CHE251 – Final Term Report

Process Simulation and Optimization of Acetone Production from Isopropanol

Course: CHE251
Instructor: Dr. Harshvardhan Katkar
Date: 8 November 2025

Team: Prakhar Gupta, Arun Chauhan, Prince Meena, Anubhav Jha, Aman Agrawal, Arjit Agrawal, Tripti

1. Background and Motivation

Acetone is a major solvent and intermediate widely used in pharmaceuticals, polymers, and coatings. Producing it from isopropanol (IPA) via catalytic dehydrogenation provides a cleaner and more efficient alternative to petrochemical routes. The reaction is endothermic and equilibrium-limited, which restricts single-pass conversion.

This project evaluates optimization strategies—specifically recycle and purge systems—using DWSIM, with compound separators replacing distillation columns for simplified separation.

2. Process Flow Diagram

Figure 1 shows the process flow diagram (PFD) for the system. The major equipment units are:

- Preheater/Vaporizer
- Reactor
- Condenser
- Flash Separator
- Distillation Column for acetone
- IPA Recovery Column
- Recycle Splitter and purge

3. Resources

The values and data we used were referred from ResearchGate Article on Acetone Production.

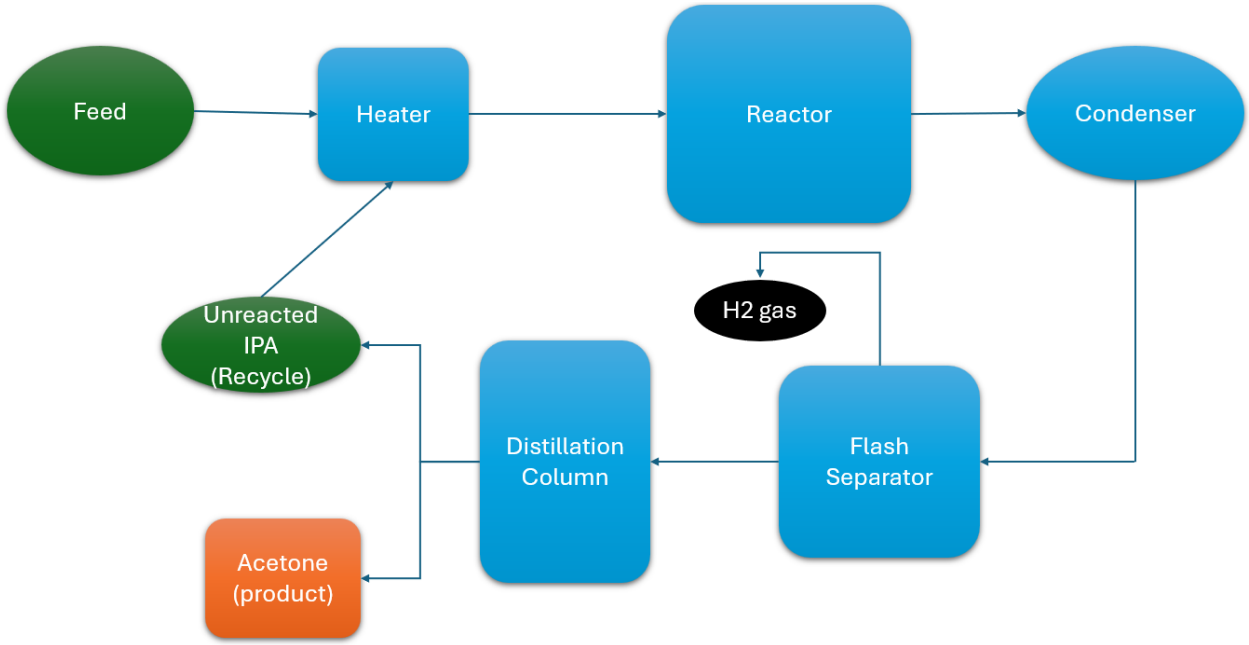

Figure 1: Process Flow Diagram for acetone production from IPA with recycle and purge.

4. Stream Information

Using the mass flow data from the reference article (12,000 t/y IPA feed, 10,000 t/y acetone product), the following molar flows were estimated:

$$F_{\text{IPA,feed}} = \frac{12,000 \times 10^3}{60.096} \approx 1.997 \times 10^5 \text{ kmol/yr} \approx 22.8 \text{ kmol/h}$$

$$F_{\text{Acetone,product}} = \frac{10,000 \times 10^3}{58.08} \approx 1.72 \times 10^5 \text{ kmol/yr} \approx 19.7 \text{ kmol/h}$$

5. Problem Statement

The catalytic dehydrogenation of IPA to acetone is reversible and highly energy-dependent. Single-pass conversion is limited, and inert buildup reduces system stability.
Based on literature data, 12000 tonnes/year IPA produces 10000 tonnes/year acetone. Converted to flow rate, this gives approximately 22.8 kmol/h feed.
Three simulation cases were developed:

- Case 1: Base process (no recycle, no purge)
- Case 2: Recycle loop without purge
- Case 3: Recycle + purge (optimized)

Peng–Robinson 1978 EOS was used throughout.

