ChE453: Capstone Project

Bi-weekly report number: 3

Group No: 4

Team members:

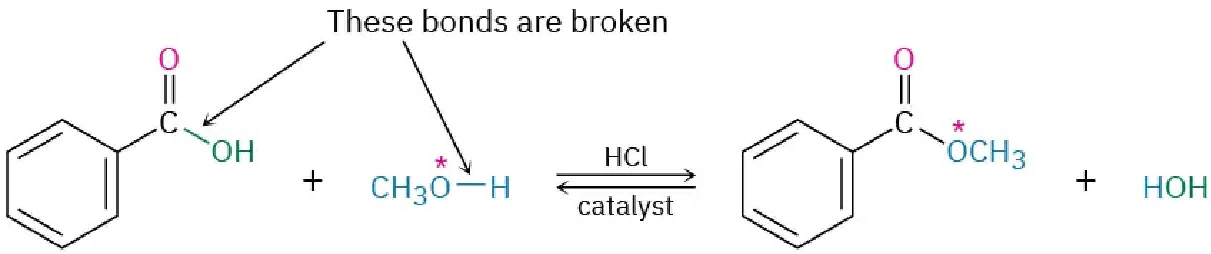
Aaditya Amlan Panda	**220007**
Abhijit Dalai	**220030**
Adarsh Pal	**220054**
Akash Kumar Gupta	**220095**
Kushagra Tiwari	**220574**
Saurabh Yadav	**220991**
Snehil Tripathi	**221071**
Tushar Verma	**221147**

Recap:

We are preparing the **Methyl benzoate,** which is an important aromatic ester widely used as a fragrance and flavouring agent, a solvent for resins and oils, and an intermediate in pharmaceuticals and agrochemicals.

It is typically synthesised via the **esterification of benzoic acid with methanol**, a reversible, equilibrium-limited reaction catalysed by strong acids such as sulfuric acid or hydrochloric acid(HCl / H_2SO_4).

Benzoic Acid + Methanol → Methyl Benzoate + H_2O

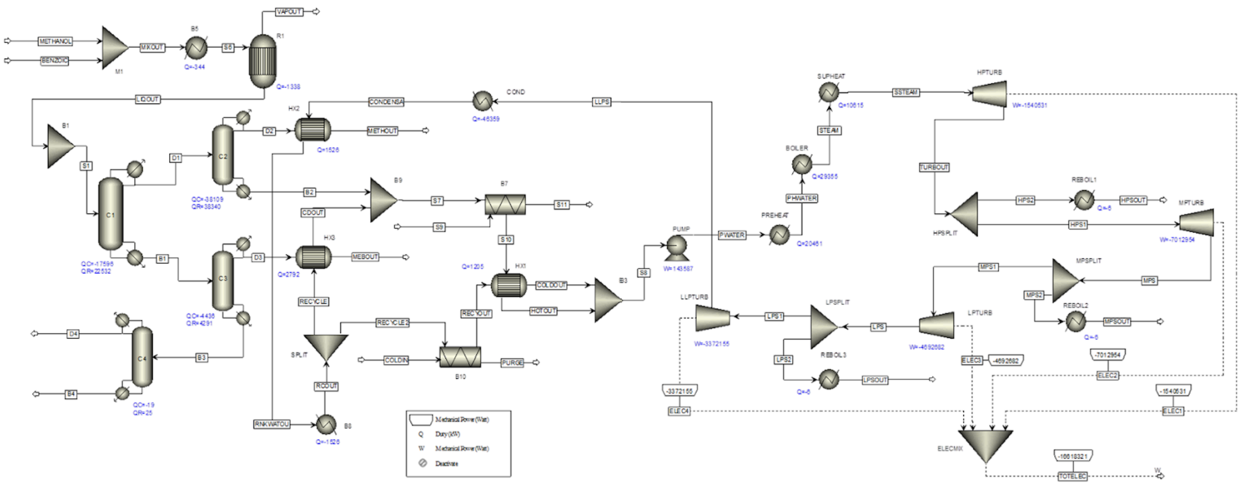


This esterification is an **equilibrium reaction**, and high conversion requires process intensification strategies. Common approaches include:

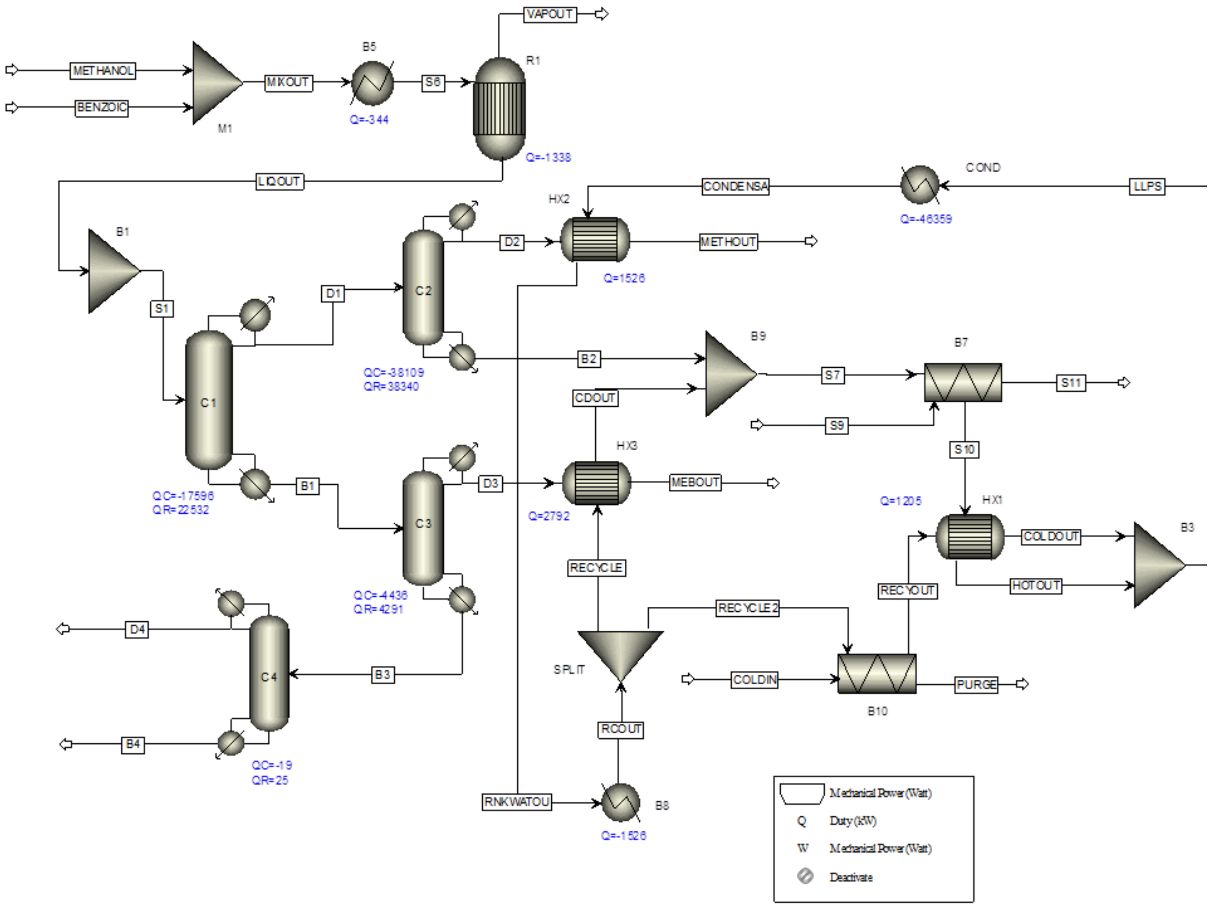
- Using an excess of methanol as a reactant shifts the equilibrium towards ester formation.
- Employing strong mineral acids or solid acid catalysts to enhance the reaction rate.

