Article

Process Development for Methyl Isobutyl Ketone Production Using the Low-Pressure One-Step Gas-Phase Selective Hydrogenation of Acetone

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Abstract: Methyl isobutyl ketone (MIBK) is a highly valuable product in the chemical industry. It is widely used as an extracting agent for heavy metals, antibiotics, and lubricating oils. Generally, MIBK can be produced by three-step and one-step liquid-phase methods. These methods are expensive and energy-demanding due to the high pressure and low conversion of acetone. A novel nano-Pd/nano-$ZnCr_2O_4$ catalyst was developed to produce MIBK with high conversion and selectivity of 77.3% and 72.1%, respectively, at 350 °C and ambient pressure, eliminating the need for high pressure in conventional MIBK processes. This study is the first that proposes a newly developed process of methyl isobutyl ketone (MIBK) production using the low-pressure one-step gas-phase selective hydrogenation of acetone. In this work, a novel process flow diagram has been developed for the production of MIBK using the developed nano-catalyst. The process was heat integrated, resulting in a 26% and a 19.5% reduction in the heating and cooling utilities, respectively, leading to a 12.6% reduction in the total energy demand. An economic analysis was performed to determine the economic feasibility of the developed process, which shows that the process is highly profitable, in which it reduced both the capital and operating costs of MIBK synthesis and showed a return on investment (ROI) of 29.6% with a payback period of 2.2 years. It was found that the ROI could be increased by 18% when the reactor temperature is increased to 350 °C. In addition, the economic sensitivity analysis showed that the process is highly sensitive to product prices and least sensitive to utility prices, which is due to the versatility of the process that requires only a low amount of energy.

Keywords: methyl isobutyl ketone (MIBK); acetone self-condensation; selective hydrogenation; process development; heat integration; economic analysis; nano-Pd/nano-$ZnCr_2O_4$ catalyst

1. Introduction

Methyl isobutyl ketone (MIBK) is an industrially important chemical worldwide. It can be used in a wide variety of important applications, including protective surface coating, vinyl, and acrylic resins, the extraction of metallic salts, and the removal of paraffin from mineral oils [1–5]. It is also used in the production of paints and rubber, as well as a solvent in a variety of pharmaceuticals and adhesives [6,7].

The global production of MIBK was 430,000 metric tons in 2020 [8]. The market for MIBK is expected to grow at a compound annual growth rate (CAGR) of more than 6% by 2026. This is due to the increasing demand for MIBK, especially in the synthesis of antioxidant additives for rubber, and the growing demand for solvents in chemical processes [9].

In addition to MIBK, a crucial byproduct is also produced, which is isopropyl alcohol (IPA). It has tremendous industrial, medical, and hygienic applications, including alcohol wipes, hand sanitizers, disinfectants, and swabs, which increases the prospects of applying the MIBK process with minimal waste. According to the Centers for Disease Control and

Prevention (CDC) in the United States, alcohol-based hand sanitizers and cleansing wipes contain between 60% and 90% of alcohol, and the use of 70% of IPA is recommended [10]. Medical IPA was scientifically proven as a disinfectant that inactivates viruses such as the COVID-19 virus.

MIBK can be produced by several processes, but essentially by a three-step [11] method and a single-step method [12–17]. Each of these processes can be carried out with different catalysts, raw materials, and reaction conditions [12]. The three-step method involves aldol condensation of acetone over homogeneous aqueous-based catalysts, such as sodium and calcium hydroxide, forming diacetone alcohol (DAA), which is subsequently dehydrated to mesityl oxide (MO). The final step is the selective hydrogenation of the C=C bond of MO to MIBK using Cu or Ni catalysts [18,19]. The most commonly occurring side reactions are over-condensation and unselective hydrogenation [20].

The three-step process produces a considerable amount of wastewater containing acidic impurities due to the homogeneous catalyst, which creates a corrosive environment associated with high capital and operating costs for the neutralization process, acetone condensation, and product purification [18,19,21]. Alternatively, the one-step process using a metal-supported catalyst was demonstrated to be more efficient [22–28]. The support catalyzes acetone condensation to mesityl oxide (MO), an α,β-unsaturated ketone, followed by in situ catalytic reductions to MIBK using palladium on acidic ion-exchange resins [18,29,30], while there are other processes that use Pd/zirconium phosphate [31]. In the one-step liquid-phase process, hydrogen and acetone are passed over metal base catalysts at moderate temperature and high pressure to produce MIBK in a single step, saving enormous costs that are required in the three-step method [32]. Under these reaction conditions, aldol condensation and dehydration are reversible [33], but the catalyst shifts the equilibrium toward MO, irreversibly hydrogenating it toward MIBK [28].

Despite the many advantages offered by the liquid-phase one-step process, it suffers from high pressure, ranging from 3 to 10 MPa [13], which significantly increases the capital and operating costs. This is in addition to the large recycle flow rate due to the low conversion of acetone, which increases the size of equipment in the recycle loop as well as the additional energy that is needed for recovering the unreacted acetone in the distillation column. Therefore, it is an industrial objective to reduce the pressure and increase the conversion and selectivity to make the process more profitable.

