Mid-Semester Project Report
Production of Acetone from Isopropyl Alcohol

September 30, 2025

1 Introduction

The mid-semester report outlines the process design for the production of acetone by the catalytic dehydrogenation of isopropyl alcohol (IPA). Reported values include a feed of 12,000 t/y IPA, reactor conditions of 350 °C and 2 bar, and an assumed single-pass conversion of 98%.

2 Team Members

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

3 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

4 Resources

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

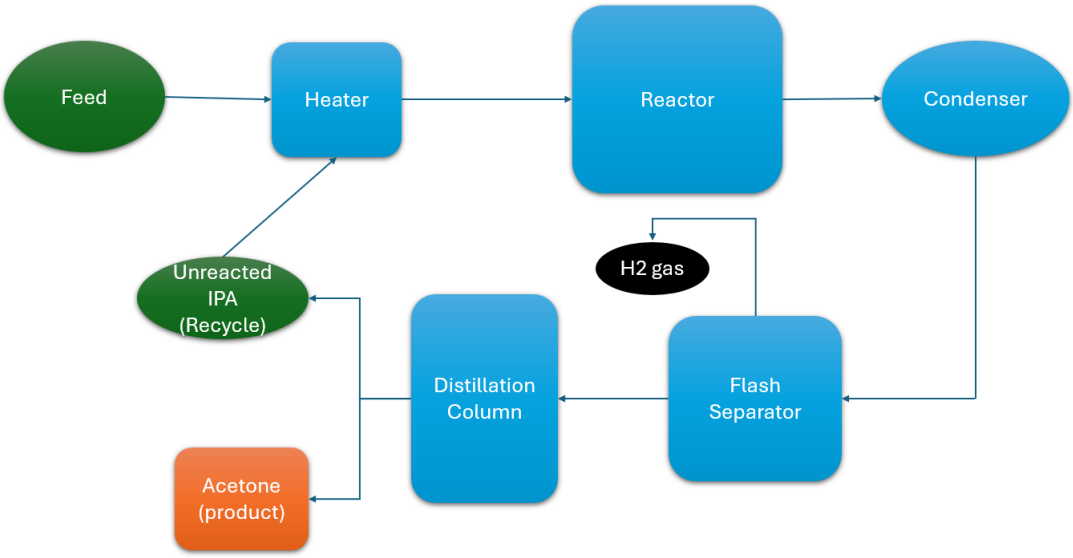

Figure 1: Process Flow Diagram for acetone production from IPA with recycle and purge.

5 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:

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

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

6 Governing Equations

6.1 Reactor

$$\text{IPA} \;\rightarrow\; \text{Acetone} + \text{H}_2$$
$$F_{A,\text{out}} = F_{A0}(1 - X_A)$$
$$\dot{n}_{\text{acetone}} = \dot{n}_{\text{H}_2} = F_{A0} X_A$$
$$Q_{rxn} = F_{A0} X_A \Delta H_{rxn}$$

6.2 Flash Separator

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

$$F \;\longrightarrow\; V + L$$

- **Vapor outlet :** Hydrogen-rich stream, containing mainly H_2 along with light inerts (e.g. N_2) and traces of acetone/IPA.
- **Liquid outlet :** Condensed liquid stream, containing mostly acetone, unreacted IPA, and heavier by-products. This stream is sent to the distillation section for acetone recovery and IPA recycle.

For the mid-term report, the flash is treated as a simple phase separator where gas and liquid phases are split based on expected volatilities. Rigorous vapor–liquid equilibrium (VLE) calculations (e.g. Peng–Robinson EOS) will be implemented in the final simulation model.

6.3 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.

6.4 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%).

For the mid-term stage, the recycle is modeled as a simple split with purge. In the final simulation, the purge fraction will be optimized to balance between minimizing product losses and controlling inert accumulation.

Table 1: Stream summary with unknowns and reactions

Stream / Unit	**Unknowns (to be solved)**	**Reactions / Notes**
Feed (IPA)	Inert fraction z_{I0}, exact T, P	Input basis: 12,000 t/y IPA
Preheated feed	Heater duty Q_{vap}, outlet T	Physical heating only
Reactor inlet	Mixed composition with recycle	
Reactor	Outlet flow rates; energy duty Q_{rxn}	Main reaction: $\mathrm{C_3H_8O} \rightarrow \mathrm{C_3H_6O} + \mathrm{H_2}$ Assume $X_A = 0.98$, $T = 350°\mathrm{C}$, $P = 2$ bar
Reactor effluent	Flow + composition	Contains acetone, IPA, H_2, traces inerts
Condenser exit	Cooling duty Q_{cool}	Physical cooling only
Flash Separator	Split ratio V/L; vapor fraction ϕ	$F \rightarrow V + L$; Vapor (S-06) = H_2-rich
Flash vapor	Flow, composition, H_2 purity	H_2 product stream
Flash liquid	Flow, acetone purity	Sent to distillation train
Acetone column	Distillate rate D, reflux ratio, stages	Produces acetone (product)
IPA recovery column	Reboiler duty Q_{reb2}, bottoms flow R	Recovers IPA to recycle (S-08)
Recycle stream	Flow R, composition $x_{i,loop}$	Unreacted IPA returned to loop
Recycle Splitter	Purge fraction p	Balance: $R \rightarrow (1-p)R + pR$
Recycle return	Flow $(1-p)R$	Mixed with fresh feed
Acetone product	Purity ($> 99\%$), actual flow	Target 10,000 t/y
Purge gas	Purge rate pR, composition	Controls inert build-up: $x_{I,\mathrm{loop}} = \dfrac{F_0 z_{I0}}{pR}$
H_2 product	Flow, purity	$\dot{n}_{\mathrm{H_2}} = F_{A0} X_A$ (stoichiometric)