CHE251 (CHEMICAL PROCESS CACULATIONS)

TERM PROJECT

Title:
Process Simulation and Optimization of Acetone Production from Isopropanol

Group 5

Next Slide

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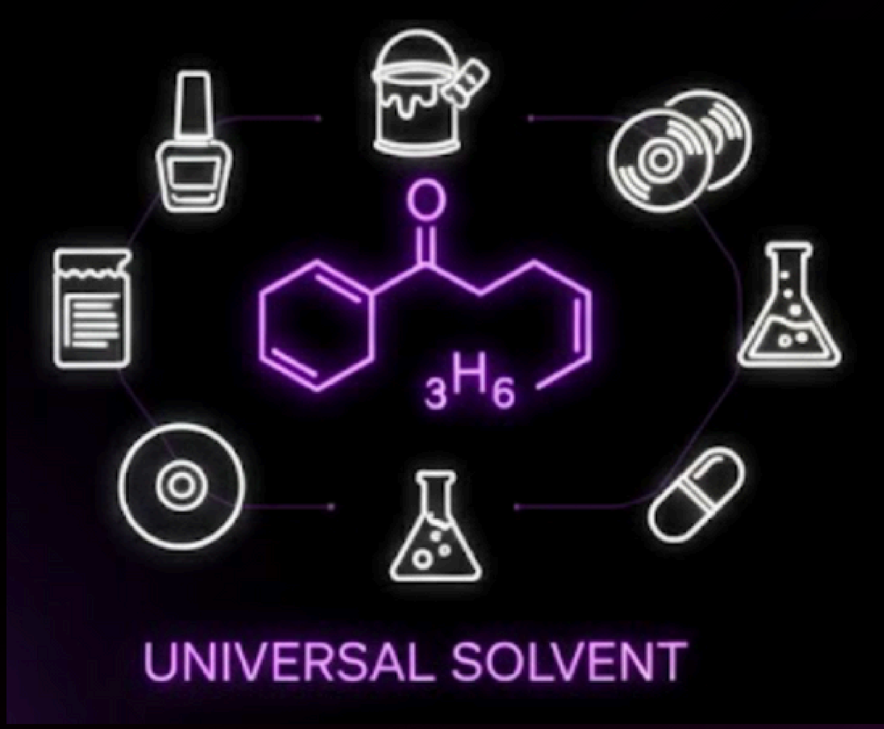
Process Overview

- Process Overview
- Importance of acetone
- Application of acetone
- Chemical Reaction
- Base case simulation
- Recycle Analysis
- Purge Analysis
- Comparison
- Environmental & Economic Impact:
- Reference Article

Importance of Acetone as an Industrial Solvent:



- Acetone (CH_3COCH_3) is a versatile and fast-evaporating solvent, valued for its ability to dissolve a wide range of organic compounds.
- It plays a critical role in chemical and pharmaceutical manufacturing, enabling purification, extraction, and synthesis processes.
- Its low boiling point and miscibility with water and most organic liquids make it ideal for cleaning, degreasing, and blending operations.
- Acetone is environmentally safer compared to many chlorinated solvents—low toxicity and easy biodegradability.

Applications of Acetone:

1. Pharmaceuticals

- Used as a solvent in the manufacture of drugs, vitamins, and antibiotics.
- Helps in crystallization and purification of active pharmaceutical ingredients (APIs)
- Essential in cleaning and sterilizing laboratory and medical equipment..

2. Coatings and Paints

- Acts as a thinner and viscosity reducer in paints, lacquers, and varnishes.
- Ensures quick drying and smooth film formation.

3. Plastics and Polymers

- Key solvent in production of acrylics, polycarbonates, and synthetic resins.
- Used in processing cellulose acetate for films and molded articles.

4. Textiles

- Employed for degreasing and removing contaminants from fabrics.
- Used in dyeing and finishing processes to improve color uniformity.