Recently, Qianling et al. reported a bifunctional catalyst TiO_2/Al_2O_{32} and Pd/Cor for one-pot liquid-phase synthesis of MIBK from acetone, which provides acetone conversion of (35–45)% with a selectivity of (80–90)% to MIBK at 150 °C and 2.0 MPa [34]. However, the process still suffers from the high-pressure requirement with moderate acetone conversion. Baining et al. proposed an alternative support with high thermal stability and adjustable acid-base property using phosphor-doped h-BN that catalyzes the aldol condensation and dehydration to provide an acetone conversion of 58.24% and selectivity of 68.39% to MIBK [35]. In addition, various kinds of support, including metal oxides [19,36,37] and sulfonated graphene [38,39], have also been a prime focus in the development of the process.

In this context, a novel nanocrystalline zinc chromite-supported nanopalladium (nano-Pd/nano-ZnCr$_2$O$_4$) catalyst was developed by Bagabas et al. and Al-Rabiah et al. [20,40,41], which enables the production of MIBK in a one-step gas-phase reaction at atmospheric pressure. This can overcome the infirmities that the conventional process suffers from. However, the process requires a temperature of (200–350) °C, which is higher than the conventional process, which uses a temperature of (120–160) °C [15].

The reaction involves base–acid coupling of acetone to form mesityl oxide (MO), followed by its hydrogenation to methyl isobutyl ketone (MIBK). The products with this catalyst are methyl isobutyl ketone (MIBK) as the main product, isopropyl alcohol (IPA) as the main byproduct, and diiasobutyl ketone (DIBK), mesityl oxide (MO), and mesitylene (M) are also formed [20,40,41]. The MIBK produced by low-pressure one-step gas-phase acetone condensation has an acetone conversion of (20–78)% and MIBK selectivities of

(40–73)% for reaction temperatures of 200–350 °C with a hydrogen-acetone molar feed ratio of 1 to 6 [20,40,41].

This research work focuses on the development of a novel process for the production of methyl isobutyl ketone (MIBK) from hydrogen and acetone in a one-step gas-phase reaction at ambient pressure using a novel nano-Pd/nano-ZnCr$_2$O$_4$ catalyst. Heat integration is conducted to reduce the process utilities. In addition, this work investigates process economics to measure the profitability and the impact of market volatility on the profitability of the process.

2. MIBK Process Development

The developed process flow diagram for the production of methyl isobutyl ketone is shown in Figure 1. A process simulation was conducted using CHEMCAD v.7.1 software based on a production of 30,000 metric tons of MIBK per annum with 30 days assigned for maintenance. The thermodynamic model chosen was UNIFAC as a cubic equation of state. The reactor conversion, selectivity, and feed ratio used in the simulation were based on the aforementioned experiment.
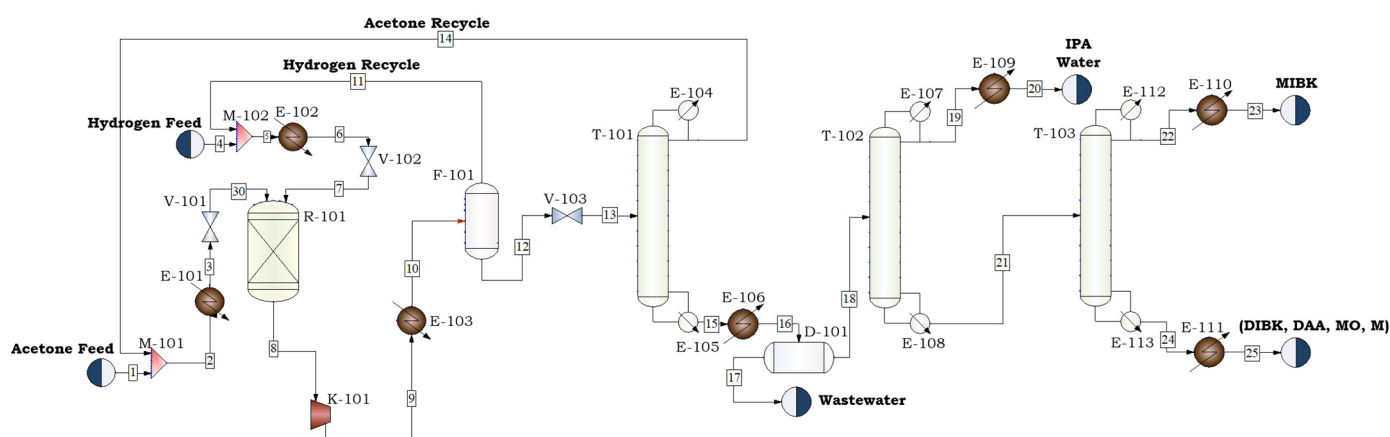

Figure 1. Developed process flow diagram (PFD) of the MIBK process.