In the last report, we mentioned the molar ratio of our reactant (Methanol: MEB: HCl = 16.59: 2.7: 0.1215). This is according to Roberts & Urey (1938)[1]; this ratio enabled a large amount of water in the product because water helped in the energy-efficient separation of methanol to help with efficient methanol recovery.

Complete Flowsheet at a glance:



Material Flowsheet:



Component description:

M1 (Mixer): Benzoic acid exists in the solid state at room temperature. Therefore, it is fed into a mixer along with Methanol, which acts as a carrier for benzoic acid to the reactor.

R1 (Equilibrium reactor): The flowsheet utilises an **equilibrium reactor** for the esterification reaction. A near-complete conversion of Benzoic Acid has been observed in the equilibrium reactor, yielding a large k, which we will correct once we obtain the detailed kinetics.

C1 (Distillation column 1): In distillation column 1, methanol and water (coming out as distillate in D1) are separated from the other components (coming out as bottoms in B1).
For 99.9% water recovery: -

- No of Trays: 20
- Feed Stage: 11
- Reflux Ratio: 0.018697
- Reboiler Duty: 22531.7 kW
- Condenser Duty: -17596.4 kW

C2 (Distillation column 2): This distillation column separates methanol in the distillate (D2) from water in the bottoms (B2).
For 99.99% methanol recovery & 99.9% water recovery: -

- No of Trays: 20
- Feed Stage: 14
- Reflux Ratio: 1.7256
- Reboiler Duty: 38339.7 kW
- Condenser Duty: -38109 kW

C3 (Distillation column 3): This distillation column separates the final product methyl benzoate in the distillate (D3) from benzoic acid + phthalic acid in the bottoms (B3).
For 99.7% Methyl Benzoate recovery: -

- No of Trays: 20
- Feed Stage: 11
- Reflux Ratio: 0.3033
- Reboiler Duty: 4291.45 kW
- Condenser Duty: -4435.88 kW

C4 (Distillation column 4): This distillation column separates benzoic acid as distillate (D4) from the impurity phthalic acid (B4) in the bottoms.
For 99.9% Benzoic Acid recovery: -

No of Trays: 20
Feed Stage: 10
Reflux Ratio: 1.19132
Reboiler Duty: 25 kW
Condenser Duty: -18.84 kW

HX2 (Heat Exchanger 2): The output steam from the Rankine cycle, after being condensed, is passed through HX2 to cool the methanol distillate stream (D2) from C2 up to 26 °C. The water output of HX2 is split into two streams, with one stream, RECYCLE, used to cool the methyl benzoate in HX3.

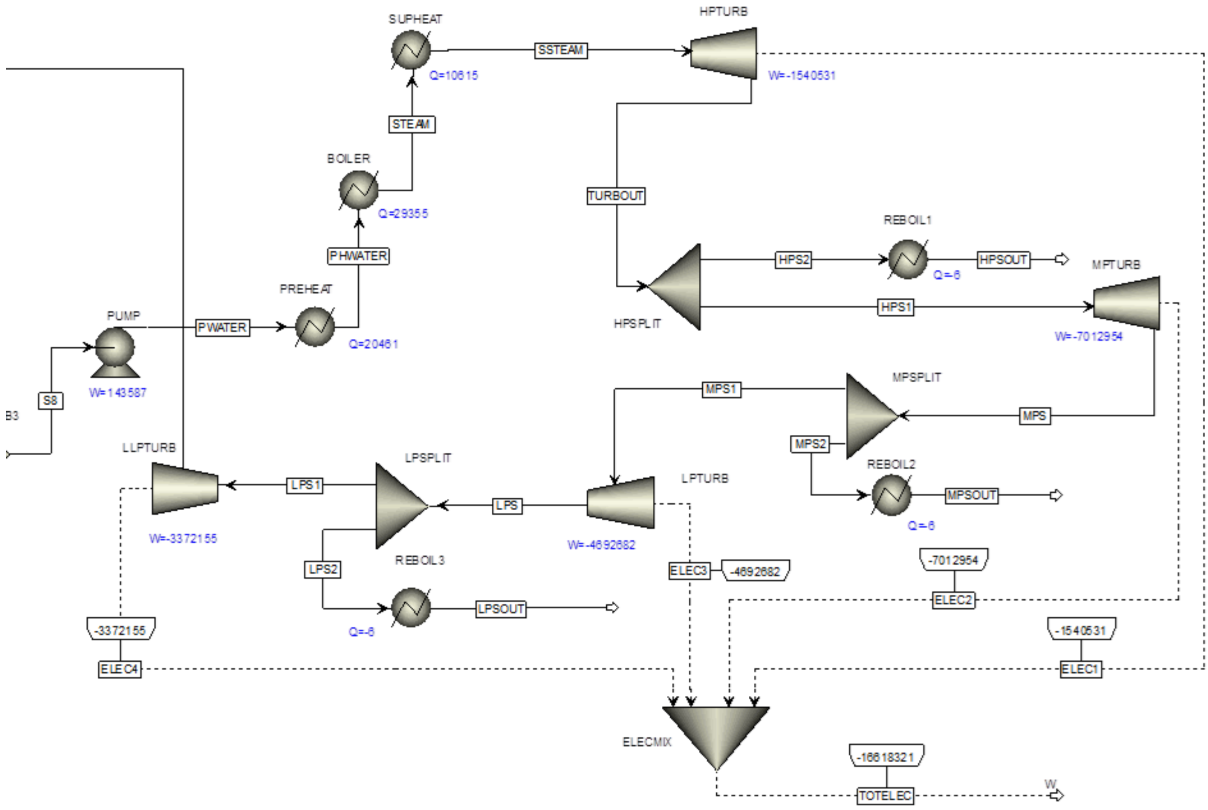
HX3 (Heat Exchanger 3): The water outlet stream from HX2 is cooled at B8 and then split into two streams: the RECYCLE stream is passed through HX3 to cool the methyl benzoate, coming out of column C3 as distillate.

