor	Activation Energy
Dehydration	$1.54*10^4$	86.56 kJ/mol
Hydrogenation	$7.16*10^3$	57.80 kJ/mol

Reactor Design and Optimization Procedure

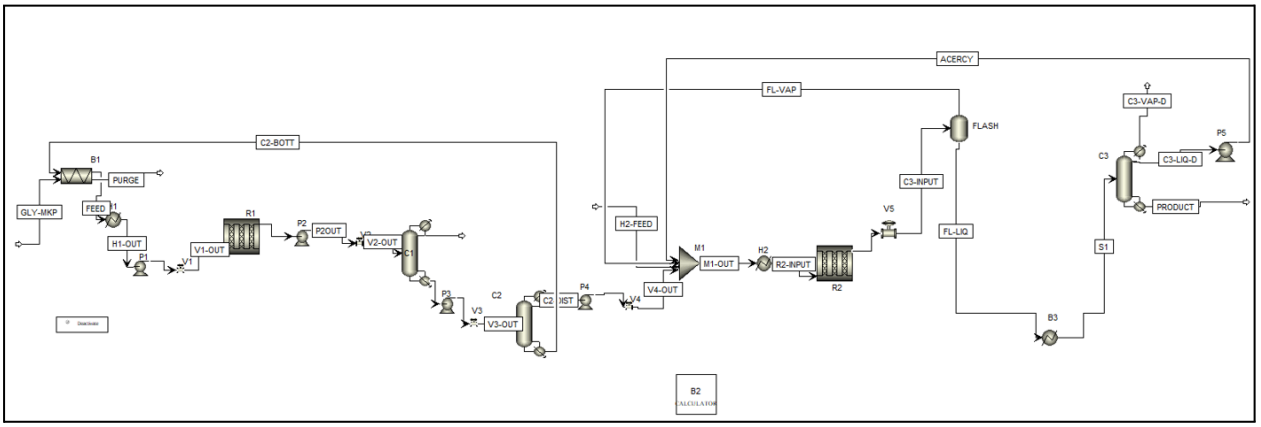
The simulation of the two-stage catalytic process was executed within the Aspen Plus environment, utilizing the **Design Specification** feature to determine the final, optimized lengths of the two Plug Flow Reactors (PFRs) required to meet specific single-pass conversion targets. With the reactor diameters fixed, the procedure involved sequentially manipulating the length of **Reactor 1 (Dehydration)** within the 10m to 100m range until the target conversion of 60.0% **Glycerol** was achieved. Subsequently, the length of **Reactor 2 (Hydrogenation)** was adjusted within its specified range of 1m to 100m to meet the target conversion of 90.0% **Acetol**, with the final converged lengths establishing the definitive design basis.

The reactor diameter is selected based on the allowable superficial velocity, while the reactor length is determined from the required conversion. Once the throughput and kinetics are defined, the resulting superficial velocity must be verified to remain below the maximum allowable limit to prevent catalyst attrition and ensure safe hydrodynamic operation.

The Langmuir–Hinshelwood rate expression was used because the reaction occurs on a catalytic surface and involves adsorption of reactants prior to the surface reaction step. This model accounts for competitive adsorption, surface coverage effects, and rate inhibition at high concentrations, making it more accurate than a simple power-law expression for heterogeneous catalytic reactions.

Reactor	Design Specification	Length (metre)	Diameter (metre)
Reactor 1 (Dehydration) (PFR)	Single Pass Conversion (Glycerol) = 60%	37.890	3.5
Reactor 2 (Hydrogenation) (PFR)	Single Pass Conversion (Acetol) = 90%	40.348	5

Simulation of the overall process including recycle loops



In the **R2 reactor**, the products include **hydrogen and acetol**. Since hydrogen has a **very low (negative) critical temperature**, it **cannot be condensed under typical distillation conditions**. As a result, hydrogen cannot be separated efficiently in a conventional distillation column. Distillation relies on condensation of the light component, but hydrogen remains in the gas phase even at very low temperatures, making separation through standard column operation impractical.

