

Conversion Improvement of Propylene to Acrylic Acid Process

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Abstract

Acrylic acid ($C_3H_4O_2$) is a chemical compound used widely in industry. This study aims to develop a modified process for Acrylic Acid production through direct oxidation. The objective is to improve Acrylic Acid conversion over conventional methods. Process modeling and simulation were conducted using Aspen Plus, and the systems were optimized for operating conditions. In conclusion, both proposed methods offer viable and environmentally favorable alternatives for sustainable propylene production, with the DC2M route offering superior economic performance.

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1. Introduction

Acrylic acid ($C_3H_4O_2$) is the simplest unsaturated carboxylic acid commercially produced by the oxidation of propylene in a two-step process: first acrolein is formed, then oxidized to acrylic acid, with the use of molybdenum and vanadium-based catalysts to maintain high selectivity [2]. This compound is a clear, colorless liquid with a pungent odor, has a double functional structure ($-COOH$ and $C=C$) that is highly reactive to free radical polymerization, making it a key monomer in the synthesis of poly(acrylic acid), superabsorbents, and acrylate esters [3]. More than 3.4 million tons of acrylic acid are produced globally each year (old data), with market demand continuing to increase and estimated to reach around 6.2 million tons in 2020, of which around 50% is processed into glacial grade (98–99.5%) for applications such as sap, polyelectrolytes, and esters for coatings and adhesives [4].

Purification of acrylic acid (AA) is necessary to avoid spontaneous polymerization and maintain the stability of the monomer during storage and processing. Vacuum distillation is often used to separate AA from impurities—such as water, acetic acid, and dimers—with the column temperature maintained between 90–110 °C at low pressure (~30–50 mm Hg). This method is effective in producing high-content products and preventing thermal degradation and thermo-initiated polymerization. In addition, liquid-liquid extraction using solvents such as di-isopropyl ether (DIPE), followed by vacuum distillation, has been shown to be able to obtain high-concentration AA solutions and separate water and acetic acid before the final purification step. Furthermore, membrane techniques such as reverse osmosis (RO) have been used to increase the concentration of AA prior to distillation, significantly reducing energy consumption and wastewater production [5].

In addition to production and purification aspects, storage and handling of acrylic acid (AA) are also important concerns in industry because of

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its chemical nature which is prone to spontaneous polymerization if not properly stabilized. Typically, AA is stored under controlled conditions with the addition of inhibitors such as hydroquinone monomethyl ether (MEHQ) or phenothiazine, and in a closed container with an inert atmosphere such as nitrogen to prevent contact with oxygen and excessive heat [6]. Storage temperatures are generally maintained below 25 °C to avoid the initiation of exothermic reactions that have the potential to cause fire or explosion hazards. In addition, AA storage and transportation equipment must be corrosion-resistant and free from transition metals such as iron or copper that can catalyze uncontrolled polymerization [7].

On the other hand, in recent years, research on the production of bio-based acrylic acid has begun to show significant development as a more sustainable alternative. One promising approach is the conversion of lactic acid or 3-hydroxypropionate (3-HP) from biomass sources to AA through a dehydration process with the help of solid catalysts such as zeolite or modified alumina [8]. This method not only reduces dependence on fossil-based propylene, but also opens up opportunities for processing biomass waste into high-value products. Although its efficiency and selectivity are still challenges, the integration of this process with biorefinery and the improvement of catalyst performance are continuously being developed to approach industrial scale. As the global demand for environmentally friendly chemical processes increases, this bio-acrylate pathway is projected to play an important role in the transition to a green chemical economy [9].

To improve the production of ethylene dichloride in terms of economics and good conversion, This study will examine the impact of this study will examine the impact of removing the recycle stream.. The research study shows that overcoming this problem can be done by implementing sustainable design procedures at various stages of the process. Optimizing conversion and minimizing carbon emissions by selecting purification methods are in line with key targets in the industrial sector.