B10 (Makeup block): This was used to pump in fresh cooling water into the Rankine cycle, as the water from the bottom of C2 was alone insufficient to cool down the hot outgoing methanol distillate, which was in high quantity.

HX1 (Heat Exchanger 1): This block is optional to be put in the system. Basically, it has been used to cool down the mixture of outgoing water bottom and water from the HX3 unit (which cools down MeB) (around 80 °C) using the incoming cooling water recycle (+makeup), so that both of them come to an almost equal temperature. This allows their (errorless) mixing (the Bot+HX3 mixture and recycled water) before being sent into the cogeneration unit.

B7 (Makeup block): Its primary function is purging some amount of water from the C2 Bot+HX3 mixture before being added to the Rankine cycle recycle stream. Fsplit was found to be error-prone, so we used a makeup block that returned near zero makeup.

Cogeneration Flowsheet (Continued...):



S8: The cold water outlet is fed to **PUMP,** which increases its pressure, and then fed to a preheater, boiler and a superheater, and yields a superheated steam.

HPTURB: The superheated steam is fed to a high-pressure steam turbine, which yields high-pressure steam at a pressure of 40 bar and generates **1540 kW** of electricity. This high-pressure steam can be used for heating purposes, where the temperature is more than the MP steam limit.

HPSPLIT: A splitter is used to split the high-pressure steam in **TURBOUT** into two streams, one HPSOUT, which will be used for future purposes, and the other HPS,1 which is fed to MPTURB.

MPTURB: The high-pressure steam in **HPS1** is fed to a mid-pressure steam turbine, which yields mid-pressure steam at 10 bar and generates **7012.9 kW of** electricity.

MPSPLIT: This splitter splits the mid-pressure steam fed into two streams, MPSOUT, which will be used later in the process for heating, and the other MPS1, fed to the LPTURB.

LPTURB: The mid-pressure steam in MPS1 is then fed to a low-pressure steam turbine, which yields a low-pressure steam at 3 bar and generates **4692.6 kW of** electricity.

LPSPLIT: The low-pressure steam is split into two streams, one stream is LPSOUT, which will be used later in the process, and the other is LPS1, which is fed to the LLPTURB.

LLPTURB: This low-pressure steam turbine generates **3372 kW** of electricity with the 3 bar steam as input and yields a 1 bar steam.

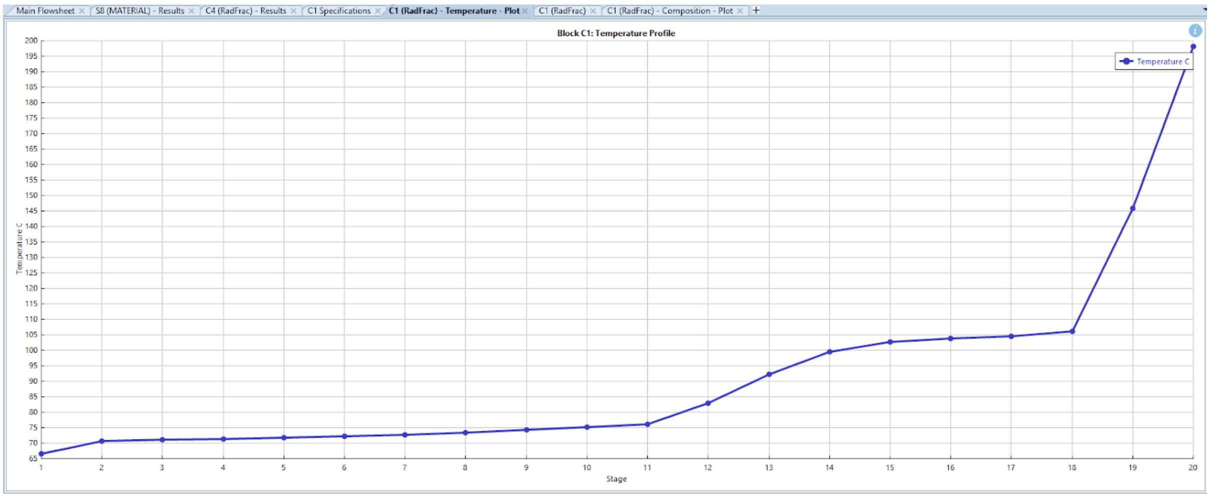
LLPS: The low-pressure steam at 1 bar is then proceeded for condensation and fed to HX2 to be reused in the recycle.