To handle this, the process uses a **flash separator**, which is the most suitable option. A flash unit allows phase separation based on vapor–liquid equilibrium without requiring full condensation of hydrogen. Hydrogen naturally exits as the vapor stream, while acetol and heavier components remain in the liquid phase. This vapor-phase hydrogen stream is then **recycled back to the reactor**.

Following the flash, a **distillation column with a partial condenser** is employed. Only trace amounts of hydrogen appear in the overhead, along with acetol. The acetol is subsequently recovered and **recycled** for improved conversion, while the residual hydrogen leaves with the vapor.

Why a flash separator is the best option:

- Hydrogen cannot be liquefied under normal process conditions due to its extremely low critical temperature (−240 °C).

- Distillation cannot condense hydrogen, so a column would fail to create vapor–liquid equilibrium for H_2 separation.
- Flash separation relies only on natural phase splitting and does not require hydrogen condensation, making it simple, energy-efficient, and inherently compatible with hydrogen-rich mixtures.
- Flash units operate at moderate temperatures and pressures and allow easy recovery of unreacted hydrogen for recycling.

Results & key insights of flash column (operated at 298K, 1 bar)

Basis: Mole

Condenser / Top stage performance

Name	Value	Units
Temperature	417.961	K
Subcooled temperature		
Heat duty	-342917	Watt
Subcooled duty		
Distillate rate	0.00137805	kmol/sec
Reflux rate	0.00647382	kmol/sec
Reflux ratio	4.6978	
Free water distillate rate		
Free water reflux ratio		

Reboiler / Bottom stage performance

Name	Value	Units
Temperature	459.173	K
Heat duty	467000	Watt
Bottoms rate	0.0142691	kmol/sec
Boilup rate	0.00895983	kmol/sec
Boilup ratio	0.627919	
Bottoms to feed ratio		

	Units	C3-INPUT	FL-LIQ	FL-VAP
Average MW		69.2182	75.8927	2.06244
− Mole Flows	**kmol/hr**	**61.9282**	**56.3297**	**5.59849**
H2O	kmol/hr	0.0036	0.00358911	1.08894e-05
H2	kmol/hr	5.6046	0.0097142	5.59489
GLYCEROL	kmol/hr	0.0507883	0.0507883	9.96294e-10
PROPDIOL	kmol/hr	50.662	50.6611	0.000939232
ACETOL	kmol/hr	5.60722	5.60457	0.0026494
N2	kmol/hr	0	0	0
O2	kmol/hr	0	0	0
− Mole Fractions				
H2O		5.81318e-05	6.37161e-05	1.94506e-06
H2		0.0905016	0.000172453	0.999357
GLYCEROL		0.000820115	0.000901625	1.77958e-10
PROPDIOL		0.818076	0.899366	0.000167765
ACETOL		0.0905439	0.0994959	0.000473236
N2		0	0	0
O2		0	0	0
+ Mass Flows	**kg/sec**	**1.19071**	**1.1875**	**0.00320738**

Property	Key Values	Inference
Hydrogen in vapor	5.59489 kmol/hr	Confirms flash is perfect for H_2 recycle; cannot use distillation.
Hydrogen in liquid	0.0097 kmol/hr	Shows negligible solubility.
Acetol in liquid	5.60457 kmol/hr	Acetol is retained for recycling.
Propylene glycol in liquid	50.661 kmol/hr	Desired product remains in the reactor liquid phase.
Total vapor flow rate	5.59849 kmol/hr	Determines compressor/recycle design.
Liquid flow rate	56.3297 kmol/hr	Used for pump, downstream column design.