The fresh acetone feed (stream 1) enters the process at 70 °C and 1.8 atm in a liquid phase and is mixed with the recycled acetone (stream 14), which enters at 74 °C and 1.8 atm. Before entering the reactor R-101, the mixed stream is heated to 300 °C. The hydrogen feed is mixed with recycled hydrogen (stream 11) before being heated to 300 °C and fed into reactor R-101. Both reactor feeds pass through valves, V-101 and V-102, to reduce the pressure in the reactor. The hydrogen–acetone molar feed ratio is maintained at 2:1, as recommended [40,41]. The reaction proceeds isothermally in the gas phase at 300 °C and 1 atm in a fixed bed catalytic reactor (R-101). The conversion of acetone is 66%, with a selectivity of 69.4% to methyl isobutyl ketone (MIBK). Other products, such as isopropanol (IPA) and diiasobutyl ketone (DIBK), are also produced. The selectivity of each of these substances was determined based on the experimental work, which is shown in Table 1. The reactor effluent will then be compressed to 6.5 atm to compensate for pressure losses through the pipelines and to enhance the separation of hydrogen without major product losses from the process stream at low pressure and high temperature, preventing the use of cryogenic conditions. MIBK losses at 1 atm are approximately 6 kmol/h. Consequently, compression is mandatory to avoid cryogenic conditions. At 6.5 atm, the losses drop to about 0.7 kmol/h of MIBK. After compression, the stream is cooled to 35 °C in E-103 before being fed into the flash drum F-101. The overhead stream from flash drum F-101 contains nearly 99.996% of the unreacted hydrogen, which is recycled and mixed with the fresh hydrogen. The bottom stream from flash drum F-101 (stream 12) is then throttled to 1.8 atm in V-103 before entering the distillation column, T-101. Nearly 99% of the unreacted acetone is recovered in the overhead stream of T-101, using 48 stages, before being mixed

with the fresh acetone. The acetone/water system forms an azeotropic mixture at higher compositions; therefore, about 0.04 of the entered water into the column is recovered into the top stream to maintain the mixture in the column below the azeotropic point. The bottom stream from T-101 is cooled to 70 °C in E-106 before being sent to a water decanter, D-101, where 90% of the water is removed. The second outlet stream from the decanter enters the distillation column, T-102, which consists of 34 stages, where 99.28% of the isopropanol (IPA) is recovered. The remaining water is also separated with IPA in the distillate stream, and the mixture is then cooled to 40 °C in E-109. The purity of IPA in the top stream of T-102 is almost 68%, which is highly recommended to be used as sanitizer in the medical industry, and therefore, there is no need to install a further distillation column for increasing the purity of the IPA. The bottom stream from T-102 enters another distillation column, T-103, which consists of 67 stages where 99% of the MIBK is recovered in the overhead stream with a purity of 99.83 wt.%, achieving the product specifications [14]. The MIBK stream is then cooled to 40 °C in E-110 before being sent to the storage tank. The bottom stream from T-103, which contains the heavy components (e.g., DAA, MO, M, and DIBK), is cooled to 40 °C in E-111.

Table 1. The conversion and selectivity of the MIBK process at different temperatures [20,40,41].

Temperature (°C)	Acetone Conversion%	Selectivity					
		MIBK	DIBK	MO	M	IPA	DA & Others
200	20.1	40.6	10.2	6.1	2.1	40.7	0.3
250	40.7	53.9	12.3	4.4	2.5	25.8	1.1
300	66	69.4	12.4	2.1	2.6	11.2	2.3
350	77.3	72.1	13.5	2.2	2.7	5.4	4.1

3. Heat Integration in the MIBK Process

Heat integration is an essential part of the process development. The reduction in energy usage not only reduces the operating costs but also prevents harmful carbon emissions in the environment. The required heating and cooling utilities were identified for the process as shown in Figure 1. Each process stream was drawn with a tail and a head representing the supplied temperature and the target temperature, respectively. The final heat exchanger network is shown in Figure 2, where the red and blue lines denote the hot and cold streams, respectively. The constructed network utilizes the energy content and high temperature of the reactor effluent to heat up the feed streams. The acetone feed (stream 2) leaving mixer M-101 will first be heated by the reactor effluent from 74.3 °C to 242 °C, in which no further heating can occur due to the process constraint prohibiting phase change before the inlet of the compressor. The reactor effluent will be further cooled by the hydrogen feed (stream 5) until it reaches a minimum temperature approach of 10 °C to avoid an excessive large area. The outcome of the heat integration, as shown in Figure 3, is a reduction in the heating and cooling utilities by 26% and 19.5%, respectively. The reduction in the total utility demand is about 12.6%. In terms of economics, the implemented heat integration has resulted in an increase in the annualized capital cost by $12,134/year (for 10 years of operation). However, operating costs have decreased by $611,852/year, indicating a highly plausible energy utilization that satisfies both technical and economic aspects.