The independent variables include pressure, temperature, and flow composition, while the dependent variable or target is the conversion rate of propylene to acrylic acid. Although the modified process achieved a higher conversion (96.34%) compared to the unmodified one (94.85%).

2. Method

The plant design in Ferrier's study [1] utilizes a fluidized bed reactor to convert

propylene, air, and steam into acrylic acid through a partial oxidation reaction. The reactor effluent is first cooled and partially condensed before entering a flash drum (V-1), where non-condensable gases are separated. The liquid stream is then sent to the bottom of a liquid-liquid extraction column (T-1), while a stream of diisopropyl ether (DIPE) is introduced at the top. This extraction step transfers acrylic acid and acetic acid into the organic phase, reducing water content before distillation. The resulting organic extract is fed to a distillation column (T-2), where acrylic acid is separated as a bottom product. The overhead stream from T-2, containing DIPE and light components, is cooled and split between a recycle stream returning to T-1 and a waste stream. The medium-pressure steam generated in the reactor is used to supply energy to the T-2 reboiler, improving energy efficiency within the system.

The simulation of Acrylic Acid production process was carried out using Aspen HYSYS V12. The simulation model was based on a syngas feed containing H₂O, Steam, and Propylene and includes multiple unit operations such as reactors, separators, compressors, and heat exchangers. The process used is through oxidation of propylene. Based on the simulation in the HYSYS V.11 program, the molar flow and mass flow error percentages were 3.4546% and 0.0057%, respectively. This can be caused by the imbalance of the inlet and outlet flows in the reference journal, where the inlet flow is 2202.362 kmol/h and the outlet flow is 2135.487 kmol/h. This can be due to the limitations of MPS modeling in the reactor system. In this case, Moving Particle Semi Implicit (MPS) modeling is used to analyze the free surface flow of incompressible fluids without using a grid. MPS is very suitable for simulating the movement of sensitive liquid fuels and the flow and interaction with very complex reactor structures. The main advantage of MPS is its ability to handle large deformations and dynamic changes in fluid shape, which are difficult to do by traditional grid-based methods. In addition, the MPS scheme shows a higher level of stability. However, parallelization of MPS, especially in PPE (Prediction-Correction Semi-Implicit), is indeed more difficult compared to SPH (Smoothed Particle Hydrodynamics). because it has complexity in iteration so that the parallelization efficiency of MPS is not as high as SPH.

Raw materials with certain pressure and temperature are fed into the mixer for homogenization of raw materials. Then, before entering the reactor, the raw materials must pass through a control valve to adjust the pressure and temperature required for the reaction process in

the reactor. After the reaction is complete, the feed is cooled using cooling water in preparation for entering the separator. In the separator, the gas phase and the liquid phase are separated, where the liquid phase is a mixture of the final product. However, the product is still not pure enough to contain acrylic acid. Furthermore, the gas phase output from the separator is fed into the absorber to remove impurity gases using water based on the principle of solubility. Then, the liquid phase product still contains water and other by-products in the form of acetic acid and water. To obtain pure acrylic acid, a distillation device is used to separate these components so that acrylic acid is obtained at the bottom. For storage purposes, the temperature and pressure of acrylic acid that comes out of the distillation are adjusted using cooling water and a control valve.

After the reaction, the outflow from the reactor will contain a mixture of water, steam, and Propylene. This mixture is then directed to the Acrylic Acid separation column, where the Acrylic Acid is separated from the other components. Propylene and water will be further separated in the Propylene separation column to be recycled back into the reactor.

3. Results and Discussion

3.1 Process Flow Overview

The process flow diagram illustrates the production of acrylic acid from propylene via an oxidation process using a series of unit operations. The feed streams, including propylene, steam, and air, enter the system and are pumped into a mixer (MIX-100) to form a homogeneous mixture. This mixture is then heated in a heat exchanger (E-201) before entering the reactor (R201), where the main oxidation reaction occurs with a conversion rate of approximately 79.89%. The reactor effluent, containing a mixture of products and unreacted reactants, passes through a cooler (E-202) to reduce its temperature, then continues to E-100 for further cooling.