Results of distillation column after flash column (operated at 298K, 1 bar)

	Units	S1	C3-LIQ-D	C3-VAP-D	PRODUCT
Average MW		75.8927	74.1293	71.1006	76.0776
− **Mole Flows**	**kmol/hr**	**56.3297**	**4.71294**	**0.24805**	**51.3687**
H2O	kmol/hr	0.00358911	0.00277028	0.000818787	4.4536e-08
H2	kmol/hr	0.0097142	3.02995e-05	0.00968391	2.89162e-26
GLYCEROL	kmol/hr	0.0507883	1.5456e-21	3.36383e-25	0.0507883
PROPDIOL	kmol/hr	50.6611	0.194696	0.002417	50.4639
ACETOL	kmol/hr	5.60457	4.51545	0.23513	0.853997
N2	kmol/hr	0	0	0	0
O2	kmol/hr	0	0	0	0
− **Mole Fractions**					
H2O		6.37161e-05	0.000587802	0.0033009	8.66987e-10
H2		0.000172453	6.42899e-06	0.0390402	5.62914e-28
GLYCEROL		0.000901625	3.27949e-22	1.35611e-24	0.0009887
PROPDIOL		0.899366	0.0413109	0.00974402	0.982386
ACETOL		0.0994959	0.958095	0.947915	0.0166248
N2		0	0	0	0
O2		0	0	0	0
+ **Mass Flows**	**kg/sec**	**1.1875**	**0.0970465**	**0.00489903**	**1.08556**

Calculator Block

A calculator block was used to calculate the appropriate amount of additional hydrogen to be given as feed so that the **ratio** of total feed hydrogen to the acetol received from the second distillation column is **1:1.**

