Article

Performance Analysis of the Perhydro-Dibenzyl-Toluene Dehydrogenation System—A Simulation Study

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Abstract: The depletion of conventional energy resources has drawn the world's attention towards the use of alternate energy resources, which are not only efficient but sustainable as well. For this purpose, hydrogen is considered the fuel of the future. Liquid organic hydrogen carriers (LOHCs) have proved themselves as a potential option for the release and storage of hydrogen. The present study is aimed to analyze the performance of the perhydro-dibenzyl-toluene (PDBT) dehydrogenation system, for the release of hydrogen, under various operational conditions, i.e., temperature range of 270–320 °C, pressure range of 1–3 bar, and various platinum/palladium-based catalysts. For the operational system, the optimum operating conditions selected are 320 °C and 2 bar, and 2 wt. % Pt/Al_2O_3 as a suitable catalyst. The configuration is analyzed based on exergy analysis i.e., % exergy efficiency, and exergy destruction rate (kW), and two optimization strategies are developed using principles of process integration. Based on exergy analysis, strategy # 2, where the product's heat is utilized to preheat the feed, and utilities consumption is minimized, is selected as the most suitable option for the dehydrogenation system. The process is simulated and optimized using Aspen HYSYS® V10.

Keywords: LOHC; simulation; exergy analysis; dehydrogenation; optimization

1. Introduction

With the increase in the world's population with time, followed by the increased demand for better living standards, it can be forecasted that future energy demand will be increased tremendously, and meeting this extreme energy requirement is a challenging task for the world. In the existing state, most of the energy requirement of the world is linked with heating and transportation, and is met using fossil fuels, mainly natural gas, coal, and crude oil. However, these energy resources are non-sustainable and non-renewable, as their use is linked with the increased greenhouse gases emissions, and these resources are depleting rapidly with time, respectively [1–3]. Therefore, the world has diverted its attention towards two important aspects: (1) the investigation and use of such energy resources in the existing infrastructure, that are sustainable and renewable, (2) use of energy resources in a way that these resources are capable of meeting the energy demand and do not cause any harm to the environment [4].

For more than 120 years ago, hydrogen has been considered an ideal energy carrier. The heating value (HHV) of the fuel is linked with the hydrogen contents, i.e., the more the hydrogen contents in the fuel, the higher will be its HHV. Therefore, pure hydrogen has proved itself as an ideal energy source since it has the highest value of HHV amongst all energy fuels. Hydrogen has been termed as the "fuel of the future" because of various

reasons: (1) the combustion of hydrogen is clean, as NO_x, and SO_x are not produced, (2) the combustion results in the generation of water with a net heat release of 242 kJ/mol, (3) in comparison to the petroleum products, the energy density of hydrogen is 3 times higher, i.e., 120 kJ/g [4,5]. Based on the energy contents (kJ/g), the comparison of hydrogen with other fuels is presented in Table 1 [6].

Table 1. Energy contents of various fuels [6].

Fuel	Energy Contents (kJ/g)
Hydrogen	120.00
LNG	54.40
Propane	49.60
Automotive Gasoline	46.40
Automotive Diesel	45.60
Ethanol	29.60
Coke	27.00
Methanol	19.70
Wood (dry)	16.20
Bagasse	9.60

For hydrogen storage, various methods have been reported in the literature. A comparative analysis, based on energy demand and cost estimation, is presented in Table 2. For the cost estimation, the following important parameters are considered: (1) catalyst cost, (2) operational expenses, (3) electricity cost, (4) depreciation cost, and (5) substation of LOHC material [5,6]. The analysis shows that liquid organic hydrogen carriers (LOHC) are the most suitable option for the storage and release of hydrogen since the energy demand and cost required for the LOHC system is the lowest, followed by compressed hydrogen storage, and liquid hydrogen storage [7].

Table 2. Comparative analysis of various hydrogen storage system [5,6].