The cooled stream enters a flash separator (T-201) to separate light gases (Stream 10) and liquid components (Stream 11). The bottoms from T-201 are sent to a valve (VLV-101) and then into a distillation column (T-100) for product purification. Here, lighter impurities are removed at the top (Stream 13) and heavier components including the desired acrylic acid are drawn off as bottom products (Stream 14). The bottom product is further cooled in E-101, with cooling water (CW) as the utility. The light gases removed from T-100 (Stream 13) are pressurized using P-100 and recycled via RCY-1 to the front end of the process to increase overall efficiency. The system is controlled by a set point controller (SET-1) and an adjuster (ADJ-1) to ensure optimum reactor performance and conversion. The second process configuration, as shown from Figure 3 and Figure 4, demonstrate a superior acrylic acid conversion of 96.34 %, compare to 94.85% observed in the original configuration that can be seen from Figure 1 and Figure 2.

The optimization of the acrylic acid production process was systematically evaluated using the Case Study tool in Aspen HYSYS. This tool facilitated parametric analysis by varying independent variables (pressure, temperature, and flow composition) to assess their impact on propylene conversion. The simulation revealed that the original process, incorporating a recycle stream, underperformed due to two primary factors: (1) Dilution of reactants: Recycled components reduced the partial pressure of propylene in the plug flow reactor (PFR-100), diminishing reaction kinetics; (2) Accumulation of inerts/by-products: These impurities interfered with catalyst activity and thermal stability.

In contrast, the modified system, which operates with a single-pass configuration, benefits from a more concentrated and consistent feed composition. Furthermore, the slightly reduced heat input (8.01×10^7 kJ/h in the modified case versus 8.209×10^7 kJ/h in the original) suggests improved thermal control, minimizing

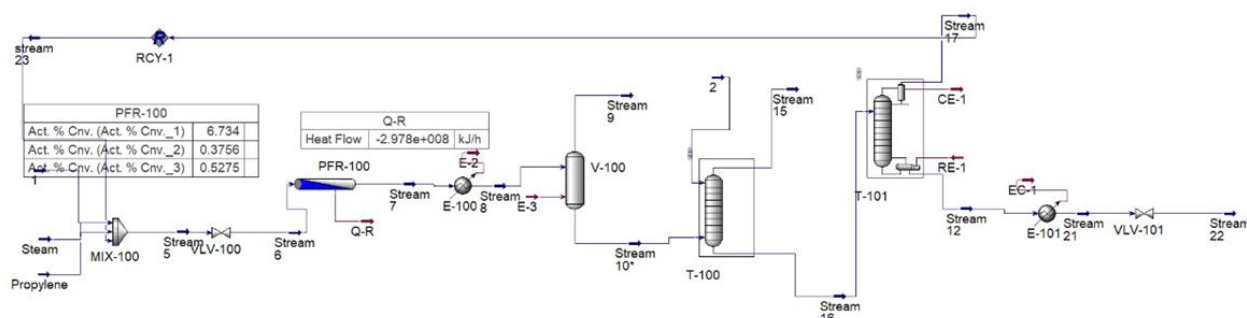


Figure 1. Modified process flow diagram of acrylic acid production using Aspen HYSYS.

side reactions and enhancing selectivity towards acrylic acid. These combined factors contribute to the improved reactor performance, indicating that under the specific operating conditions examined, the removal of the recycle stream results in a more favorable conversion profile.

3.2 Reactor Performance

The reactor itself is a plug flow reactor, This resulted in a volume of 56.5 m³). To cool the highly exothermic reaction, boiler feed water (BFW) is used and converted to medium pressure steam

(MPS). Plug flow reactors are a type of reactor in which the reactant concentration changes along the reactor. This is because in the modeling of plug flow reactors, the reactants are assumed to be continuously consumed as long as the reactant flow flows along the reactor. The consumed reactants were converted into products, so that the product concentration increased.

