Bi-Weekly Report 4

Team number: 1

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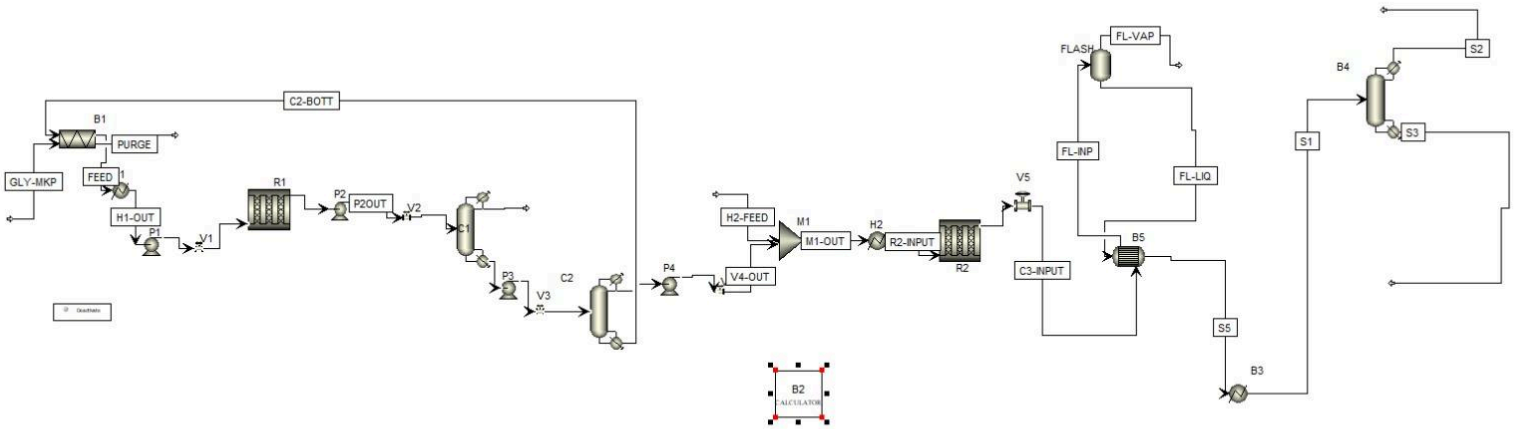
Objectives

This report focuses on four key deliverables: the design of additional separation units to enhance overall process efficiency; the detailed design and sequencing of reactors based on comprehensive kinetic analysis; the complete design of a selected heat exchanger to ensure optimal heat transfer performance; and the simulation of the overall process, incorporating recycle loops to evaluate system integration and performance.



Reaction Kinetics

The rate laws (rate expressions) for the dehydration and hydrogenation reactions described in the context of glycerol hydrogenolysis are based on a two-site Langmuir-Hinshelwood (L-H) kinetic model.

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 (Reactor 1: 3 m, Reactor 2: 4m), 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.

Reactor	Design Specification	Length (metre)	Diameter (metre)
Reactor 1 (Dehydration) (PFR)	Single Pass Conversion (Glycerol) = 60%	97.6974	3
Reactor 2 (Hydrogenation) (PFR)	Single Pass Conversion (Acetol) = 90%	57.8484	4

Heat Exchanger Design

The outlet stream from Reactor 2 is cooled before being fed to the flash column. The flash liquid stream is used for this cooling, during which its temperature increases before it enters the final RadFrac column. This heat integration scheme will be further optimized in our study.