Description (Unit)	Liquid Hydrogen Storage	Compressed Hydrogen Storage	Liquid Organic Hydrogen Carriers
Cost Estimation (€/kg hydrogen)	0.732	0.243	0.238
Energy Demand (kWh$_x$/kWh$_{hyd}$)	21%	3.5%	1.1%

Based on the reported literature, a good LOHC system must have the following characteristics, so these systems can be utilized for practical application (on a large scale):

- Non-toxic and safe during transportation and use, with an acceptable eco-toxicology profile.
- Low production cost and compatibility with current fuel infrastructure.
- To attain the stability of LOHC molecules, an enthalpy of 40–70 kJ/mol is required.
- Gravimetric storage capacities are greater than 6 wt. % and volumetric storage capacities greater than 56 kg/m^3 are required.
- To simplify hydrogen purification and to require low dynamic viscosity for fast pumping, a high boiling point is required, i.e., greater than 300 °C.
- Lower melting point i.e., less than—30 °C is required for two reasons: (1) to eliminate the requirement for the addition of external solvents, and (2) to eliminate the requirements for solid-based fuel infrastructure [8–10].

The comparison between various LOHC systems, as reported in the literature, is presented in Table 3. MCH-Toluene system (MTH) remained a well-known system in the early stages of the LOHC system. However, there are certain drawbacks associated with the use of this system, i.e., (1) thermodynamically, MCH requires harsh conditions, owing

to the high heat demand for the dehydrogenation process, (2) catalyst deactivation/coke-formation, and by-product formation at higher temperatures $\geq 350\,°C$, (3) lower values of flashpoints and boiling points are problematic towards selectivity, reversibility, etc. The major hurdle associated with the implementation of the benzene-toluene system is the carcinogenic property of the benzene. There are several problems associated with the naphthalene-decalin system, which makes this system unfavorable for the operation, (1) the solid nature of naphthalene which causes difficulties in transportation and storage, and (2) high energy requirement for the dehydrogenation.

In comparison to these three systems, the perhydro-dibenzyl-toluene and dibenzyl-toluene (PDBT-DBT) system provides several advantages: (1) none of the components is carcinogenic, (2) liquid nature, therefore no handling, storage, and transportation issues, (3) lower vapor pressure of DBT allow easy release of hydrogen in the liquid phase, low vapor pressure is advantageous with respect to the safety and storage of PDBT-DBT, low vapor pressure means that these compounds can be stored at atmospheric conditions and when needed, these can be dehydrogenated via reaction, (4) lower volatility helps in obtaining comparatively higher purities of hydrogen, and (5) higher value of volumetric density [7,10–14]. Regarding the high energy requirements of dehydrogenation in this system, it has been reported that the process can be performed efficiently by using a micro-structured reactor [14,15]. Therefore, the PDBT-DBT system is taken as the LOHC system in this study. The overall working of the LOHC system is depicted in Figure 1 [16].

Table 3. Comparison of various LOHC system [7,10–14].

| Characteristics	MCH-Toluene System	Cyclohexane-Benzene System	DBT-PDBT System	Naphthalene-Decalin System
Pressure (bar)	10–50	10–50	10–50	20–50
Temperature (°C)	200–300	150–250	180	150–250
Phase under ambient conditions	Liquid	Liquid	Liquid	Solid + Liquid
Heat of reaction (kJ·mol^{-1})	204.8	205.9	588.5	319.5
Gravimetric H$_2$ density (wt. %)	6.16	7.20	6.20	7.29
Volumetric H$_2$ density (kg-H$_2$.m^{-3})	47.4	55.9	57	65.4
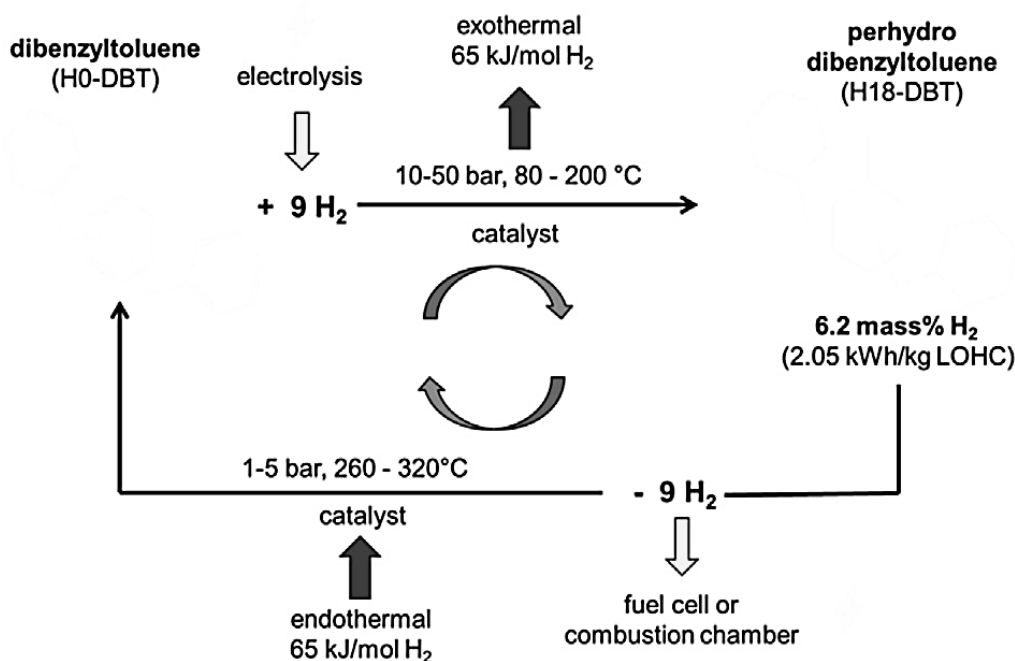
Figure 1. LOHC system based on PDBT-DBT (Adapted from [16]).