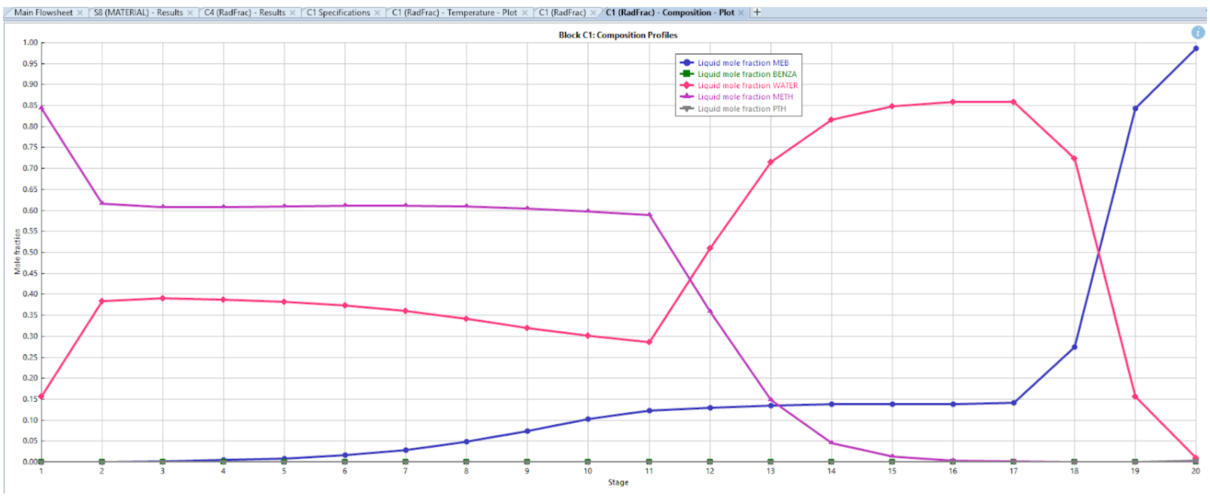
Mass and Energy Balance in Distillation Columns:

		Column C1			
	Mass In (S1)		Mass Out(B1)	Mass Out(D1)	MassOut_total
Methyl Benzoate	36622.21057		36620.80996	1.400610149	36622.21057
Benzoic Acid	1.996230958		1.996230958	2.47E-24	2.00E+00
Water	4845.815842		48.45815348	4797.357689	4845.815842
Methanol	45692.64392		0.017089908	45692.62683	45692.64392
Pthalic Acid	166.13324		166.13324	1.97E-39	1.66E+02
TOTAL	87328.7998				87328.7998

		Column C1		
	Heat In (kW)			Heat out (kW)
Feed (S1)	-141828.2926		Distillate C1 (D1)	-113817.4079
Reboiler Duty C1 (Qr)	22532		Bottoms C1 (B1)	-23075.58014
Condenser Duty C1 (Qc)	-17596			
Total	-136892.2926		Total	-136892.988

Column-1 Temperature and Composition Profile

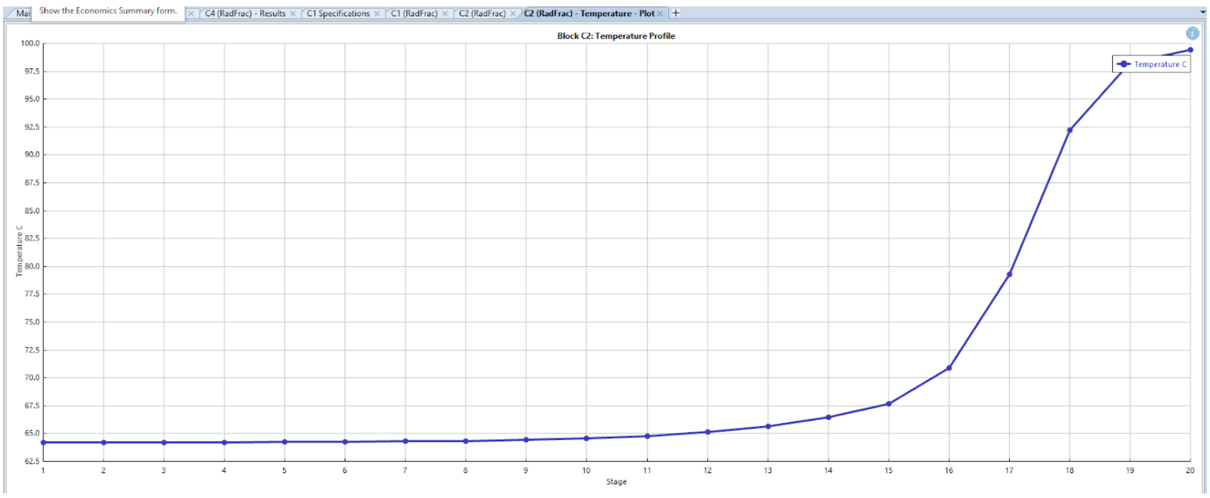


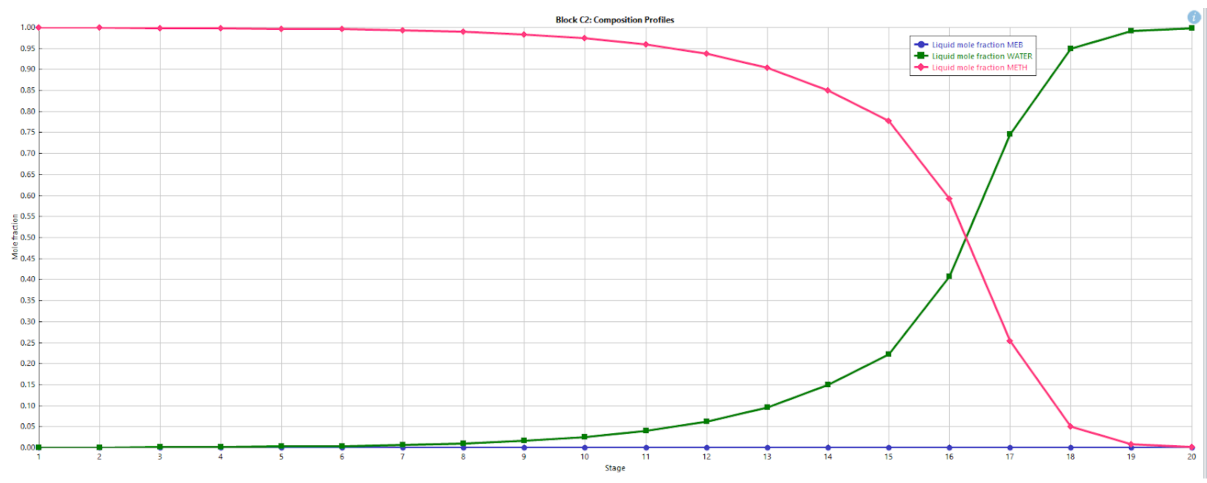


		Column C2			
	Mass In (D1)		Mass Out(B2)	Mass Out(D2)	MassOut_total
Methyl Benzoate	1.400610149		1.400610149	0	1.400610149
Benzoic Acid	2.47E-24		0	0	0
Water	4797.357689		4792.560331	4.797357688	4797.357689
Methanol	45692.62683		9.138525366	45683.4883	45692.62683
Pthalic Acid	1.97E-39		0	0	0
TOTAL	50491.3851				50491.38513