Chemical Reaction:

1. The Reaction (Dehydrogenation)

Concept: Isopropyl Alcohol (IPA) is decomposed to produce Acetone and Hydrogen gas.

$$CH_3CH(OH)CH_3 \longrightarrow CH_3COCH_3 + H_2$$

2. Operating Conditions

Catalyst: Copper or Copper/Chromium Catalyst (Common industrial choice).

Temperature (T): High approx 350°C (Required for the endothermic reaction).

Pressure (P): Low/Moderate ≈2 bar.

Base Case Simulation:

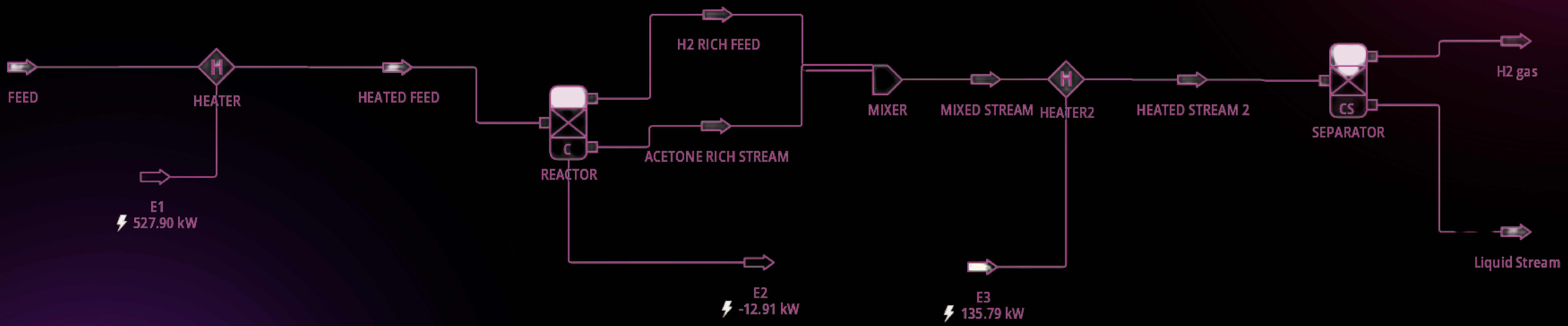
- Simulator: DWSIM
- Components: Isopropyl Alcohol (IPA), Acetone, and Hydrogen.
- Fluid Package: Peng-Robinson (PR) equation of state
- Reaction: Conversion reaction based on the stoichiometry

$$(CH_3)_2CHOH \rightarrow (CH_3)_2CO + H_2$$

- Base Component: IPA (as the only reactant decomposing)

Next Slide

Base case Flowchart:



Base case Analysis:

▸ Feed Conditions:

Temp: 25°C

Pressure : 1 bar

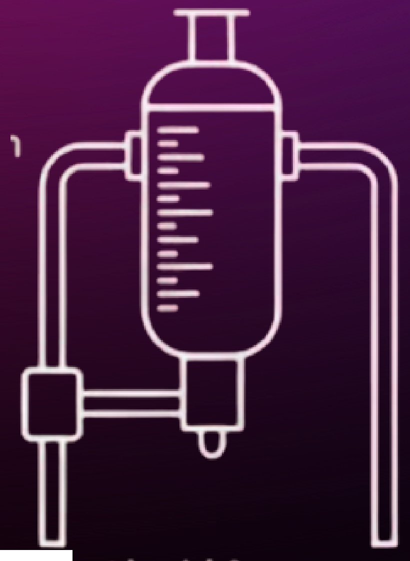
Molar Flow : 22.8 kmol/hr

▸ Heater 1 Condtions :

Temp : 350°C

Pressure : 2 bar

▸ Inside Reactor :



$$CH_3CH(OH)CH_3 \rightarrow CH_3COCH_3 + H_2$$

(conversion : 92.8%)