Equation Used:

```
H2 = ACET-H2RCY+ACERCY
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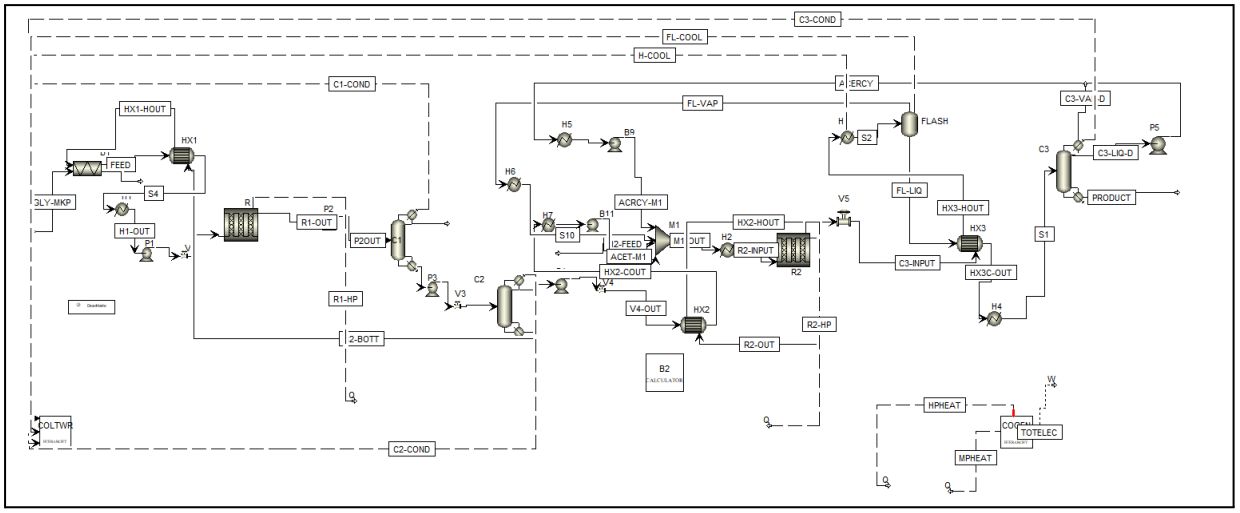
Heat Exchanger Design



H1 : Inlet and Outlet Conditions for Hot and Cold Streams

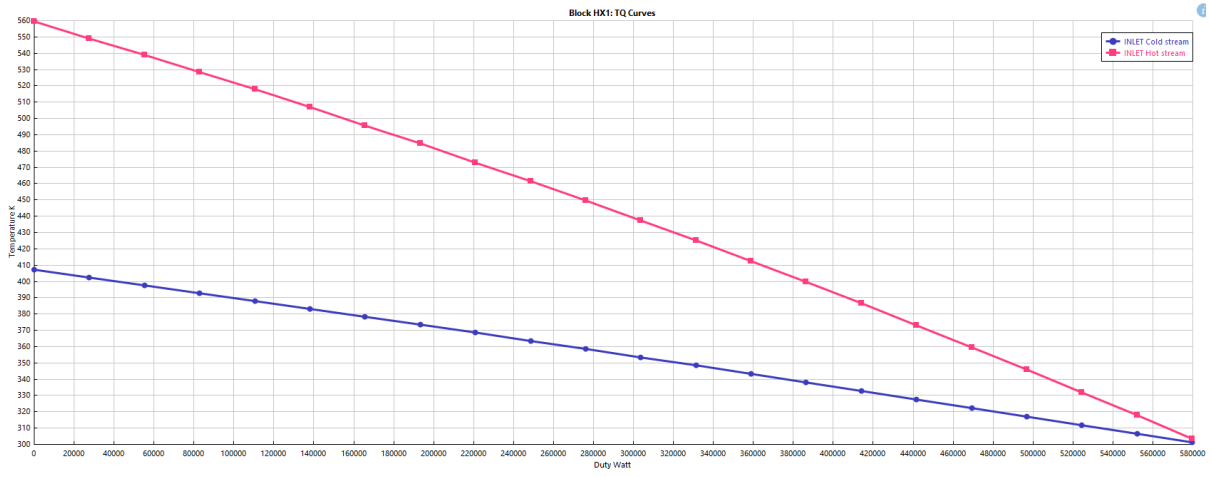
Parameter	Hot Stream (Inlet)	Hot Stream (Outlet)	Cold Stream (Inlet)	Cold Stream (Outlet)
Temperature (K)	559.35	311.307	304.219	407.266
Pressure (N/sqm)	100001	98136.1	98135.7	93670.2
Vapor Fraction	0	0	0	0
1st Liquid / Total Liquid	1	1	0	0

H1: Thermal Performance

Parameter	Shell Side	Tube Side
Mean metal temperature (K)	369.504699	350.947
Bulk film coefficient (W/m²·K)	184.266	123.462
Wall film coefficient (W/m²·K)	184.266	123.462
Thermal resistance (m²·K/W)	0.005420695	0.008099068
Film % overall resistance	39.9823	59.6733

H1 ΔP Results

Parameter	Shell Side (N/m²)	Tube Side (N/m²)
Total pressure drop	1864.54802	4465.48
Frictional pressure drop	1864.58	4465.42
Window pressure drop	2.99369	0



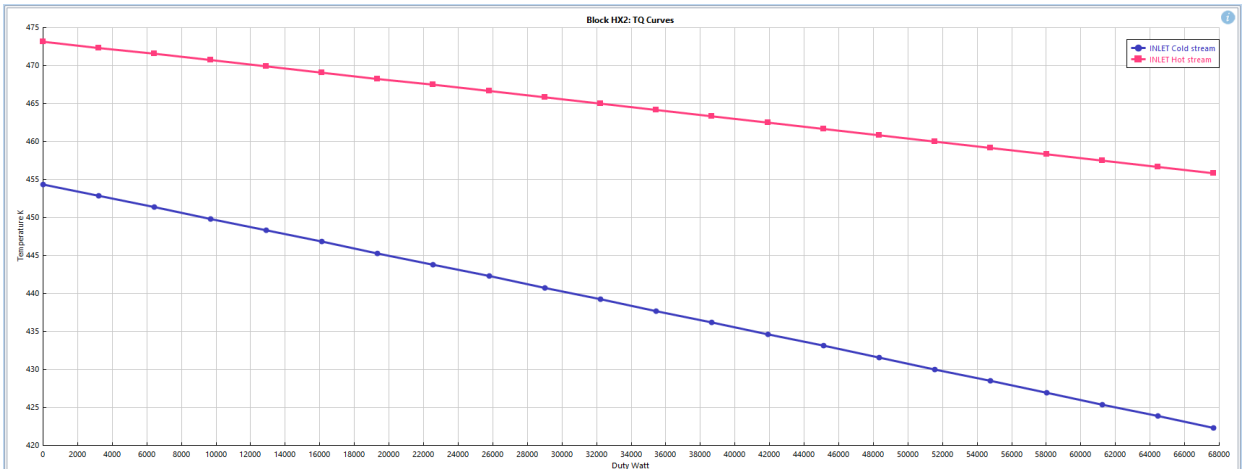
TQ Curve for H1 Exchanger

H2 : Inlet and Outlet Conditions for Hot and Cold Streams

Parameter	Hot Stream (Inlet)	Hot Stream (Outlet)	Cold Stream (Inlet)	Cold Stream (Outlet)
Temperature (K)	473.15	455.86	422.306	454.343
Pressure (N/m²)	2e+06	1.99273e+06	2e+06	1.99018e+06
Vapour fraction	0.081985	0.0790778	0	0
Liquid fraction	1	1	1	1

H2 ΔP Results

Parameter	Shell Side (N/m²)	Tube Side (N/m²)
Total pressure drop	7270.99846	9823.84
Frictional pressure drop	7262.76	9788.24
Window pressure drop	566.767	0

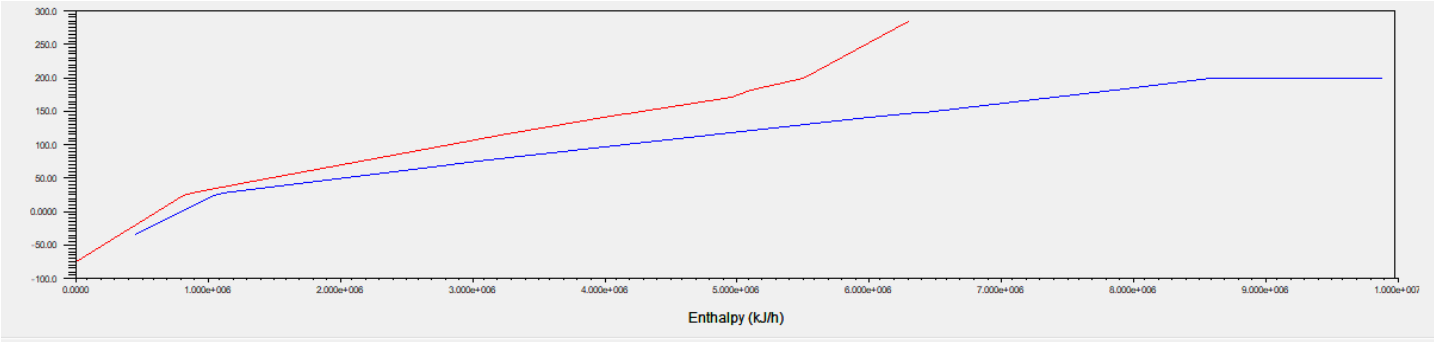


TQ Curve for H2 Exchanger

H3 : Inlet and Outlet Conditions for Hot and Cold Streams

Parameter	Hot Stream (Inlet)	Hot Stream (Outlet)	Cold Stream (Inlet)	Cold Stream (Outlet)