	Units	C3-INPUT	FL-LIQ	FL-INP	S5
− **MIXED Substream**					
Phase			Liquid Phase		
Temperature	K	454.473	298.15	359.8	425.03
Pressure	N/sqm	200000	300000	200000	300000
Molar Vapor Fraction		0.180648	0	0.0917063	7.93502e-05
Molar Liquid Fraction		0.819352	1	0.908294	0.999921
Molar Solid Fraction		0	0	0	0
Mass Vapor Fraction		0.100972	0	0.00394437	1.23288e-05
Mass Liquid Fraction		0.899028	1	0.996056	0.999988
Mass Solid Fraction		0	0	0	0
Molar Enthalpy	J/kmol	-4.08429e+08	-4.86994e+08	-4.31932e+08	-4.61155e+08
Mass Enthalpy	J/kg	-5.90228e+06	-6.41874e+06	-6.24193e+06	-6.07818e+06
Molar Entropy	J/kmol-K	-442642	-586564	-500000	-514056
Mass Entropy	J/kg-K	-6396.7	-7731.11	-7225.59	-6775.43
Molar Density	kmol/cum	0.28657	12.636	0.69069	11.0065
Mass Density	kg/cum	19.8302	958.698	47.7947	835.071
Enthalpy Flow	Watt	-6.43975e+06	-6.98467e+06	-6.81034e+06	-6.61408e+06
Average MW		69.1985	75.8706	69.1985	75.8706

− **Mole Flows**	**kmol/sec**	**0.0157671**	**0.0143424**	**0.0157671**	**0.0143424**
H2O	kmol/sec	2.27453e-07	2.27224e-07	2.27453e-07	2.27224e-07
H2	kmol/sec	0.00143183	7.42169e-06	0.00143183	7.42169e-06
GLYCEROL	kmol/sec	1.41078e-05	1.41078e-05	1.41078e-05	1.41078e-05
PROPDIOL	kmol/sec	0.0128891	0.0128891	0.0128891	0.0128891
ACETOL	kmol/sec	0.00143183	0.0014316	0.00143183	0.0014316
N2	kmol/sec	0	0	0	0
O2	kmol/sec	0	0	0	0
− **Mole Fractions**					
H2O		1.44258e-05	1.58428e-05	1.44258e-05	1.58428e-05
H2		0.090811	0.000517464	0.090811	0.000517464
GLYCEROL		0.000894763	0.000983645	0.000894763	0.000983645
PROPDIOL		0.817469	0.898667	0.817469	0.898667
ACETOL		0.090811	0.0998161	0.090811	0.0998161
N2		0	0	0	0
O2		0	0	0	0
+ **Mass Flows**	**kg/sec**	**1.09106**	**1.08817**	**1.09106**	**1.08817**

Heat Exchanger Results

	Units	S1	S2	S3
Cost Flow	$/sec			
− MIXED Substream				
Phase			Vapor Phase	Liquid Phase
Temperature	K	423.15	267.75	270.6
Pressure	N/sqm	300000	1	1.12
Molar Vapor Fraction		7.36138e-05	1	0
Molar Liquid Fraction		0.999926	0	1
Molar Solid Fraction		0	0	0
Mass Vapor Fraction		1.08374e-05	1	0
Mass Liquid Fraction		0.999989	0	1
Mass Solid Fraction		0	0	0
Molar Enthalpy	J/kmol	-4.61577e+08	-4.18088e+08	-5.00563e+08
Mass Enthalpy	J/kg	-6.08374e+06	-5.52865e+06	-6.57534e+06
Molar Entropy	J/kmol-K	-515050	-330650	-629661
Mass Entropy	J/kg-K	-6788.54	-4372.4	-8271.16
Molar Density	kmol/cum	11.0392	4.49204e-07	12.7328
Mass Density	kg/cum	837.553	3.39698e-05	969.311
Enthalpy Flow	Watt	-6.62013e+06	-3.04723e+06	-3.53094e+06
Average MW		75.8706	75.6221	76.1273

− Mole Flows	**kmol/sec**	**0.0143424**	**0.00728849**	**0.00705392**
H2O	kmol/sec	2.27224e-07	2.27224e-07	1.15224e-25
H2	kmol/sec	7.42169e-06	7.42169e-06	5.99362e-67
GLYCEROL	kmol/sec	1.41078e-05	4.1164e-29	1.41078e-05
PROPDIOL	kmol/sec	0.0128891	0.00584924	0.00703982
ACETOL	kmol/sec	0.0014316	0.0014316	7.46577e-16
N2	kmol/sec	0	0	0
O2	kmol/sec	0	0	0
− Mole Fractions				
H2O		1.58428e-05	3.11757e-05	1.63348e-23
H2		0.000517464	0.00101827	8.49686e-65
GLYCEROL		0.000983645	5.6478e-27	0.002
PROPDIOL		0.898667	0.802531	0.998
ACETOL		0.0998161	0.19642	1.05839e-13
N2		0	0	0
O2		0	0	0
+ Mass Flows	**kg/sec**	**1.08817**	**0.551171**	**0.536996**