In the overall LOHC system, there are various sub-systems. Among them, the dehydrogenation process plays a vital role towards overall system efficiency, as the % conversion is dependent on various parameters, i.e., temperature range, pressure range, a suitable catalyst, etc. Usually, the % conversion of the hydrogenation process is above 98%. Therefore, dehydrogenation of the DBT-PDBT system is considered for this study.

In recent years, research has focused on the PDBT (H18-DBT)—DBT (H0-DBT) system [17]. H0-DBT is a heat transfer oil that is widely used in industry and is available as high purity/quality oil on a large scale [18]. H0-DBT is a wide liquid range, as it exists in the liquid phase, both under process conditions and room temperature. It has low vapor pressure and high thermal stability, allowing it to be used in a reversible phase for a long time. It also meets the Department of Energy's storage requirement, with a storage capacity of 6.2%. It also meets all the previously stated safety criteria, such as non-toxicity and low flammability [9,19–21].

The dehydrogenation of perhydro-dibenzyl-toluene for hydrogen production was first reported by Bruckner et al. in 2014 [22]. Since then, the DBT/PDBT pair has become the center of attention for many researchers [19,21,23,24]. Various researchers have conducted investigations for the identification of the characteristics of the dehydrogenation reaction conditions. They have reported the following operational conditions for the dehydrogenation system: (1) temperature range of 290–320 °C, (2) pressure below 5 bar [25]. For cycloaliphatic hydrogen carrier molecules, platinum (Pt) is a well-known dehydrogenation catalyst. Several authors have investigated the dehydrogenation system using Pt-based catalysts for dehydrogenation and have reported these catalysts as most suitable for the system [26,27].

Shi et al. [28] integrated both dehydrogenation and hydrogenation systems based on DBT and investigated the effect of temperature on the degree of dehydrogenation (DoD) for a time interval of 300 min using a catalyst of 5 wt. % Pt/Al_2O_3. With the increase in temperature from 270 to 320 °C, the value of DoD was increased from 50.8 to 81.3%. Modisha et al. [29,30] studied the impact of various parameters on hydrogen production through catalytic dehydrogenation of PDBT. When using a 1 wt. % Pt/Al_2O_3 catalyst, the DoD was increased from 40 to 90%, by increasing reaction temperature from 290 to 320 °C. With the increase in temperature, the rate of hydrogen production increased while the purity of hydrogen decreased due to the creation of by-products. However, when 2 wt. % Pt/Al_2O_3 was used at 320 °C, a DoD of 96% was obtained. Pd, Pt, and Pt-Pd catalysts had shown DoD values of 11, 82, and 6%, respectively. As a result, both in monometallic and bimetallic systems, Pd was reported to be not suitable for PDBT dehydrogenation.

For the catalytic dehydrogenation of PDBT, the kinetic model was presented by Peter et al. [16]. To determine the kinetic parameters, the catalyst selected was Pt/Al_2O_3, with a temperature range of 260–310 °C, for hydrogen release. To verify the complete sequence of LOHC-bound hydrogen-to-electric power conversion, the hydrogen release from PDBT was coupled with a solid oxide fuel cell device model. The maximum efficiency of LOHC-bound hydrogen-to-electricity was calculated as 45% (at full load). Fikrt et al. [26] evaluated a PDBT-based LOHC for dynamic power supply using a fixed-bed reactor loaded with 0.5 wt. % Pt/Al_2O_3. The dehydrogenation reaction was carried out at 1.2–1.5 bar hydrogen pressure with a temperature range of 563–593 K. As the pressure level of the release unit improved from 0.9 to 2.1 wt. % per cycle, while light byproducts remained below 0.3 wt. %, the hydrogen supply response time from a LOHC system was observed to be the highest. Thermal cracking of the molecule created heavy byproducts, which were measured and increased on a cycle-by-cycle basis. The increase in the number of heavy byproducts resulted in a decrease in catalyst activity.