Temperature (K)	445.423	375.423	298.15	389.659
Pressure (N/m²)	192729	192729	100000	100000

Vapour fraction	0.126669	0.079851	0	1.88227e-05
Liquid fraction	1	1	1	1



Composite Curves (Pinch can be seen at the start)

Energy Savings Due to Heat Exchanger Integration

Steam Type	Before (kW)	After (kW)	Reduction (kW)
HP Steam	4904.84	1059.8	3845.04
MP Steam	920.00	366.69	553.31

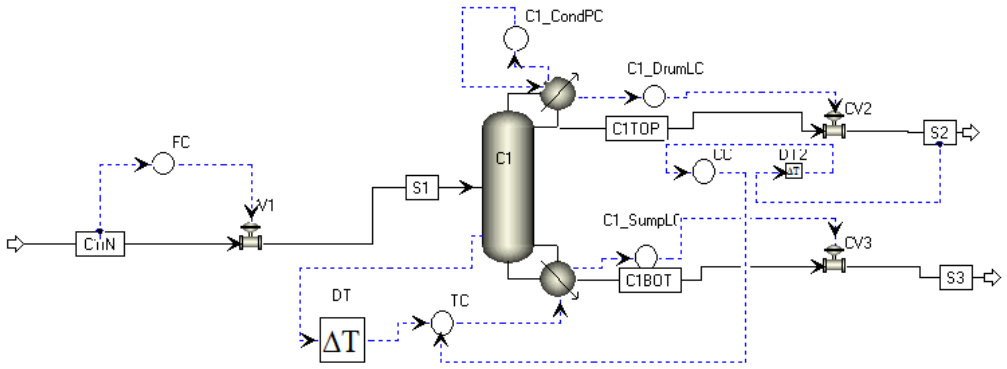
Dynamics and control design for the distillation block

The distillation block on which we implemented the complete dynamics and control configuration is characterized by the following key specifications:

Design Spec - 0.09 acetol from distillate

Feed Stage - 15

The figure shows a standard distillation column control configuration consisting of pressure (PC), level (LC), flow (FC), temperature (TC), and composition (CC) controllers connected to their respective control valves (CVs). Together, these maintain column stability and ensure product purity under varying operating conditions.



Feed Flow Control (FC)

The feed flow controller maintains a constant feed rate to the column by measuring inlet flow and adjusting the feed valve (V1). This direct-acting control loop stabilizes the vapor–liquid traffic within the column and prevents disturbances from propagating to the separation section.

Pressure Control (C1_CondPC)

The column top pressure controller manipulates condenser duty. When pressure increases, condenser cooling is increased to condense more vapor; when pressure drops, cooling is reduced. This direct-acting PID controller ensures vapor–liquid equilibrium, prevents flooding or weeping, and maintains safe operating pressure.

Reflux Drum Level Control (C1_DrumLC)