The blue columns in Figure 3 represent the utility demand before the heat integration, while the green columns represent the current value of the utility demand in the MIBK process after heat integration. In addition, the figure is divided into three sections, starting from the total utility demand, including the combined heating and cooling utilities, then the heating utility in the middle, while the cooling utility is placed on the right side. The process was re-simulated after the heat integration using CHEMCAD v.7.1. The developed flowsheet after heat integration is shown in Figure 4. The material balances for the key streams of the developed MIBK process are shown in Table 2.
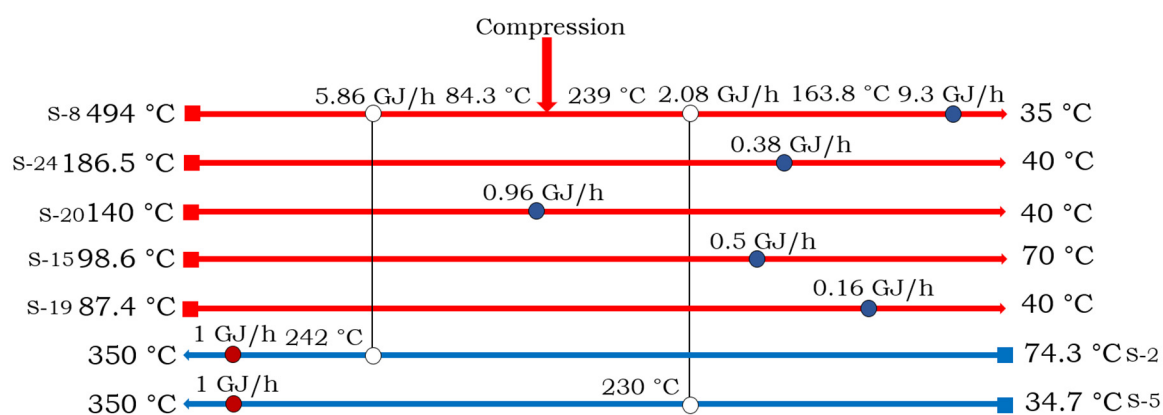
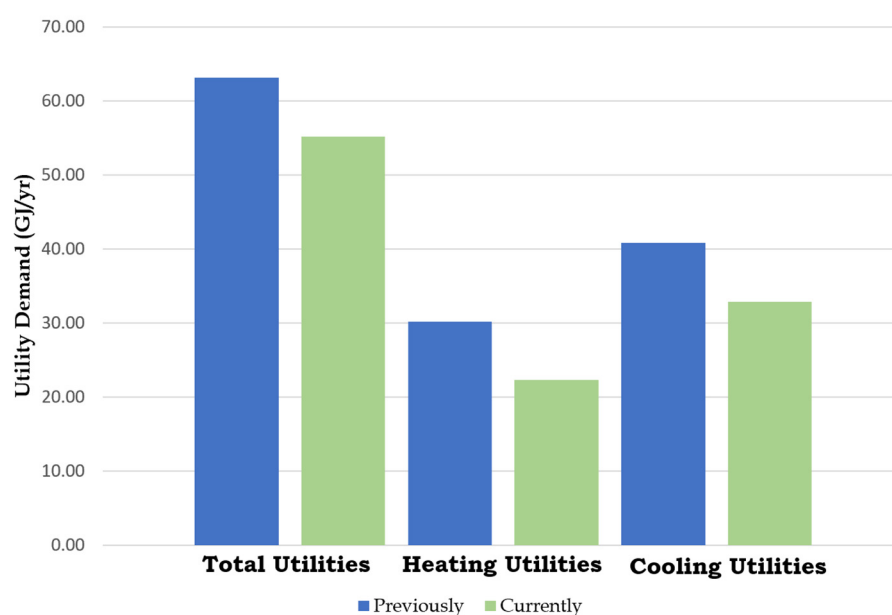**Figure 2.** Heat exchanger network of the process streams for the developed process.

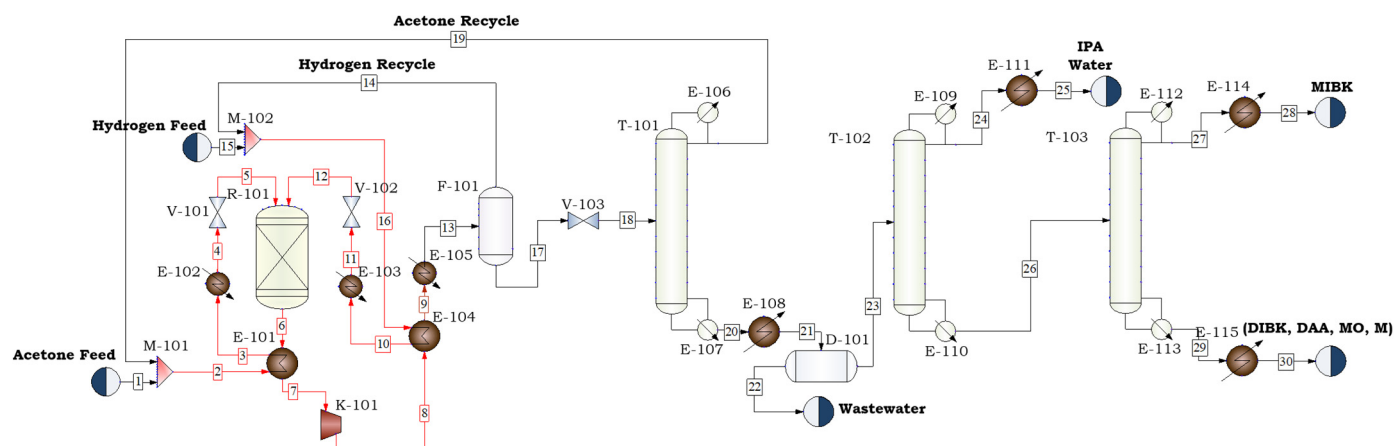**Figure 3.** Heat integration outcome for the developed process.

Figure 4. Developed process flow diagram (PFD) of the MIBK process after heat integration.

Table 2. Material balance of key streams for the developed MIBK process.