6. Flowchart

Case 1 – Base Process

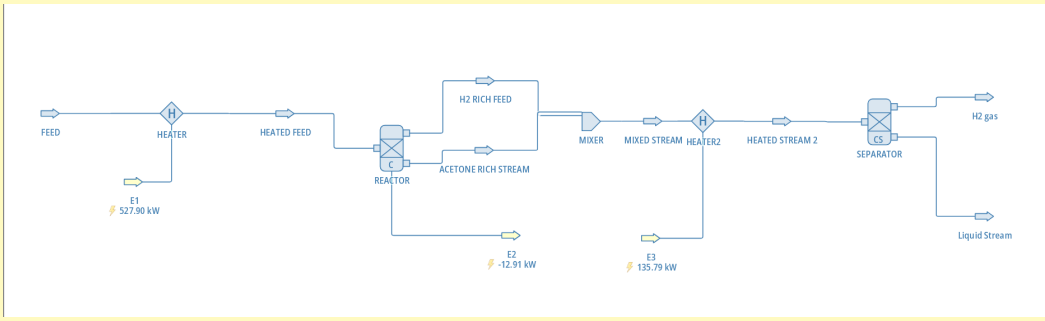

Figure 2: Base Process without Recycle or Purge

Case 2 – Process with Recycle

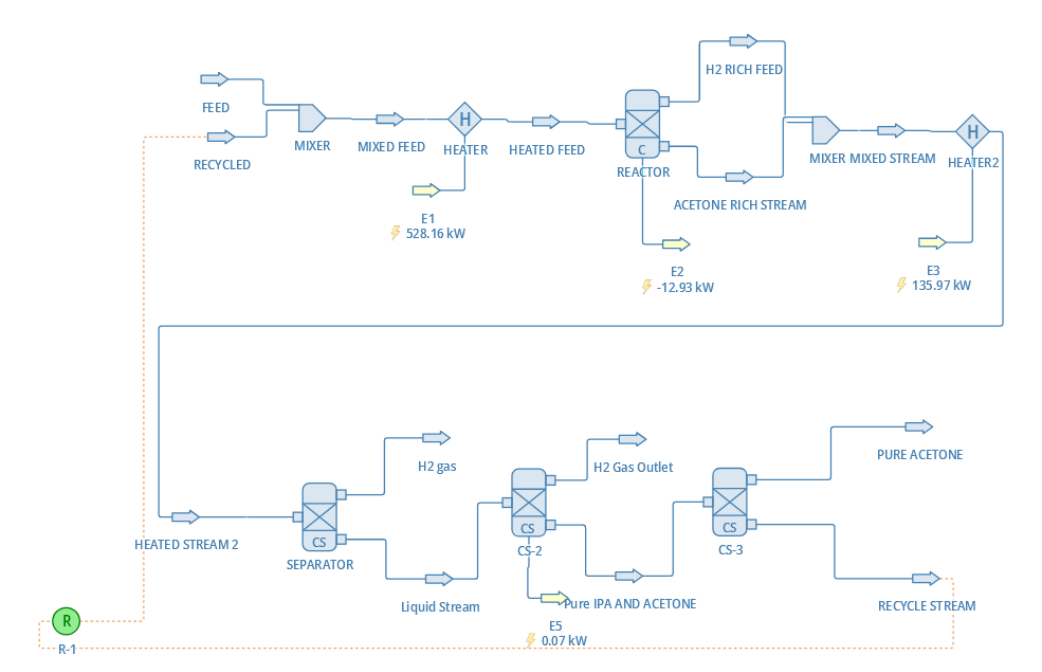

Figure 3: Process with Recycle Loop

Case 3 – Process with Recycle and Purge

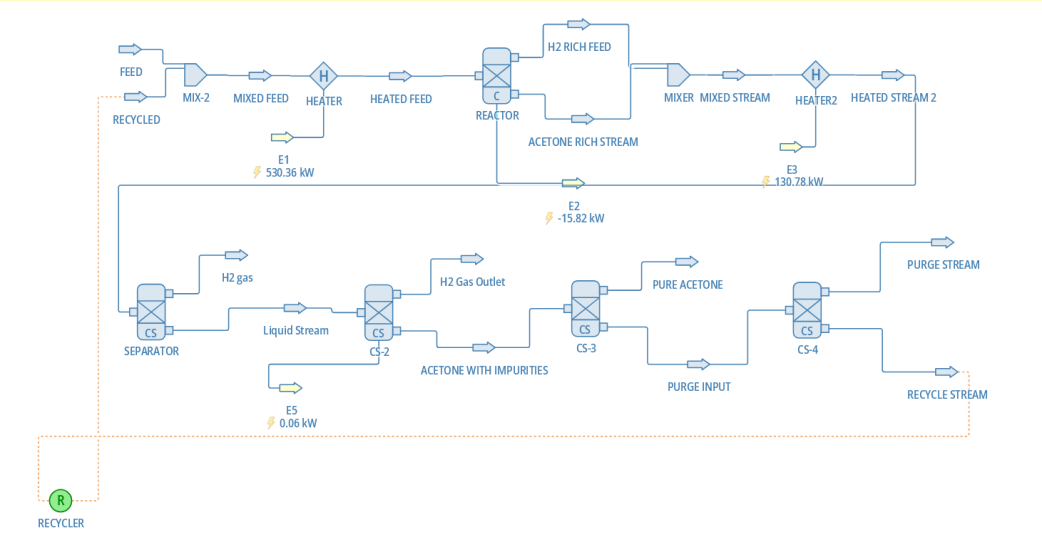

Figure 4: Process with Recycle and Purge Stream

7. Base Case Analysis

Feed: 100% IPA at 25°C, 1 bar, 22.8 kmol/h.

Heater

Heats the feed to 350°C and 2 bar as required for reaction.

Reactor

The reactor converts IPA to acetone + hydrogen with 92.8% efficiency. Outlet temperature drops to 49.82°C. The composition of both the streams are taken from the reference article, also the flow rates automatically matched as given in article. Two outlet streams:

- **H_2-rich stream:** 34.1464 kmol/h, 61.9% H_2, 36.5% acetone, 1.6% IPA.
- **Acetone-rich stream:** 9.81 kmol/h, 88.62% acetone, 11% IPA and rest H_2.

Mixer + Heater

Both streams are mixed and heated to 120°C and 2.2 bar.

Compound Separator

Separates the mixture into:

- gas stream (H_2-rich)
- liquid stream (acetone-rich)

Acetone Product Stream

Flow rate = 21.1498 kmol/h Purity = 96.5%

$$\text{Acetone obtained} = 21.1498 \times 0.96509 = 20.411 \text{ kmol/h}$$

$$\text{Yield} = \frac{20.411}{22.8} \times 100 = 89.52\%$$

8. Recycle Case Analysis

We first tried using distillation column but it was'nt working so we used multiple compound seperators. Product stream is passed through two compound separators:

- first removes leftover hydrogen
- second removes IPA which is recycled

Recycle stream: 0.029 kmol/h, 100% IPA Product stream: 20.438 kmol/h, 100% acetone

$$\text{Yield} = \frac{20.438}{22.8} \times 100 = 89.64\%$$

Yield increases by 0.14%.

9. Recycle + Purge Case Analysis

Feed: 24 kmol/h consisting of:

- 22.8 kmol/h IPA (99.5%)
- 1.2 kmol/h N_2 (5%)

Acetone obtained: 20.438 kmol/h Yield remains:

$$89.64\%$$

Purge is essential when inert buildup becomes significant.

10. Governing Equations

10.1 Reactor

$$C_3H_8O \rightarrow C_3H_6O + H_2$$

Conversion= 92.8%

10.2 Flash Separator

The cooled reactor effluent enters the flash separator, where the total stream flow F is divided into two outlet streams:

$$F \longrightarrow V + L$$