3.3 Properties and Reaction During Process

Acrylic acid (AA) is polar and has a high boiling point (~141 °C), but under vacuum

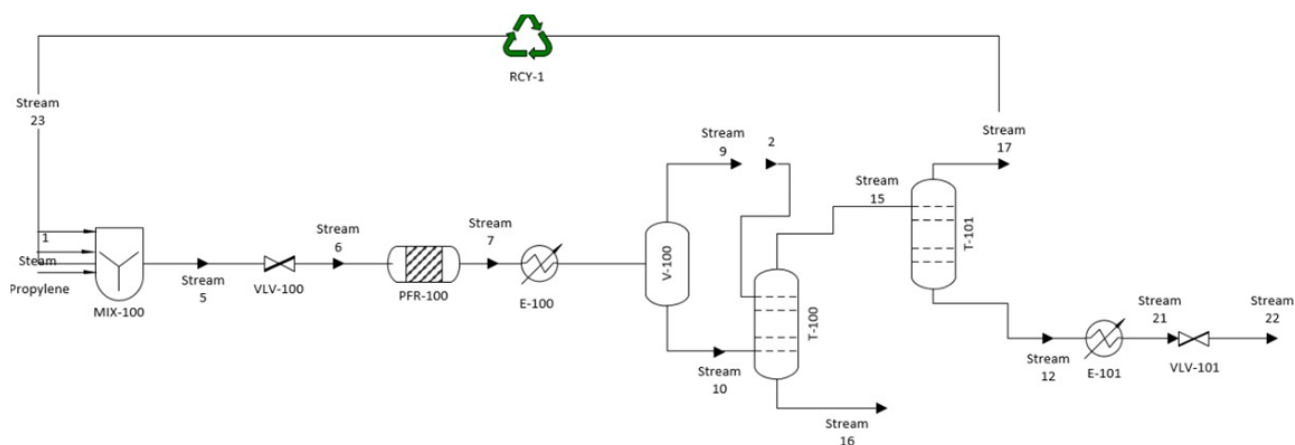


Figure 2. Process flow diagram of basic process of acrylic acid production.

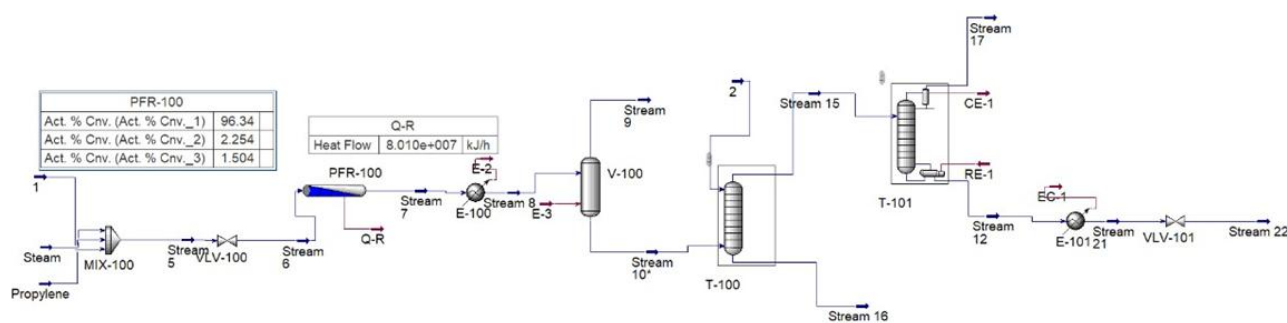


Figure 3. Modified process flow diagram of acrylic acid production using Aspen HYSYS.