Streams	Acetone Mixed Feed (S-2)	Hydrogen Mixed Feed (S-16)	Reactor Effluent (S-6)	Acetone Recycle (S-19)	Hydrogen Recycle (S-14)	Waste-Water (S-22)	(IPA + Water) Product (S-25)	MIBK Product (S-28)	(DIBK, DAA, MO, M) Product (S-30)
Temperature (°C)	74.29	34.74	300	61.49	35	70	40	40	40
Pressure (atm)	1.8	5.9	1	1.8	5.9	1.4	1.4	1.9	2.4
Enthalpy (MJ/h)	−37,473.6	−2720.4	−35,506.3	−10,788	−2695.83	−12,968.1	−5515	−12,209.8	−3039.6
Molar vapor fraction	0.29	1	1	1	1	0	0	0	0
Molar flow rate (kmol/h)	160.11	342.63	443.12	50.13	283.34	45.94	18.02	37.46	8.25
Mass flow rate (kg/h)	9224.8	1266.14	10,491	2837.35	1146.63	827.54	−5515	3748.6	1054.04
Component flow rates (kmol/h)									
Hydrogen	0.0109	331.31	272	0.0109	272	0	0	0	0
Acetone	158.3	7.64	56.4	48.27	7.64	0	0.49	0	0
MIBK	0	0.75	38.75	0	0.75	0	0.2492	37.37	0.38
Water	1.84	2.36	55.24	1.84	2.36	45.94	5.1	0	0
DAA	0	0.0012	1.26	0	0.0012	0	0	0	1.26
MO	0	0.0115	1.16	0	0.0115	0	0	0.0065	1.15
M	0	0.0148	0.9637	0	0.0148	0	0	0	0.9489
IPA	0.00645	0.5225	12.79	0.0065	0.5225	0	12.18	0.0883	0
DIBK	0	0.0155	4.54	0	0.0155	0	0	0	4.53

4. Economic Analysis

An economic analysis was performed to verify the profitability of the process based on several economic indicators, including the return on investment, payback period, net present worth, and discounted cash flow rate of return.

The return on investment (ROI) is expressed on an annual basis, and it is defined as the average net profit divided by the total fixed capital investment as shown in Equation (1) [42].

$$\text{ROI} = \frac{\text{Yearly net profits}}{\text{Fixed capital investement}} \tag{1}$$

The payback period (PBP) is defined as the required time to recoup the original depreciable fixed capital investment as shown in Equation (2) [42].

$$\text{PBP} = \frac{\text{Depreciable fixed capital investment}}{\text{Avg. profit/yr} + \text{avg. depreciation/yr}} \tag{2}$$

The net present worth (NPW) is defined as the difference between the present value of the annual cash flow and the initial required investment as shown in Equation (3).

$$\text{NPW} = \frac{\text{Net cash flow at time t}}{(1 + \text{interest rate})^{\text{time of cash flow}}} \tag{3}$$

The discounted cash flow rate of return (DCFRR) represents the maximum interest rate that a project can afford to pay for its total capital investment [43] as shown in Equation (4) [42].

$$\text{NPW} = \sum_{n=1}^{n=T} \frac{\text{Cash flow at time t}}{(1 + \text{DCFRR})^n} - \text{Total capital investment} = 0 \tag{4}$$

In order to determine the economic indicators, the following should be calculated: (i) the cost of the equipment; (ii) the costs of raw materials and utilities; (iii) the total capital cost; and (iv) the total production cost.

4.1. Purchase Cost

In order to determine the purchase costs, the process equipment sizes must first be calculated; the process simulator was used for this purpose. In addition, the costs were estimated using the CHEMCAD costing package, adjusting all the costs to 2022 using the Chemical Engineering Plant Cost Index (CEPCI) [44]. Figure 5 depicts the distribution of the process equipment costs. Note that the condensers and reboilers of the distillation columns are compiled with heat exchangers. The cost distribution of the process equipment indicates that the distillation columns account for the largest share of fixed capital costs of around 40% as the most expensive units of the process, which is due to the byproducts generated by the process.
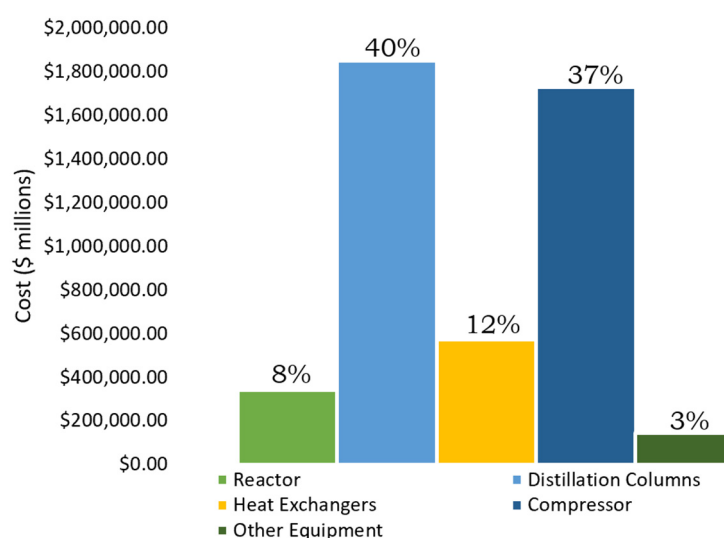

Figure 5. Fixed capital cost distribution for the developed process.

4.2. Raw Material and Utility Costs

Besides the fixed capital costs, the raw materials and utility costs are major components of the production cost. The prices of the raw materials, utilities, and products are shown in Table 3.

Table 3. Cost input for the developed MIBK process [45,46].