- **Vapour outlet :** 89.6%H_2 ,IPA 7.07%, Acetone 3.27%. light inerts (e.g. N_2) (only taken in case of purge)
- **Liquid outlet :** Acetone 96.51%, 3.35% H_2, rest is left IPA.

10.3 Distillation Section

The liquid outlet from the flash separator is fed to the distillation train:

- **Acetone Column :** Separates high-purity acetone as the distillate product . The design target is $> 99\%$ purity acetone. The bottom stream mainly contains unreacted IPA and heavier components.
- **IPA Recovery Column :** Processes the bottom stream from. Its distillate may contain light impurities, while the bottoms contain recovered IPA, which is recycled to the reactor feed.

In this report, the distillation is represented as a separation step with product acetone and a recycle stream. Detailed column design parameters (e.g. number of stages, energy duties) will be determined in the final simulation.

10.4 Recycle and Purge

The recycle stream from the IPA recovery column is split into two parts:

$$R \longrightarrow (1-p)R + pR$$

- **Recycle return:** The majority fraction $(1-p)R$ is mixed with the fresh feed and sent back to the preheater and reactor. This allows unreacted IPA to be reused.
- **Purge stream :** A small fraction pR is removed from the system to prevent the build-up of inerts and light by-products in the recycle loop. The purge rate p is tuned so that inert concentrations remain below acceptable limits (e.g. 2–3 mol%).

.....

11. Results and Discussion

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 prevents accumulation
H_2 Recovery	Moderate	High	High	-	Valuable byproduct

Recycle improves yield slightly and stabilizes operation. Purge becomes necessary when feed contains non-condensables like N_2.

12. Conclusion

The simulation study of acetone production from IPA in DWSIM demonstrated the progressive impact of recycling and purge integration. The recycled one was optimal if the feed is almost pure, else using purge one is optimal. But the optimal one demands greater energy and so we need to see by which way there is more net profit. Rest the results for the base case were precise to that mentioned in reference article.

13. References

ResearchGate Article on Acetone Production.