Jorshick et al. [31] demonstrated the complex realization of the LOHC principle. The dehydrogenation reaction was carried out with platinum on an alumina catalyst in a tube reactor at 300 °C. In addition, the so-called one-reactor model was developed. The authors reported that hydrogenation and dehydrogenation can be done in the same pressure swing reactor with this concept. Ali et al. [32] performed dehydrogenation of PDBT (4.26 wt. %

and 2 wt. %) using 1 wt. % Pt/C at 290 °C, for the analysis of the amount of evolved hydrogen. The research proved the amount of hydrogen evolved was almost twice in the case of 4.26 wt. % of PDBT as compared to 2 wt. %. In comparison to pure DBT equivalents, Jorshick et al. [33] suggested combining H12-BT (perhydro-benzyl-toluene) with H18-DBT (PDBT) to reduce viscosity and increase hydrogen release/productivity. At 10 °C, the viscosity was reduced by 79%, with the addition of 20% H12-BT to H18-DBT. The hydrogen release rate was comparatively increased by 12–16%, when dehydrogenation of H12/H18 mixture was carried out, instead of H18 dehydrogenation, using Pt/Al$_2$O$_3$ catalyst at 260 °C.

For the PDBT dehydrogenation, the effect of Zn and Mg dopants on the catalytic efficiency of Pt/Al$_2$O$_3$ was investigated by Garidzirai et al. [34]. Zn-Al$_2$O$_3$ and Mg-Al$_2$O$_3$ with a target loading of 3.8 wt. % for dopants were generated by modifying Al$_2$O$_3$ supports with Mg and Zn. The catalysts Pt/Al$_2$O$_3$, Pt/Mg-Al$_2$O$_3$, and Pt/Zn-Al$_2$O$_3$ with 0.5 wt. % Pt loading was made by impregnating the modified supports with the chloroplatinic acid solution. For Pt/Al$_2$O$_3$, Pt/Zn-Al$_2$O$_3$, and Pt/Mg-Al$_2$O$_3$, the conversion of H18-DBT ranges from 90–96%, 90–97%, and 92–99%, respectively, with the selectivity ranges from 57–78%, 51–75%, and 45–71%, respectively. As a result, the catalytic efficiency of Pt/Mg-Al$_2$O$_3$ in the dehydrogenation of H18-DBT was significantly improved.

The literature survey shows that experimental studies for dehydrogenation of PDBT are reported extensively. However, these studies are not conducted yet using any simulation approach, i.e., Aspen HYSYS, Aspen Plus, etc. Further, the temperature, and pressure ranges, and various catalysts are reported in the literature using experimental studies, however, the selection of suitable parameters and catalyst is not reported in the literature yet. This novel study aims to address this research gap by examining the dehydrogenation system (for the release of hydrogen) based on various operational parameters, i.e., temperature, pressure, use of various catalysts, and then the examination of the suitable configuration (providing the highest value of the degree of dehydrogenation, corresponding to the suitable temperature, pressure, and catalyst) based on a key performance indicator, i.e., exergy analysis, followed by the development of optimization strategies of the system based on exergy analysis and concepts of the pinch. Aspen HYSYS® V10 has been used to conduct the simulation study, exergy analysis, and optimization. The thermodynamic property package used for the system is Peng-Robinson.