Item	Price Unit
Raw Materials	
Acetone	$790/ton
Hydrogen	$2500/ton
Utilities	
High-pressure steam (hps)	$5.66/GJ
Medium-pressure steam (mps)	$4.77/GJ
Low-pressure steam (lps)	$4.54/GJ
Boiler feed water	$1.532/1000 kg
Cooling water (cw)	$15.7/1000 m^3
Electricity	$0.0674/kWh
Products	
Methyl isobutyl ketone (MIBK)	$2120/ton
Isopropanol (IPA)	$1540/ton
(DAA, DIBK, MO, M)	$1300/ton

The distribution of the utility costs is depicted in Figure 6. It shows that electricity represents 35% of the total utility cost, which is due to its high prices. Low-pressure steam is the second most cost-intensive required utility that is used in the reboiler of T-101. Although cooling water is the most consumed in terms of volume, it accounts for only 5%

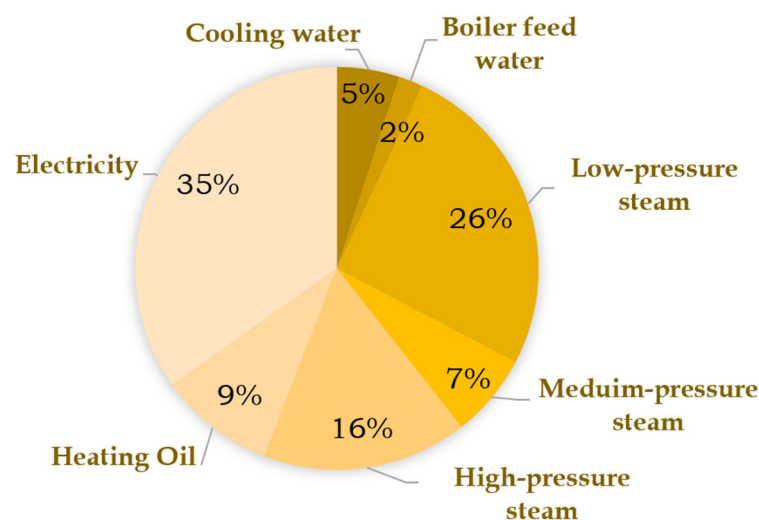of the total utility cost, which is due to the low price of cooling water compared to the other utilities.

Figure 6. Utility cost distribution for the MIBK process.

4.3. Total Capital Cost

The total production cost comprises all of the direct, indirect, and general expenses [42]. The direct costs are estimated as a fraction of the purchased equipment costs and include all the prices of the delivery and installation of the purchased equipment, installed instrumentation and control systems, installed piping, electrical systems, yard improvement, buildings, and service facilities [42]. The direct cost of the developed MIBK process is $18.34 million per annum. The indirect cost was calculated as a fraction of the direct cost provided in Plant Design and Economics for Chemical Engineers by Peter and Timmerhaus [42]. It includes the engineering and supervision costs, construction, legal, contractor, and contingency expenses, which represent $7.34 million [42]. The fixed capital investment is the summation of the direct and indirect costs [42]; it is $25.68 million for the MIBK process. The total capital investment is a combination of the fixed capital investment and the working capital. The working capital was taken as 0.15 of the total capital cost for the fluid processing plant [42]. The total capital investment in the developed MIBK process is $30.21 million.

4.4. Total Product Cost

The total product cost represents all of the annual expenses that are required for production. It includes raw material prices, utility costs, operating labor, maintenance and repairs, operating supplies, laboratory charges, royalties, taxes, financing, insurance, rent, depreciation, plant overhead, administration, distribution and selling, and research and development expenses, all of which are fractions of the fixed capital investment provided by Peter and Timmerhaus [42]. The total production cost, excluding depreciation, for the developed MIBK process is $55.78 million annually.

4.5. Profitability Evaluation

The process profitability can now be evaluated after obtaining all of the necessary information. The total raw material cost is $42.71 million per year, which accounts for 76.7% of the total product cost. The total product price is $83.81 million yearly, which shows a positive profit margin. Therefore, fluctuations in the raw material or product prices may have a considerable influence on the process profitability; consequently, a sensitivity analysis is required for the price fluctuation. The plant has shown its feasibility in being commercially applied; the return on investment for the plant is 29.6%/y, with a payback period of 2.2 years. Furthermore, the plant could generate $28.93 million profits in 10 years

of operation. The discounted rate of return on investment of the plant is 26.6%. Table 4 summarizes the economic performance of the MIBK process.

Table 4. The economic performance for the developed MIBK process.

Factor	Value
Total Raw Material Cost	$42.71 million/y
Total Utility Cost	$1.646 million/y
Fixed Capital Investment (FCI)	$25.68 million
Total Capital Investment (TCI)	$30.22 million
Depreciation	MACRS, 5 years recovery period
Total Product Cost	$55.78 million/y
Revenue	$83.81 million/y
Return on Investment (ROI)	29.6%/y
Payback Period	2.2 y
Net Present Worth (at i = 15%)	$28.93 million
Discounted Cash Flow Rate of Return (DCFRR)	26.6%