Temperature drops to (after reaction): 49.82°C

Master Property Table			
Object	H2 RICH FEED	ACETONE RICH STREAM	
Temperature	49.82	49.82	C
Pressure	2	2	bar
Molar Flow	34.1464	9.81165	kmol/h
Molar Fraction (Vapor)	1	8.41249E-07	
Molar Fraction (Overall Liquid)	0	0.999999	
Molar Fraction (Mixture) / Acetone	0.364994	0.886207	
Molar Fraction (Vapor) / Acetone	0.364994	0.365216	
Molar Fraction (Overall Liquid) / Acetone	NaN	0.886208	
Molar Fraction (Mixture) / Isopropanol	0.0155918	0.11305	
Molar Fraction (Vapor) / Isopropanol	0.0155918	0.0155992	
Molar Fraction (Overall Liquid) / Isopropanol	NaN	0.113051	
Molar Fraction (Mixture) / Hydrogen	0.619414	0.000742404	
Molar Fraction (Vapor) / Hydrogen	0.619414	0.619185	
Molar Fraction (Overall Liquid) / Hydrogen	NaN	0.000741884	

Base case Analysis:

▶Heater 2 Condtions :

Temp : 120 °C

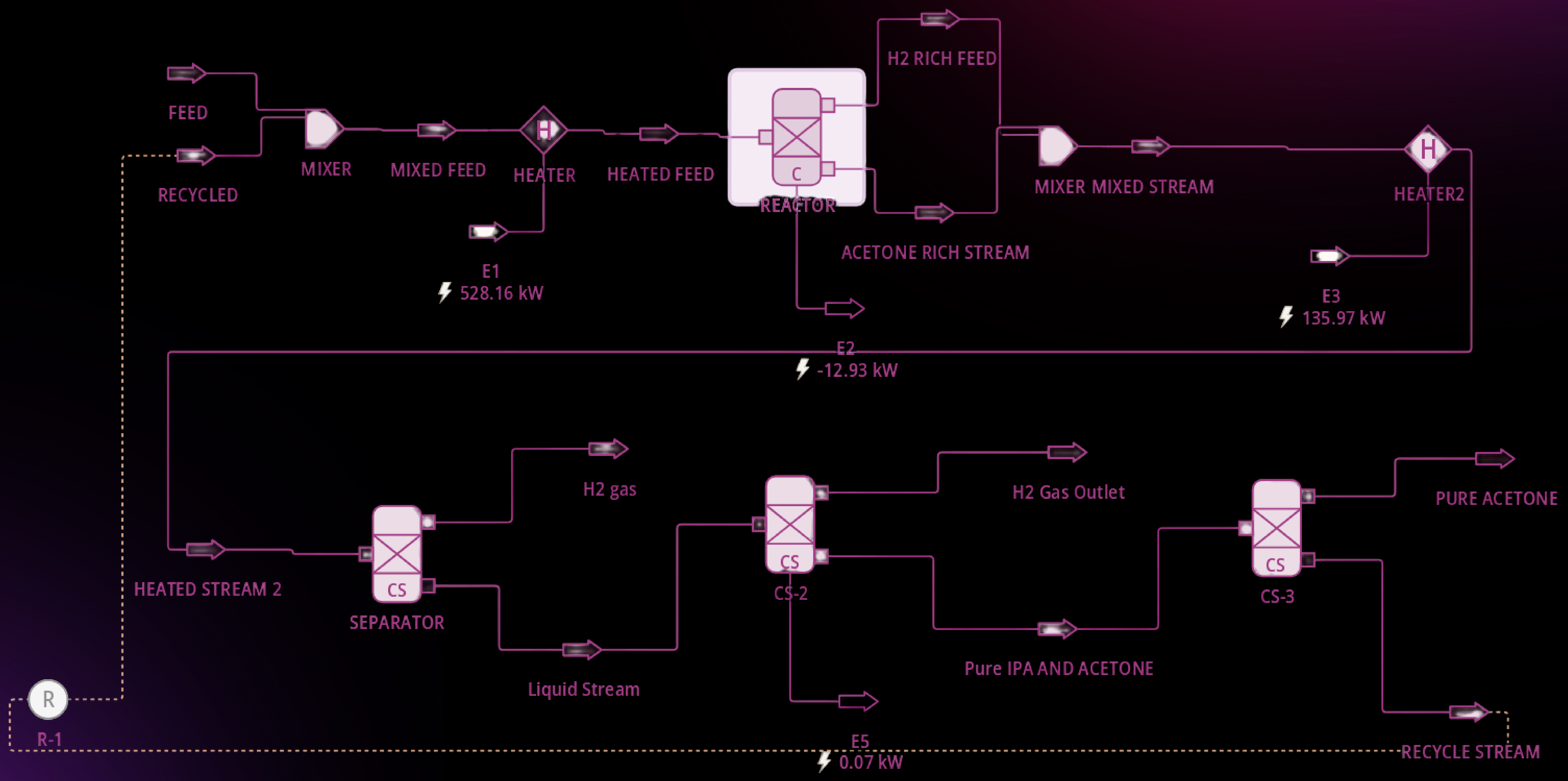
Pressure : 2.2 bar

▶Separator :

Acetone produced ->
liquid stream = 20.4115
IPA Feeded = 22.8
Efficiency : 89.524

Master Property Table			
Object	Liquid Stream	H2 gas	
Temperature	120	120	C
Pressure	2.2	2.2	bar
Molar Flow	21.1498	22.8082	kmol/h
Molar Fraction (Mixture) / Acetone	0.96509	0.0327466	
Molar Fraction (Mixture) / Isopropanol	0.00139713	0.0706793	
Molar Fraction (Mixture) / Hydrogen	0.033513	0.896574	

Recycle Flowchart:



Recycle Analysis:

Added two separators in the base case , the function of the first separator is to separate any left H_2 gas in the liquid stream , and the next separator separates our pure acetone from IPA and recycles the stream which contains IPA back to the feeding stage .

▶Separator (CS - 2) conditions :