		Column C2		
	Heat In (kW)			Heat out (kW)
Distillate C1 (D1)	-113817.4079		Distillate C2 (D2)	-92874.60482
Reboiler Duty C2 (Qr)	38340		Bottoms C2 (B2)	-20712.05695
Condenser Duty C2 (Qc)	-38109			
Total	-113586.4079		Total	-113586.6618

Column 2 Temperature and Composition profile:

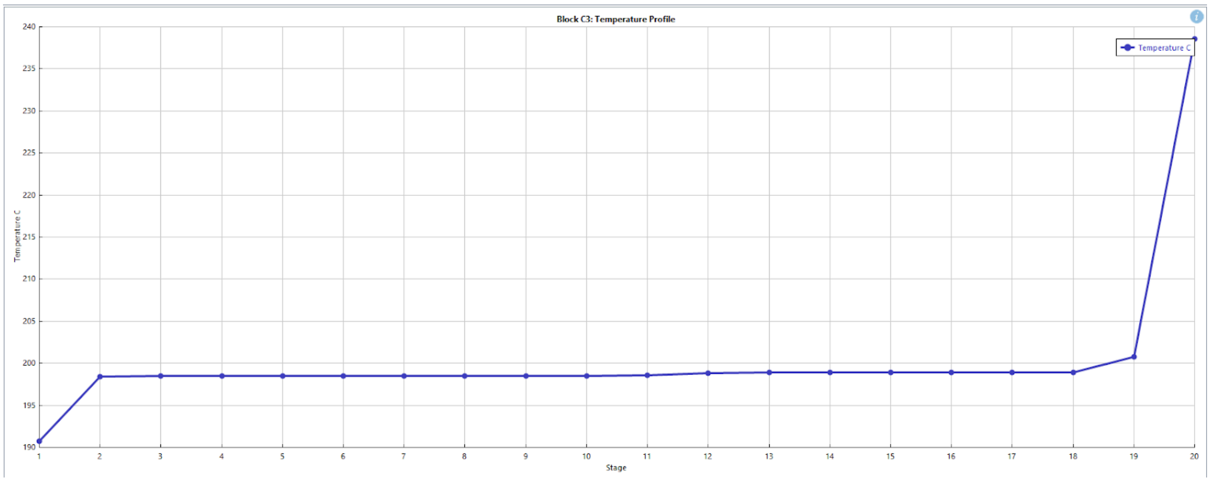


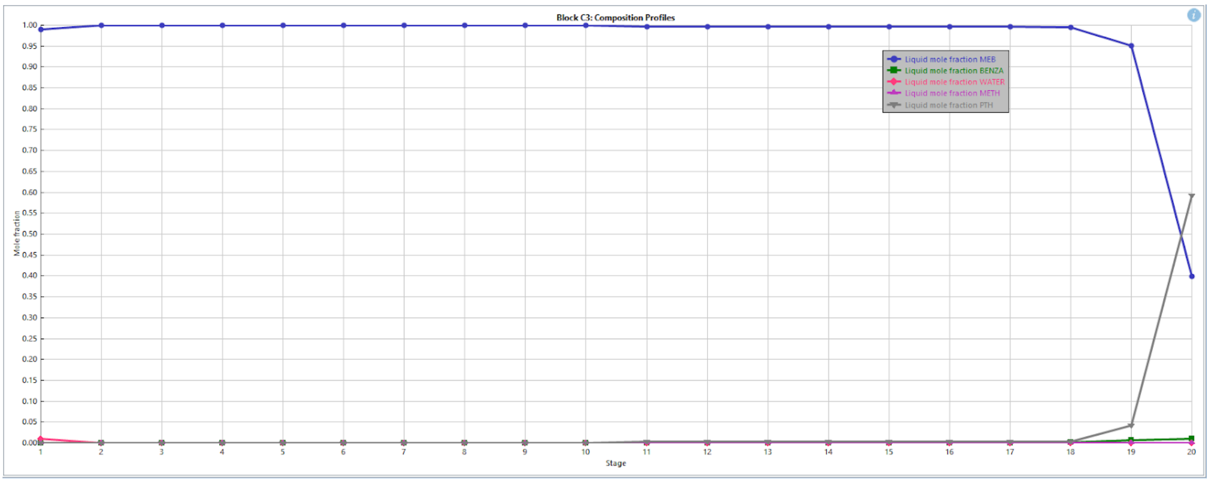


		Column C3			
	Mass In (B1)		Mass Out(B3)	Mass Out(D3)	MassOut_total
Methyl Benzoate	36620.80996		91.55202489	36529.2579	36620.80992
Benzoic Acid	1.996230958		1.967318305	0.028912653	1.996230958
Water	48.45815348		3.84E-15	48.45815344	4.85E+01
Methanol	0.017089908		9.13E-18	0.017089908	1.71E-02
Pthalic Acid	166.13324		166.13324	1.48E-12	1.66E+02
TOTAL	36837.4147				36837.41464

			Column C3		
	Heat In (kW)				Heat out (kW)
Bottoms C1 (B1)	-23075.58014			Distillate C3 (D3)	-22966.23687
Reboiler Duty C3 (Qr)	4291			Bottoms C3 (B3)	-253.7746107
Condenser Duty C3 (Qc)	-4436				
Total	-23220.58014			Total	-23220.01149

Column 3 Temperature and Composition profile:

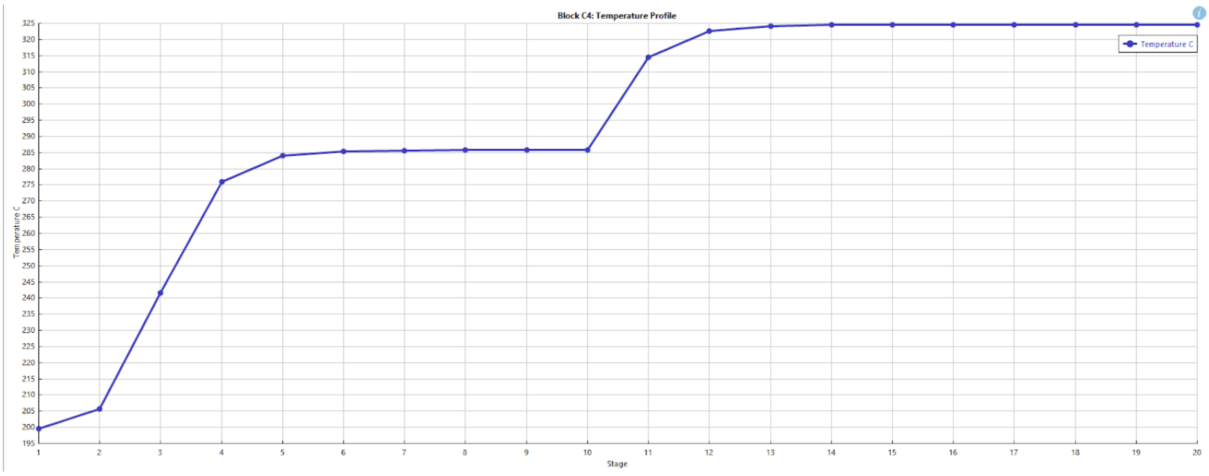


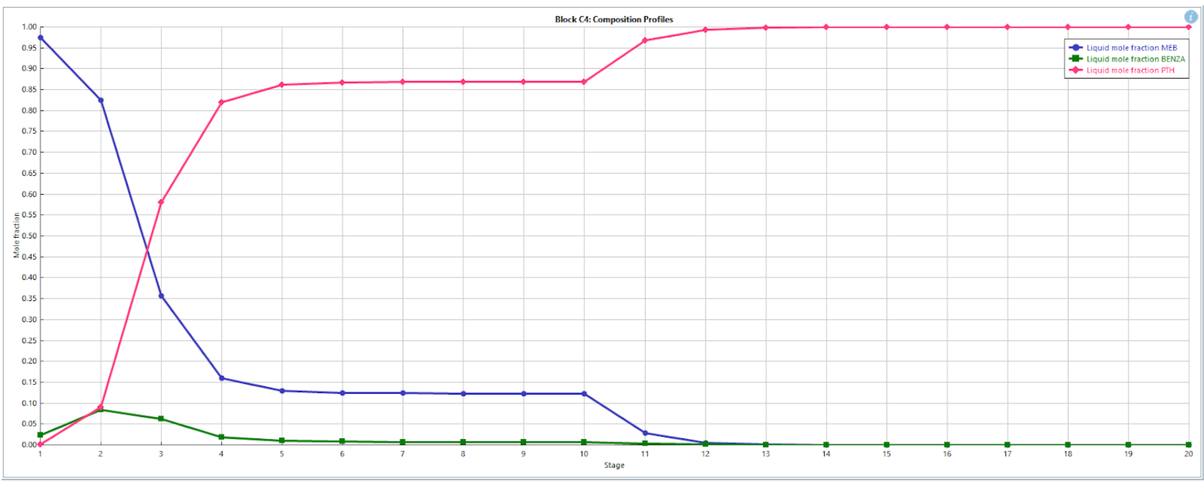


		Column C4			
	Mass In (B3)		Mass Out(B4)	Mass Out(D4)	MassOut_total
Methyl Benzoate	91.55202489		7.38E-07	91.55202415	9.16E+01
Benzoic Acid	1.967318305		1.97E-05	1.967298588	1.97E+00
Water	3.84E-15		0	0	0
Methanol	9.13E-18		0	0	0
Pthalic Acid	166.13324		165.9671068	0.16613324	166.13324
TOTAL	259.652583				259.6525832

		Column C4		
	Heat In (kW)			Heat out (kW)
Bottoms C3 (B3)	-253.7746107		Distillate C4 (D4)	-58.29793905
Reboiler Duty C4 (Qr)	25		Bottoms C4 (B4)	-189.3194072
Condenser Duty C4 (Qc)	-19			
Total	-247.7746107		Total	-247.6173463

Column 4 Temperature and Composition profile:





Mass & Energy Balance and in Heat Exchangers

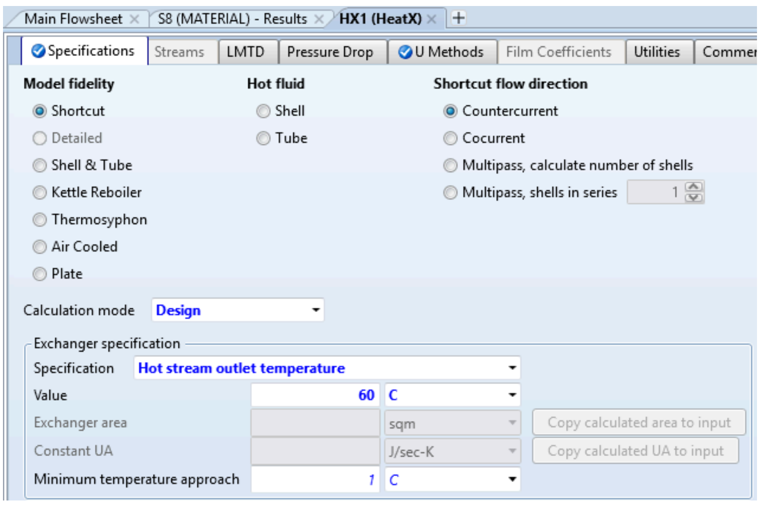
Heat Exchanger :1

		Heat Ex1		
	Mass In (kg/hr)			Mass Out (kg/hr)
RECYOUT	35000		COLDOUT	35000
S10	29999.99996		HOTOUT	29999.99996
Total	64999.99996		Total	64999.99996

	Enthalpy In (KW)			Enthalpy Out (KW)
RECYOUT	-154167.4993		COLDOUT	-152962.1945
S10	-129693.7601		HOTOUT	-130899.0632
Total	-283861.2594		Total	-283861.2576

	Temperature In (°C)			Temperature Out (°C)
RECYOUT	25.00000582		COLDOUT	54.65208065
S10	92.99341537		HOTOUT	60

The overall mass balance is satisfied for column **Hex1**, with total mass in = **64999.99996 kg/hr** and total mass out =**64999.99996 kg/hr**, confirming conservation of mass. Also, total energy in = **-283861.2594 KW** and total energy out = **-283861.2576 KW**, confirming conservation of energy.