4.6. Economic Sensitivity Analysis

The petrochemical industry is a highly volatile market that has experienced many ups and downs throughout its market history [47,48]. Therefore, to account for these perturbations, raw material costs, product costs, utility costs, and fixed capital costs were varied by ±15% of their current prices. Figure 7 shows the overall sensitivity analysis of the above factors at a constant production rate and 10 years of operation. It shows that the process is highly dependent on the product prices, in which a 10% increase could make the process an extremely lucrative process with an ROI of 54.3%. However, a 15% decrease could make the process unprofitable with an ROI of 4.1%. The fluctuation in the product prices gave maximum and minimum values of ROI in the sensitivity analysis, which represents the importance of reducing the MIBK losses throughout the process. On the other hand, raw material prices come in as a second large contributor to the process profitability, in which a 15% increase in the raw material prices decreases the ROI to 12.7%, whereas a 15% reduction in the raw material prices increases the ROI to 46%. This highlights how crucial it is to properly recover unreacted raw materials (e.g., acetone and hydrogen), in addition to the great influence that the higher selectivity can have on the process profitability. The fixed capital investment was found to be the third largest contributor, with an ROI of 23.5% if its cost increased by 15% and an ROI of 37.7% if its cost decreased by 15%. This also highlights that even though recovering more of the product and raw materials can increase the TCI, it has a lower negative influence on the process profitability than losing them. In addition, it is worth noting that the utility cost, as expected, has an insignificant impact on the ROI as the current utility cost is $1.646 million per year, representing only 2.95% of the total product cost, which is due to the low-pressure requirement in the process compared to the conventional process, which is directly associated with the electricity consumption.
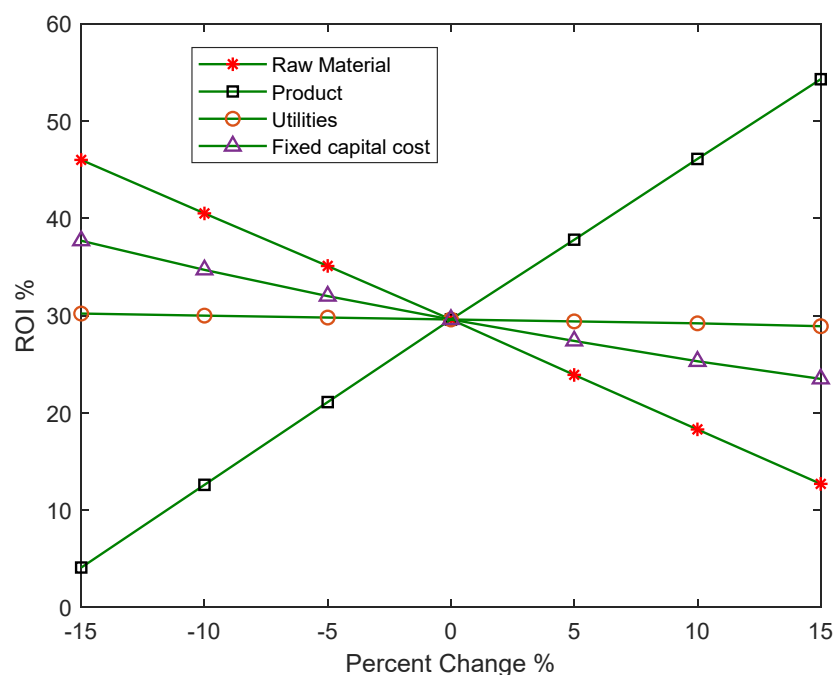
Figure 7. Return on investment under various market variations of the economic factors.

4.7. Effect of Reaction Temperature on the Process Profitability

The temperature for reactor operation proposed by Al-Rabiah et al. [40,41] is in the range of (200–350) °C. The conducted sensitivity analysis has shown that it is appealing to increase the conversion and selectivity of the process. In the current study, the used temperature is 300 °C. When the reactor temperature is increased to 350 °C, the conversion and selectivity are increased from 66% and 69.4% to 77.3% and 72.2%, respectively. Consequently, less acetone is required, and more MIBK is produced. Nevertheless, this also increases the heating requirement needed for the feed stream as well as the reactor cooling system. In order to determine the optimum temperature in terms of profitability, the process was simulated at 350 °C. All costs were determined in the same manner as previously done. Figure 8 shows that as the reactor temperature increases, the fixed capital investment decreases, which is due to the lower volume of the distillation column T-101 that is needed to separate acetone from the process stream. In addition, the rest of the columns' size remained almost the same as the production rate was fixed. In addition, the cost of the compressor decreased because the numbers of unreacted moles of acetone and hydrogen were lower. On the other hand, the heating utility that is required to maintain the reactor temperature was increased by about 10%. In addition, more heating utility was required for E-102 because the minimum temperature approach was increased from 10 °C to 30 °C to prevent a phase change prior to the compressor. It is worth noting that even though the inlet temperature to E-105 was increased from 164 °C to 180 °C, the heat duty was about 11% less due to the lower flow rate entering the heat exchanger. The condenser and reboiler heat loads of T-101 were also lower due to the lower amount of unreacted acetone. An overall assessment of energy consumption is shown in Figure 8, which indicates that increasing the temperature from 300 °C to 350 °C reduces the overall energy consumption of the process. Furthermore, the ROI increased to 34.3%, and the payback period decreased to 2 years.
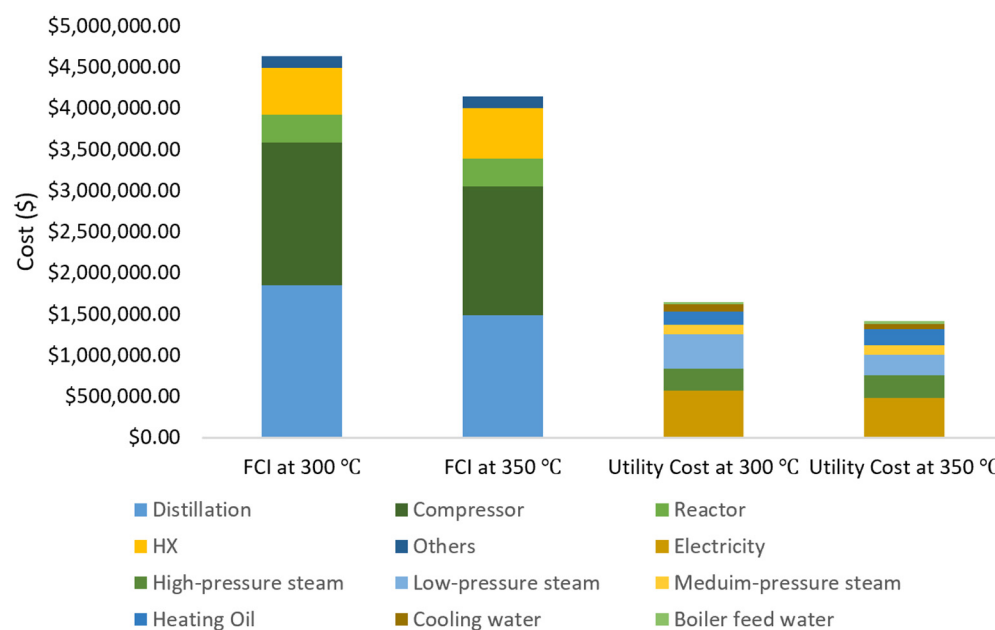
Figure 8. A comparison between the effect of the eactor temperature on the FCI and the utility cost.