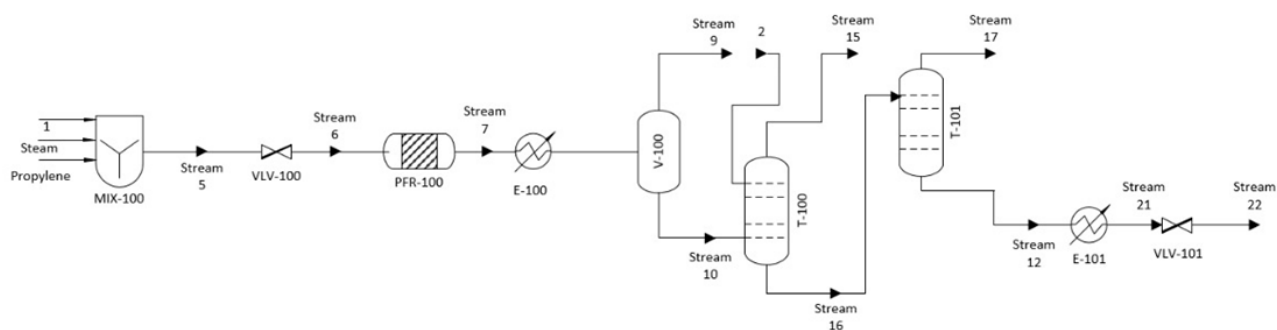
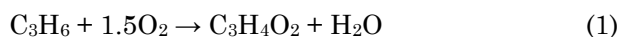


Figure 4. Flow diagram of modified process of acrylic acid production.

conditions in the module distillation column the vapor phase contains light compounds such as water or methanol, while the AA-rich liquid phase is almost glacial—as seen in the low frac mole streams in the separate modified and fabricated columns. In a propylene oxidation reactor at high temperatures (~360–400 °C), propylene is oxidized to acrolein and then to AA; the kinetics and selectivity are highly dependent on the Mo–V–Ox catalyst composition and operating conditions, where increasing temperature accelerates the conversion but the risk of overoxidation (to CO₂) also increases; this was demonstrated in a kinetic study of Bi₂Mo₃O₁₂ and vanadyl pyrophosphate [8]. The PFR reactor with plug-flow facilitates residence time control for AA conversions of >94 % at propylene conversions of up to ~96 % [10], as achieved under optimized gas–solid conditions in a two-stage fluidized bed. After the reaction, the heat from the exothermic reaction passes through an exchanger (E-100), followed by vapor–liquid separation (T-100) before distillation; the resulting heat flow Q-R reaches the order of 10⁷–10⁸ kJ/h [11], corresponding to the strong exothermic oxidation reaction energy. Overall, the thermal properties of AA, the kinetic characteristics of propylene oxidation, and the reactor design (PBR/PFR) are key elements to achieve high conversion with optimum selectivity, according to your HYSYS simulation conditions.

3.4 Main Reaction

The production of acrylic acid (C₃H₄O₂) from propylene (C₃H₆) proceeds via a two-step oxidation mechanism in the presence of oxygen (O₂), typically using a Mo–V–Te–Nb–O or Mo–Fe–Bi catalyst system. For simplicity in process modeling, the overall reaction is expressed as a single-step reaction:



The standard enthalpy change of the reaction (ΔH^0) and Gibbs free energy change (ΔG^0) at 298 K are –493.8 kJ/mol and $\Delta G^0 = -372.3$ kJ/mol, respectively.

These values indicate that the oxidation of propylene to acrylic acid is highly exothermic and thermodynamically favorable under standard conditions.

3.5 Thermodynamic Consideration

To evaluate the spontaneity and feasibility of the reaction under operating conditions, the equilibrium constant is calculated from the Gibbs free energy change:

$$\Delta G^0 = -RT \ln K \quad (2)$$

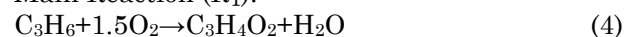
$$\ln K = -\frac{\Delta G^0}{RT} = -\frac{-372300}{8.314 \times 298} \Rightarrow K \approx 1.62 \times 10^6 \quad (3)$$

A very large equilibrium constant indicates that the reaction strongly favors the formation of acrylic acid and water under standard conditions. Furthermore, because the enthalpy change ($\Delta H^0 = -493.8$ kJ/mol) is negative, the reaction is exothermic, and higher temperatures may shift the equilibrium slightly backward according to Le Chatelier's principle. However, the increase in temperature enhances the reaction kinetics, justifying operation at elevated temperatures (e.g., 260–300 °C) in industrial reactors.