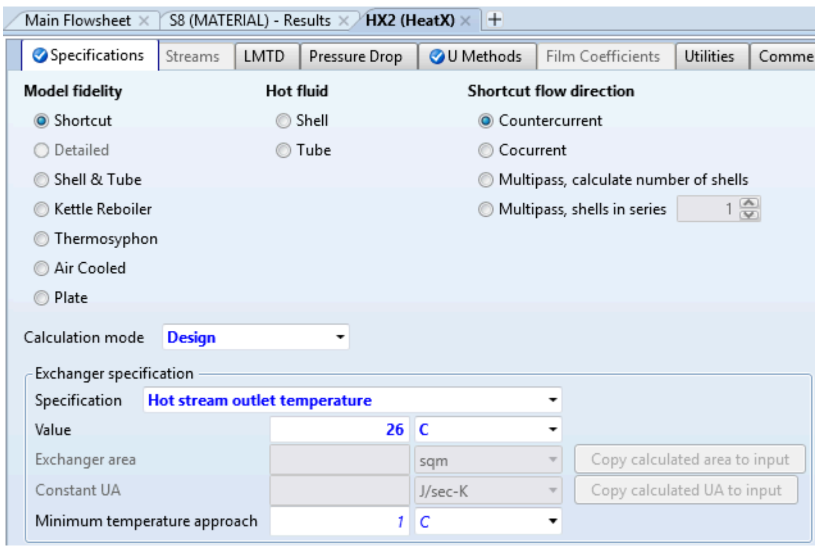
Heat Exchanger: 2

		Heat Ex2		
	Mass In (kg/hr)			Mass Out (kg/hr)
CONDENSA	64970.04089		METHOUT	45688.28569
D2	45688.28569		RNKWATOU	64970.04089
Total	110658.3266		Total	110658.3266

	Enthalpy In (KW)			Enthalpy Out (KW)
CONDENSA	-286157.7773		METHOUT	-94400.43889
D2	-92874.60488		RNKWATOU	-284631.9433
Total	-379032.3822		Total	-379032.3822

	Temperature In (°C)			Temperature Out (°C)
CONDENSA	25		METHOUT	26
D2	64.203415		RNKWATOU	45.32497494

The overall mass balance is satisfied for column **Hex1**, with total mass in = **110658.3266 kg/hr** and total mass out = **110658.3266 kg/hr**, confirming conservation of mass. Also, total energy in = **-379032.3822 KW** and total energy out = **-379032.3822 KW**, confirming conservation of energy.



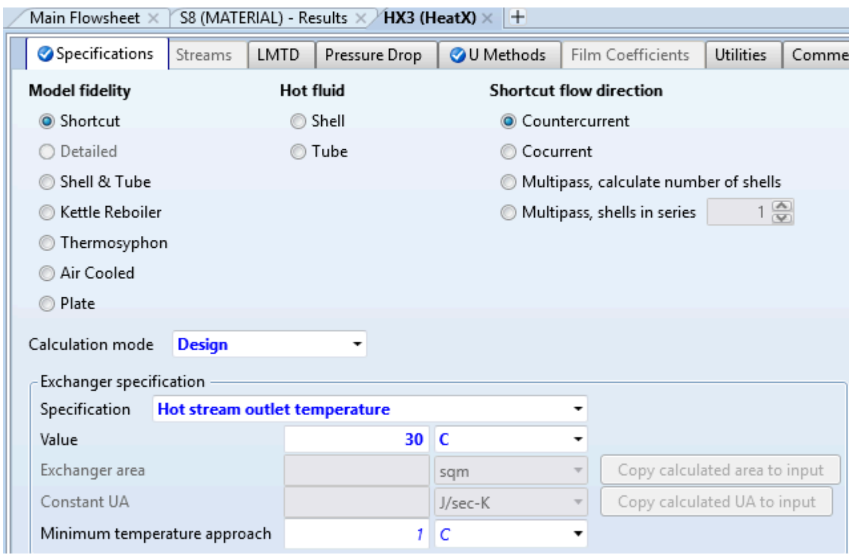
Heat Exchanger: 3

		Heat Ex3		
	Mass In (kg/hr)			Mass Out (kg/hr)
D3	36577.76419		**CDOUT**	34970.04089
RECYCLE	34970.04089		**MEBOUT**	36577.76419
Total	71547.80508		**Total**	71547.80508

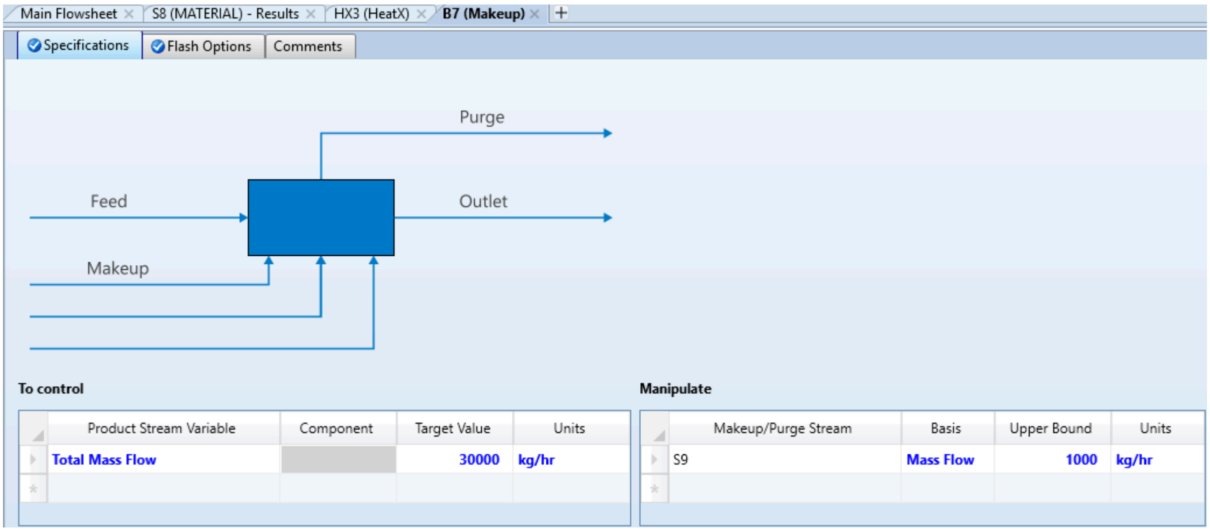
	Enthalpy In (KW)			Enthalpy Out (KW)
D3	-22966.23825		**CDOUT**	-151232.2142
RECYCLE	-154024.0553		**MEBOUT**	-25758.08211
Total	-176990.2936		**Total**	-176990.2963