RadFrac Results

	Units	FL-INP	FL-LIQ	FL-VAP
− MIXED Substream				
Phase			Liquid Phase	Vapor Phase
Temperature	K	359.8	298.15	298.15
Pressure	N/sqm	200000	300000	300000
Molar Vapor Fraction		0.0917063	0	1
Molar Liquid Fraction		0.908294	1	0
Molar Solid Fraction		0	0	0
Mass Vapor Fraction		0.00394437	0	1
Mass Liquid Fraction		0.996056	1	0
Mass Solid Fraction		0	0	0
Molar Enthalpy	J/kmol	-4.31932e+08	-4.86994e+08	-81858.8
Mass Enthalpy	J/kg	-6.24193e+06	-6.41874e+06	-40296.2
Molar Entropy	J/kmol-K	-500000	-586564	-9075.46
Mass Entropy	J/kg-K	-7225.59	-7731.11	-4467.53
Molar Density	kmol/cum	0.69069	12.636	0.121021
Mass Density	kg/cum	47.7947	958.698	0.245844
Enthalpy Flow	Watt	-6.81034e+06	-6.98467e+06	-116.625
Average MW		69.1985	75.8706	2.03143

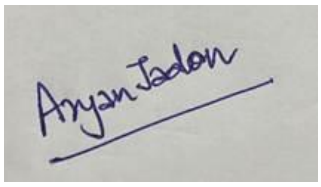
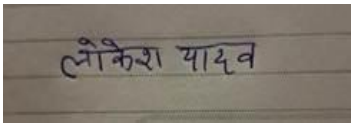
− Mole Flows	**kmol/sec**	**0.0157671**	**0.0143424**	**0.00142471**
H2O	kmol/sec	2.27453e-07	2.27224e-07	2.29703e-10
H2	kmol/sec	0.00143183	7.42169e-06	0.00142441
GLYCEROL	kmol/sec	1.41078e-05	1.41078e-05	9.2195e-14
PROPDIOL	kmol/sec	0.0128891	0.0128891	7.96105e-08
ACETOL	kmol/sec	0.00143183	0.0014316	2.25465e-07
N2	kmol/sec	0	0	0
O2	kmol/sec	0	0	0
− Mole Fractions				
H2O		1.44258e-05	1.58428e-05	1.61228e-07
H2		0.090811	0.000517464	0.999786
GLYCEROL		0.000894763	0.000983645	6.47113e-11
PROPDIOL		0.817469	0.898667	5.58783e-05
ACETOL		0.090811	0.0998161	0.000158253
N2		0	0	0
O2		0	0	0
− Mass Flows	**kg/sec**	**1.09106**	**1.08817**	**0.0028942**

Flash Column Results

Objectives that could not be accomplished with reasons: -

Recycle loop could not be converged

Reference - Kinetics of Hydrogenolysis of Glycerol to Propylene Glycol

Name (Roll No.)	Contribution	Signature
Anas Ali (220137)	Reaction kinetics, design and report formation	
Ansh Sethi (220167)	Reactor Design Heat Exchanger Design	
Aryan Jadon (220223)	Heat exchanger design, report formation	
Jatin Madan (220475)	Heat exchanger design, report formation	
Lokesh Yadav (220594)	Reactor design and optimization Other separators design	
Madhav Lata (220597)	Reactor and heat exchanger design and implementation in Aspen	

Pratyush Gupta (220813)	Reactor and heat exchanger design and implementation in Aspen	
Punam Singh (220835)	Reactor and heat exchanger design and implementation in Aspen