This controller maintains the liquid level in the reflux drum by adjusting the distillate product valve (CV2). If the drum level rises, the valve opens to remove more distillate; if it falls, the valve closes. Being reverse-acting, it ensures adequate reflux flow and prevents liquid carryover to the overhead lines.

Bottom Sump Level Control (C1_SumpLC)

The bottom level controller manipulates the bottom product valve (CV3). When the reboiler sump level increases, CV3 opens to withdraw more bottoms; when it decreases, the valve closes. This reverse-acting loop prevents reboiler dry-out, overheating, or internal flooding.

Temperature Control (TC)

The temperature controller maintains the column's separation by regulating the temperature at a selected tray (here, stage 7). It adjusts reboiler duty (ΔT) to maintain the setpoint. If temperature falls, heat input is increased; if it rises, duty is reduced. Since an increase in controller output increases temperature, this is a reverse-acting controller. Tray 7 is chosen because it shows the greatest sensitivity (ΔT) to composition changes near the feed stage.

Composition Control (CC)

A composition controller is added to ensure precise product purity, typically by regulating either overhead or bottom composition. The analyzer measures the mole fraction of a key component, and the controller adjusts a relevant manipulated variable—commonly reflux flow for top composition or reboiler duty/bottoms rate for bottom composition.

- If **overhead composition** deviates from setpoint, the controller adjusts the reflux valve (CV2) or reflux ratio to correct purity.

- If **bottoms composition** deviates, the controller adjusts bottoms withdrawal (CV3) or reboiler heat input.

This slow-acting but critical loop complements the temperature controller, correcting long-term composition drift and ensuring specification compliance.