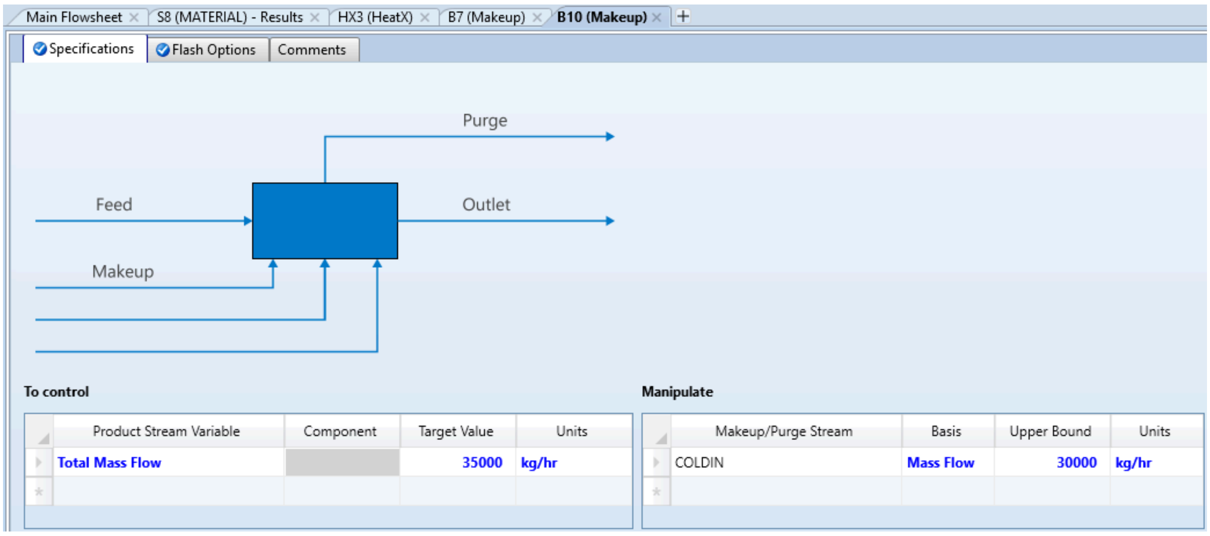
	Temperature In (°C)			Temperature Out (°C)
D3	190.7919192		**CDOUT**	92.10074176
RECYCLE	25		**MEBOUT**	30

The overall mass balance is satisfied for column **Hex1**, with total mass in = **71547.80508 kg/hr** and total mass out = **71547.80508 kg/hr**, confirming conservation of mass. Also, total energy in = **-176990.2936 KW** and total energy out = **-176990.2963 KW**, confirming conservation of energy.



<u>Specifications of the Makeup block:</u>





Mass balance for Co-generation Unit:

	MASS BALANCE		
	Input(kg/h)	Output(kg/h)	
Stream	Mass flow	Stream	mass flow
S8	65000.04	LPSOUT	10
		MPSOUT	10
		HPSOUT	10
		CONDENSA	64970.04
total input	65000.04	total output	65000.04
Total mass balance:	4E-10		

The overall mass balance is satisfied for the **Rankine cycle**, with total mass in = **65000.0408877573 kg/hr** and total mass out = **65000.04 kg/hr**, confirming conservation of mass. A small amount of energy imbalance was observed.

	ENERGY BALANCE		
	Input(kW)	Output(kW)	
Stream	Energy flow	Stream	Energy flow
S8	-283861.5566	LPSOUT	-42.709
		MPSOUT	-42.042
		HPSOUT	-40.823
		CONDENSA	-286158
total input	-283861.5566	total output	-286283
Total energy balan(	2421.794008		

Objectives that could not be accomplished with reasons:

- Even though we used the cogeneration plant's cooling water for cooling purposes, we could not make a cooling water loop with industry best practices, which uses a central cooling facility. We need to study a bit more on the same before implementing it.
- We have not found the exact use of LPS, MPS, HPS, and LLPS in our process
- We could not obtain a complete energy balance in the cogeneration loop

Any other challenges:

- The R-equilibrium block gave a massive right shift output, showing the need for detailed reaction kinetics data, which we do not have at this moment

Bibliography:

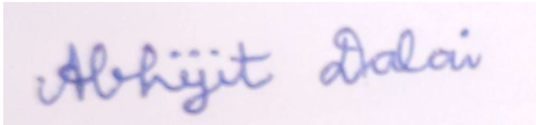
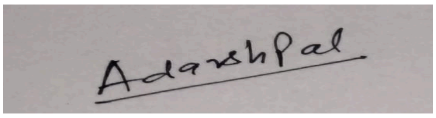
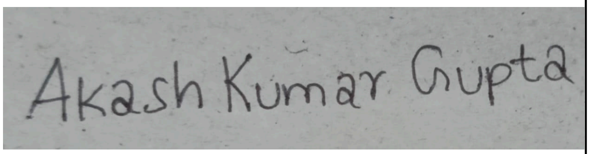
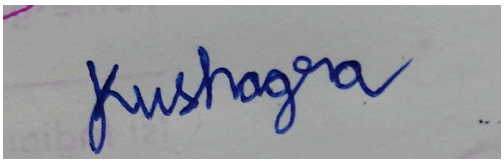
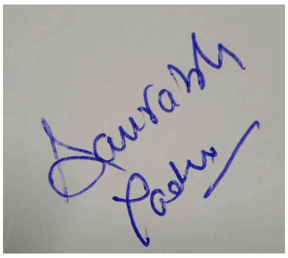
A Study of the Esterification of Benzoic Acid with Methyl Alcohol Using Isotopic Oxygen, Irving Roberts and Harold C. Urey

Number of hours spent on Capstone project during this period: 29 hours total

Contributions from individual members:

1. Aaditya Amlan Panda (Cogeneration Plant Integration)
2. Abhijit Dalai (Cooling Water Cycle Design)
3. Adarsh Pal (Distillation Column Spec Optimisation)
4. Akash Kumar Gupta (Distillation Column Spec Optimisation)
5. Kushagra Tiwari (Cogeneration Plant Integration)
6. Saurabh Yadav (Cogeneration Plant Integration)
7. Snehil Tripathi (Distillation Column Spec Optimisation)
8. Tushar Verma (Cooling Water Cycle Design)

Signatures of members:

Aaditya Amlan Panda	
Abhijit Dalai	
Adarsh Pal	
Akash Kumar Gupta	
Kushagra Tiwari	
Saurabh Yadav	
Snehil Tripathi	
Tushar Verma