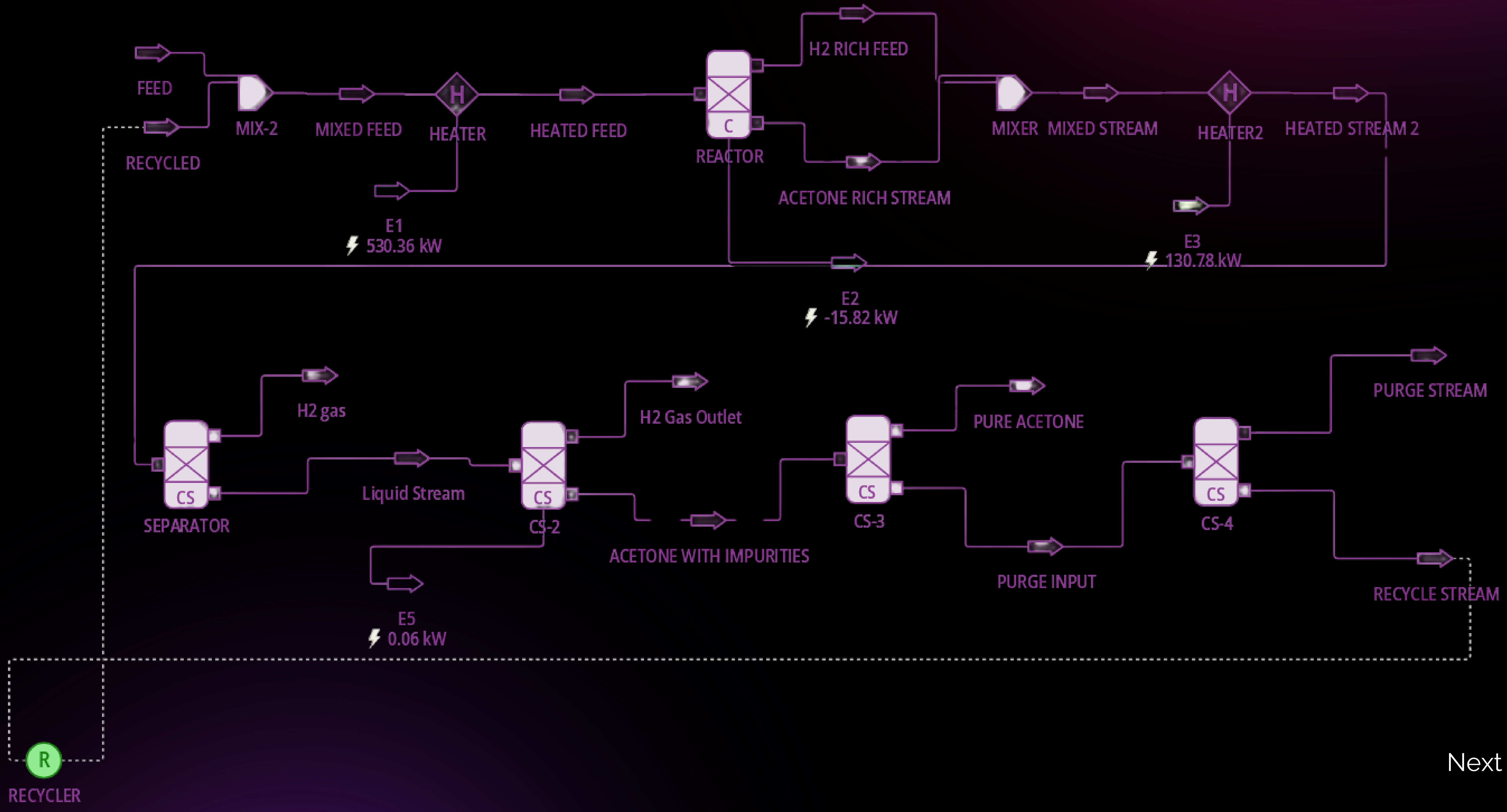
Master Property Table			
Object	Pure IPA AND ACETONE	H2 Gas Outlet	
Temperature	120	120	C
Pressure	2.2	2.2	bar
Molar Flow	20.4676	0.709714	kmol/h
Molar Fraction (Mixture) / Acetone	0.998554	0	
Molar Fraction (Vapor) / Acetone	0.998554	0	
Molar Fraction (Mixture) / Isopropanol	0.00144558	0	
Molar Fraction (Vapor) / Isopropanol	0.00144558	0	
Molar Fraction (Mixture) / Hydrogen	4.88187E-18	1	
Molar Fraction (Vapor) / Hydrogen	4.88187E-18	1	

▶Separator (CS - 3) conditions :

Master Property Table			
Object	RECYCLE STREAM	PURE ACETONE	
Temperature	120	120	C
Pressure	2.2	2.2	bar
Molar Flow	0.0295875	20.438	kmol/h
Molar Fraction (Mixture) / Acetone	0	1	
Molar Fraction (Vapor) / Acetone	0	1	
Molar Fraction (Mixture) / Isopropanol	1	0	
Molar Fraction (Vapor) / Isopropanol	1	0	
Molar Fraction (Mixture) / Hydrogen	3.37711E-15	0	
Molar Fraction (Vapor) / Hydrogen	3.37711E-15	0	

Next Slide

Purge system Flowchart:



Next Slide

Purge Case Analysis:

For the purge case we have added Nitrogen as Inert and changing the feed molar rate to 24 kmol/h with 5% Nitrogen and rest IPA. Because of this the compostion of output streams changed.