2. Model Development

Following assumptions are fixed for the simulation study:

- Steady-state
- Pressure drop (ΔP) in the heat exchangers = 10 kPa or 0.1 bar
- No pressure drop in the reactor

The process flowsheet of the overall dehydrogenation system is presented in Figure 2. The components (PDBT and DBT) are not present initially in the library of Aspen HYSYS. So, these are added as a hypothetical component by drawing their molecular structure, and then Peng-Robinson as thermodynamic property package is selected. The feed, perhydro-dibenzyl-toluene (PDBT), is pumped using the centrifugal pump to the dehydrogenation reactor. The feed is pre-heated using two heat exchangers (HEX-1 and HEX-2), with heating media being the saturated steam coming from the steam generation section. The feed is then introduced into the reactor, where the dehydrogenation reaction takes place. For the simulation study, the conversion reactor model is assumed, and the values provided in the literature are taken as the reference point. The products of the reactor are first cooled down in the 3rd heat exchanger (HEX-3), with cooling media as cooling water. The stream is then passed through the flash separator, with the top product obtained as hydrogen while the bottom product as dibenzyl-toluene (DBT).
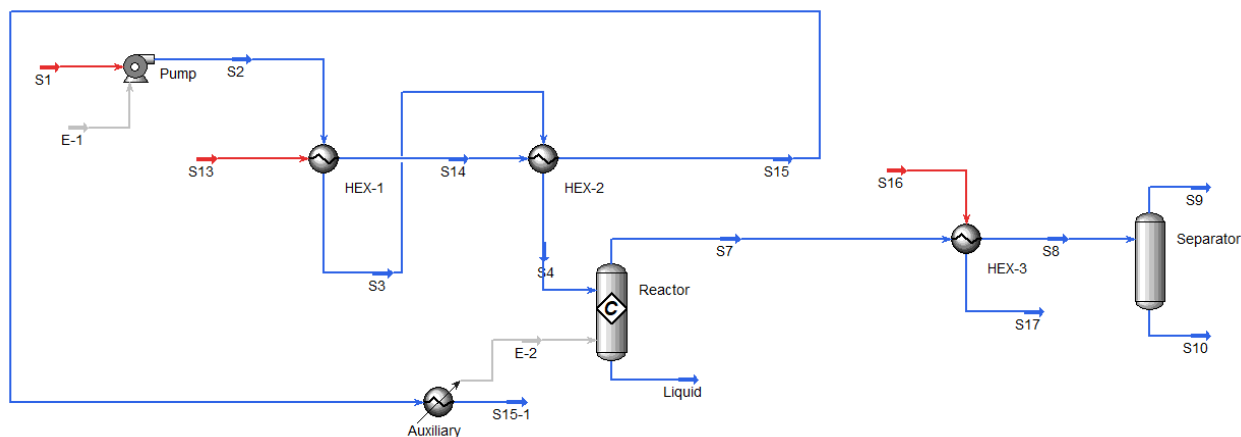
Figure 2. Process flowsheet developed and simulated in Aspen HYSYS.

Various types of catalysts for the PDBT dehydrogenation have been reported in the literature, i.e., Pd/Al_2O_3, $Pt-Pd/Al_2O_3$, and Pt/Al_2O_3. However, since palladium (Pd), and platinum-palladium (Pt-Pd) based catalyst have exhibited a maximum of 6 and 11% DoD, respectively, therefore, these catalysts were not chosen for the study. Pt/Al_2O_3 catalysts have shown comparatively better results, i.e., 40–96% for various weight fractions of platinum on alumina, therefore, this catalyst has been chosen for this study. Since variations in weight fractions of platinum on alumina exhibit a significant impact on the value of DoD, therefore, following weight fraction of Pt/Al_2O_3 catalysts were chosen for the study, and optimized based on DoD:

- 0.5 wt.% Pt/Al_2O_3 catalyst
- 1 wt.% Pt/Al_2O_3 catalyst
- 2 wt.% Pt/Al_2O_3 catalyst
- 5 wt.% Pt/Al_2O_3 catalyst [28–30].

Followed by the selection of catalyst and further optimization of the catalyst based on wt.% of platinum, the exergy analysis of the system was conducted. To analyze the performance of chemical processes, the exergy methods have been widely used in recent years [35]. The exergy methods help in evaluating various parameters i.e., the process irreversibility, utilization of energy resources, and optimal process design [36]. Exergy analysis is useful to determine the effects of key operational parameters on process efficiency [37–39]. For the exergy analysis, two key terms i.e., % exergy efficiency, and exergy destruction rate (kW) were used. % exergy efficiency is defined as the cumulative exergy value of the outlet streams divided by the cumulative exergy value of the inlet streams. The difference between the cumulative exergy value of inlet and outlet streams is called exergy destruction. The exergy of a stream is calculated by summing physical and chemical exergy values, which are calculated as presented in Equations (1) and (2) [40]:

$$\text{Physical Exergy} = E_{phy} = (h - h_o) - T_o\,(s - s_o) \tag{1}$$

$$\text{Chemical Exergy} = E_{chem} = \sum_i x_i \varepsilon_{ch,i} + RT_o \sum_i x_i \ln x_i \tag{2}$$

The formula used for each equipment in the system is presented in Table 4 [39,40].