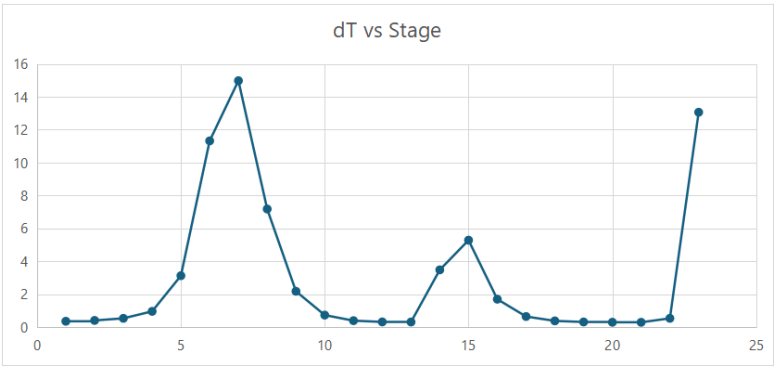
Procedure:

1. Steady-State Design:
   The column was first modeled in Aspen Plus with defined feed composition, pressure, and number of stages. Steady-state convergence ensured proper material and energy balances.

2. Switch to Dynamics Mode:
   The model was transferred to Aspen Dynamics, where control valves replaced product outlets, and PID controllers were added for pressure, level, temperature, and flow.

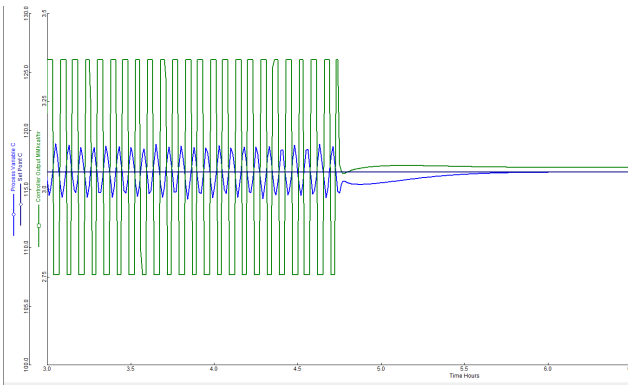
3. Controller Configuration:
   Each control loop was assigned a measurement, a controller block, and a control valve. Controller types (direct or reverse) were selected based on process behavior.

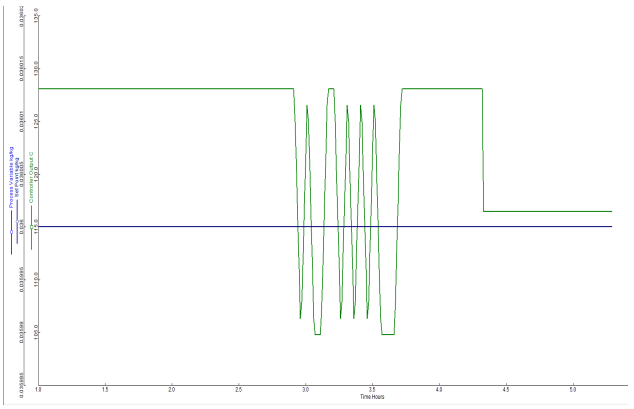
4. Dynamic Simulation:
   The column was initialized to steady-state and then subjected to disturbances (feed flow or composition changes). The response of pressure, temperature, and levels was observed over time. Controller parameters (gain, integral time) were tuned for stability.

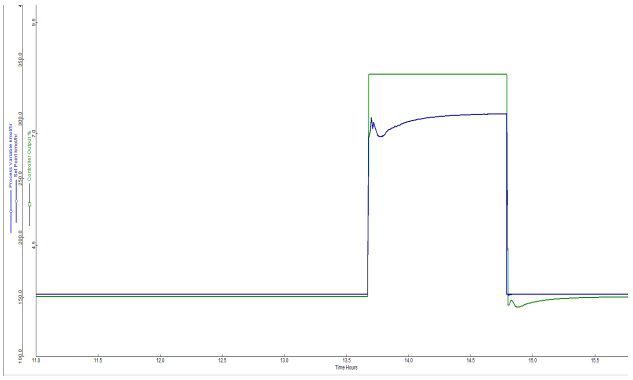


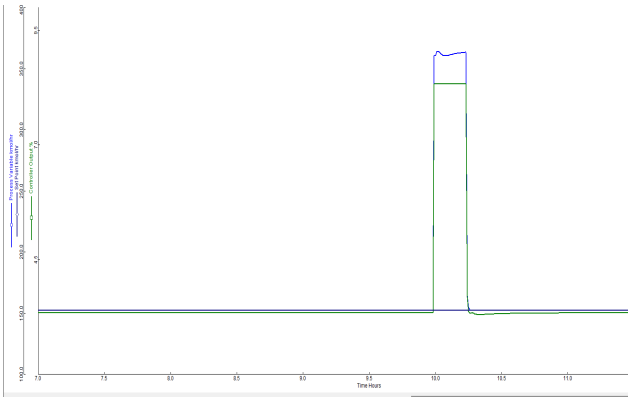
The plot shows the temperature difference (ΔT) across various column stages.The tray (here stage 7) with the largest temperature difference (around the feed stage) is best suited for the temperature control loop.

Dynamic response plots for all controllers were generated after performing Auto-Tune Variation (ATV) tests to obtain optimized PIDparameters









Technoeconomic Analysis

Parameter	Value	Remarks / Cost
Total molar flow of product	51.37 kmol/hr	
Target production	30,000 tonnes per year	
Total production time	7,684 hours per year	Calculated as target production ÷ production per hour