3.6 Kinetics Consideration

The reaction kinetics were modeled based on empirical rate laws and Arrhenius expressions for the three parallel reactions:

Main Reaction (R₁):



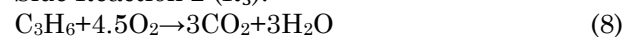
$$-r_1 = k_1 \cdot (\text{C}_{\text{C}_3\text{H}_6}) \cdot (\text{C}_{\text{O}_2}) \quad (5)$$

Side Reaction 1 (R₂):



$$-r_2 = k_2 \cdot (\text{C}_{\text{C}_3\text{H}_6}) \cdot (\text{C}_{\text{O}_2}) \quad (7)$$

Side Reaction 2 (R₃):



$$-r_3 = k_3 \cdot (\text{C}_{\text{C}_3\text{H}_6}) \cdot (\text{C}_{\text{O}_2}) \quad (9)$$

With Arrhenius constants:

$$k_1 = 1.59 \times 10^5 \cdot \exp\left(\frac{-E_{a1}}{RT}\right) \quad (10)$$

$$k_2 = 8.83 \times 10^5 \cdot \exp\left(\frac{-E_{a2}}{RT}\right) \quad (11)$$

$$k_{13} = 1.81 \times 10^8 \cdot \exp\left(\frac{-E_{a3}}{RT}\right) \quad (12)$$

where, $E_{a1} = 15,000$ kcal/kmol; $E_{a2} = 20,000$ kcal/kmol; $E_{a3} = 25,000$ kcal/kmol; $R = 1.987$ kcal/kmol; $T = 533$ K.

These kinetic expressions were implemented into a plug flow reactor (PFR) model, where reactants are continuously consumed along the reactor length, and the temperature is controlled via external cooling due to the highly exothermic nature of the reactions. The simulation showed that with optimized conditions, propylene conversion reaches 96.34%, and acrylic acid selectivity is significantly improved in the modified configuration compared to the original.

3.7 Environment, Health, and Safety Concern

In the acrylic acid (AA) production process, runaway polymerization poses a major hazard: this reaction is highly exothermic and can cause

equipment blockage, as described in a calorimetric study that recorded uncontrolled heat and explosion risks in AA storage tanks [12]. To reduce this risk, the AA temperature is kept below 92 °C, since kinetic studies have shown that Michael addition can trigger polymerization even at low temperatures and reasonable inhibitor volumes [13]. Furthermore, the fire risk is very high in propylene (LFL 2.4%, UFL 11%), so flammability studies emphasize the importance of an air-free reactor design and the use of sensors, redundant controls, and leak detection systems [14]. From an environmental perspective, life cycle analysis (LCA) suggests that increasing the selectivity of propylene to AA reduces CO₂ and VOC emissions that are detrimental to the atmosphere. Finally, the CCPS guidelines recommend electrostatic protection, grounding, and the use of stable inhibitors such as MEHQ to prevent spontaneous polymerization, maintain personnel safety and avoid thermal and fire hazards [15]. Recent studies have shown that N-alkyl phenoxazine derivatives exhibit super-stoichiometric radical scavenging activity, thus having the potential to be stronger AA stabilizers than MEHQ, especially under acidic conditions often encountered in the AA production process [16].

4. Conclusion

This study successfully achieves its objective by demonstrating that the modified process configuration enhances acrylic acid conversion from 94.85% to 96.34%. The improvement confirms the effectiveness of the design modification in optimizing the conversion performance of propylene to acrylic acid.

Credit Author Statement

Author Contributions: A. D .A .T. Barus: Conceptualization, Writing, Software, Review and Editing; A. H. Bahij: Conceptualization, Writing, Software, Review and Editing; K. B. P. Nadeak: Conceptualization, Writing, Software, Review and Editing; M. S. Farhan: Conceptualization, Writing, Software, Review and Editing. All authors have read and agreed to the published version of the manuscript.

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