In terms of profitability, the return on investment for the process when operating at 350 °C is 35.1%/y, which is 18% higher while the net present worth has upsurged by 12%. Figure 9 depicts the cash flow diagram of both process conditions.
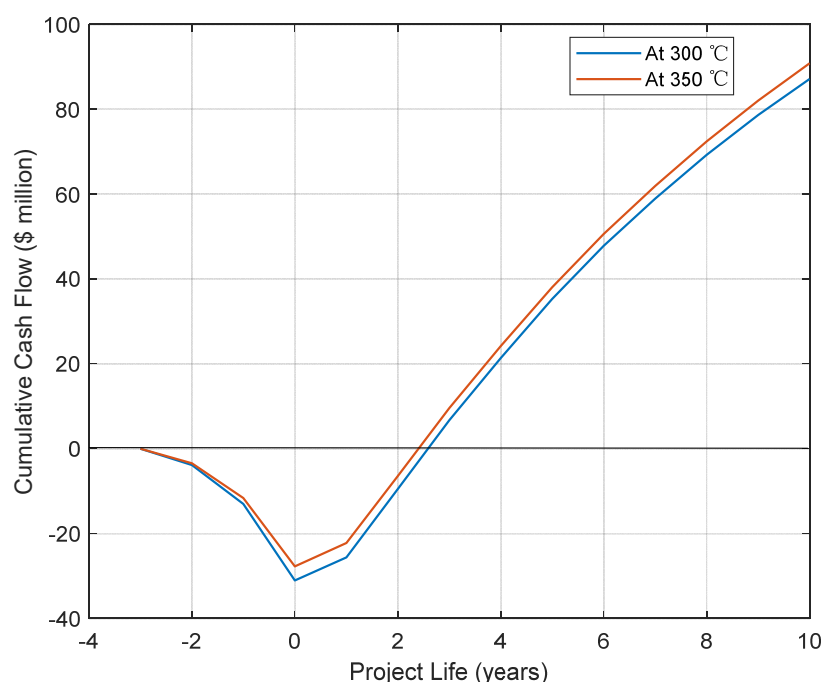

Figure 9. The cumulative cash flow diagram for both reactor temperatures.

5. Conclusions

Methyl isobutyl ketone (MIBK) is a chemical intermediate and an important solvent. It is used in several important applications in the chemical market. There are several methods to produce MIBK, either by the three-step process or by the one-step liquid-phase reaction method, which is commercially preferred. However, these methods require very high pressure, which is expensive and energy consuming. In contrast, a promising nano-Pd/nano-ZnCr$_2$O$_4$ catalyst was developed to produce MIBK in a one-step gas-phase

reaction under ambient pressure, overcoming the drawback of the conventional process. In this work, a novel process flowsheet has been developed and simulated. The developed process was heat integrated by matching the process streams to deliver the surplus heat to the heat deficit streams, resulting in a 12.6% reduction in the total energy demand. A comprehensive economic analysis of the developed process was conducted and has shown that the process is highly profitable with a return on investment (ROI) of 29.6% and a payback period of 2.2 years. It is shown that when the process is operated at a temperature of 350 °C, the economics improved, and the ROI increased to 34.3%.

6. Patents

US Patent No. 7,951,976, 31 May 2011, US Patent No. 8,101,805, 24 January 2012, EP Patent No. 2,532,642 B1, 25 January 2017, EP Patent No. 2418017B1, 21 November 2018.

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Abbreviations

Abbreviation	Definition
MIBK	Methyl Isobutyl Ketone
CAGR	Compound Annual Growth Rate
DAA	Diacetone alcohol
MO	Mesityl oxide
DIBK	Diiasobutyl ketone
M	Mesitylene
IPA	Isopropyl alcohol
W	Water
FCI	Fixed Capital Investment
TCI	Total capital investment
ROI	Return on investment
DCFRR	Discounted Cash Flow Rate of Return

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