Selling price of Propylene Glycol	Rs. 135 per kg	
Total product worth		Rs. 405 Crores per year
Raw Material Details		
Glycerol feed	100 kmol/hr (59,320 tonnes/year)	Cost: Rs. 30/kg → Rs. 178 Crores/year
Hydrogen feed	53 kmol/hr (821 tonnes/year)	Cost: Rs. 397/kg → Rs. 32.59 Crores/year
Copper Chromite (Catalyst)	216 tonnes/year	Cost: Rs. 1,050/kg → Rs. 22 Crores/year

1. Assumptions Table

Item	Value
Plant CAPEX	₹199 crore(Aspen cost index)
Land Cost	₹20 crore
Total CAPEX (Year 0)	₹219 crore
Project Life	7 years
Depreciable Capital	₹199 crore
Depreciation Method	Straight-line
Annual Depreciation	₹28.43 crore/year
Annual Revenue	₹405 crore

Annual Operating Cost (OPEX)	₹235.215 crore (Aspen simulation)
EBITDA	₹169.785 crore/year
Corporate Tax Rate (India 115BAA)**	22%
Discount Rate	10%
Salvage Value – Plant (10%)	₹19.9 crore
Salvage Value – Land (full)**	₹20 crore
Total Salvage at Year 7	₹39.9 crore

2. Profitability Calculation (with 22% Tax)

Item	Value (₹ crore/year)
Revenue	405.000
OPEX	235.215
EBITDA	169.785
Depreciation	28.430
EBIT	141.355
Tax @22%	31.098
Net Income	110.257
Add: Depreciation	28.430
Operating Cash Flow (OCF)	138.687 crore/year

3. Discounted Cash Flow (10% Discount Rate)

Year	Cash Flow (₹ Cr)	Discount Factor	Discounted CF (₹ Cr)	Cumulative DCF
0	−219.000	1.000	−219.000	−219.000
1	138.687	0.909	126.000	−93.000
2	138.687	0.826	114.600	21.600
3	138.687	0.751	104.200	125.800

4	138.687	0.683	94.700	220.500
5	138.687	0.621	86.200	306.700
6	138.687	0.564	78.200	384.900
7	178.587	0.513	91.600	476.500

4. Final Economic Indicators

Metric	Result
Simple Payback Period	1.29 years
Discounted Payback Period	≈ 2.0 years
NPV @10%	₹476.5 crore
IRR	≈ 56%
Project Lifetime	7 years
Conclusion	Strongly profitable