Master Property Table

Object	Liquid Stream	H2 gas	FEED	
Temperature	120	120	25	C
Pressure	2.2	2.2	1	bar
Molar Flow	22.1373	23.0779	24	kmol/h
Molar Fraction (Mixture) / Acetone	0.923238	0.0324059	0	
Molar Fraction (Mixture) / Isopropanol	0.00133654	0.0699437	0.95	
Molar Fraction (Mixture) / Hydrogen	0.0320599	0.887251	0	
Molar Fraction (Mixture) / Nitrogen	0.0433653	0.0103994	0.05	

Next Slide

Purge Case Analysis:

Added three separators in the base case , the function of the first separator is to separate any left H2 gas in the liquid stream , and the next separator separates our pure acetone from IPA and other impurities , the third separator separates our impurities from IPA and then this stream which contains only IPA is send to the feeding stage.

separator (CS - 2) conditions :

Master Property Table			
Object	H2 Gas Outlet	ACETONE WITH IMPURITIES	
Molar Flow	0.709719	21.4276	kmol/h
Molar Fraction (Mixture) / Acetone	0	0.953818	
Molar Fraction (Mixture) / Isopropanol	0	0.00138081	
Molar Fraction (Mixture) / Hydrogen	1	9.32631E-18	
Molar Fraction (Mixture) / Nitrogen	0	0.0448016	

Purge Case Analysis:

separator (CS - 3) conditions :

Master Property Table

Object	PURGE INPUT	PURE ACETONE	
Molar Flow	0.989577	20.438	kmol/h
Molar Fraction (Mixture) / Acetone	0	1	
Molar Fraction (Mixture) / Isopropanol	0.029899	0	
Molar Fraction (Mixture) / Hydrogen	2.01945E-16	0	
Molar Fraction (Mixture) / Nitrogen	0.970101	0	

separator (CS - 4) conditions :

Master Property Table

Object	RECYCLE STREAM	PURGE STREAM	
Molar Flow	0.0295874	0.95999	kmol/h
Molar Fraction (Mixture) / Acetone	0	0	
Molar Fraction (Mixture) / Isopropanol	1	0	
Molar Fraction (Mixture) / Hydrogen	6.75424E-15	0	
Molar Fraction (Mixture) / Nitrogen	0	1	

Comparison:

Parameter	Case 1	Case 2	Case 3	Unit	Remarks
IPA Conversion	92.8	92.8	92.8	%	High conversion
Acetone Purity	96.5	100	100	%	Meets industrial grade
Efficiency	89.52	89.64	89.64	%	Slight increase
Total Energy Duty	676.6	677.1	677	kW	Slight variation
Inert Build-up	High	High	Low	-	Purge High Low –ion
H_2 Recovery	Moderate	High	High	-	Valuable byproduct

Recycle improves yield slightly and stabilizes operation. Purge becomes necessary when feed contains non-condensables like N2.

Next Slide

Results and Conclusion:

- The DWSIM simulation showed the positive impact of recycle and purge integration on acetone production.
- Recycle system works best when the IPA feed is almost pure.
- Purge system is more effective when impurities or inerts are present in the feed.
- The optimal setup requires higher energy, so economic analysis is needed to find which option gives better net profit.
- The base case results closely matched the data from the reference research article.

Environmental & Economic Impact:

1. Environmental Impact

- Using byproduct Hydrogen as fuel.
- Recycling and purge system cut down waste and harmful gases.
- Heat reuse makes the process more eco-friendly and efficient.

2. Economic Impact

- Lower raw material cost due to recycling of unreacted IPA.
- Less energy use means reduced operating expenses.
- Higher acetone yield increases overall profit and process efficiency.

Reference Article:

Odunlami, M. O., Akintola, J. T., Amodu, O. S., Sodeinde, O. A., Ezeka, F. C., Gbadamosi, A. S., Shittu, A. A., & Omoigui, B. O. (2022, June 30). Process simulation of the synthesis of acetone from isopropyl alcohol. RJEES.

Research Article

Next Slide

Thank You!