Optimization of a chemical process has always remained a hot topic to find the most suitable parameters to obtain the highest possible efficiency of the system. During the optimization of the PDBT dehydrogenation system, the concept of process integration, and hierarchy of energy reduction, as proposed by Kemp and Lim [41,42], were considered.

Table 4. Formulae used for exergy analysis in the study [39,40].

Equipment	Exergy Efficiency ε_k (%)	Exergy Destruction $E_{d,k}$ (kW)
Pump	$\frac{\sum Ex_o - \sum Ex_i}{W}$	$W - \sum Ex_o + \sum Ex_i$
Heat Exchangers	$\frac{\sum Ex_o}{\sum Ex_i}$	$\sum Ex_i - \sum Ex_o$
Dehydrogenation Reactor	$\frac{\sum Ex_o - \sum Ex_i}{\sum Ex_q}$	$\sum Ex_i - \sum Ex_o + \sum Ex_q$
Turbine	$\frac{W}{\sum Ex_i - \sum Ex_o}$	$\sum Ex_i - \sum Ex_o - W$
Separator	$\frac{\sum Ex_o}{\sum Ex_i}$	$\sum Ex_i - \sum Ex_o$

The hierarchy of energy reduction specific to this study is: (1) avoid or reduce the energy requirement, (2) recover the heat from the process. The overall process is using external utilities, i.e., cooling water and steam. On analyzing the system based on exergy analysis, it was revealed that there is a potential to minimize the utilities consumption in the process and that can be done by enhancing the process-to-process heat recoveries. Further, it was observed (based on exergy analysis) that the hydrogen stream (S9) has the potential to produce power, thereby meeting the energy requirement of the pump, and helpful in reducing the steam consumption for feed preheating. Accordingly, the two strategies are proposed for the system:

- *Strategy #1*: It is observed during the simulation, that stream S9 (consists of hydrogen) has a considerably high temperature, which can be extracted, i.e., power can be produced, and the hydrogen stream can exchange heat with the reactor feed (in HEX-1) to reduce the steam consumption in the system. The scheme is presented in Figure 3.
- *Strategy #2*: In addition to the scheme developed in strategy # 1, the product of the reactor is at the highest temperature in the system, so its heat can also be used to pre-heat the reactor feed (in HEX-1). The scheme is presented in Figure 4.
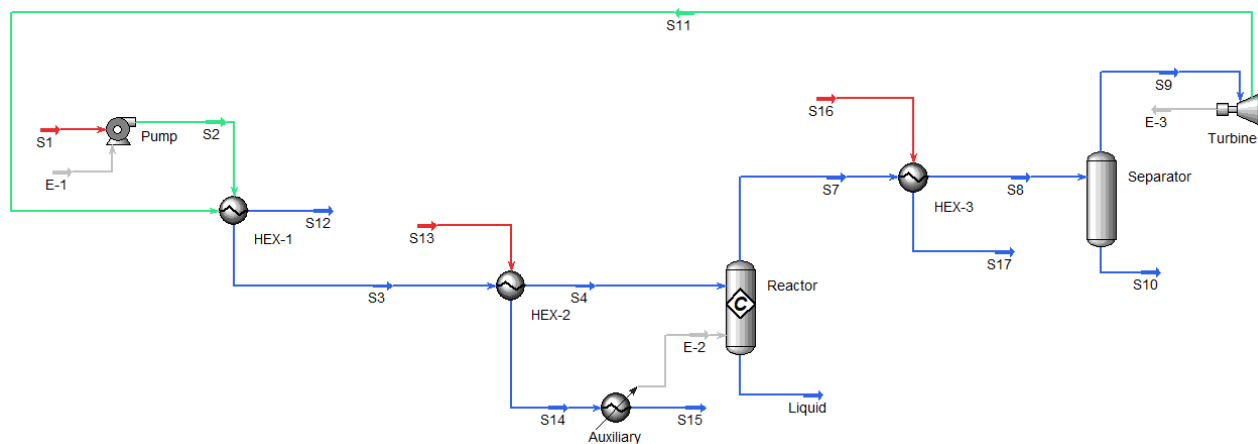
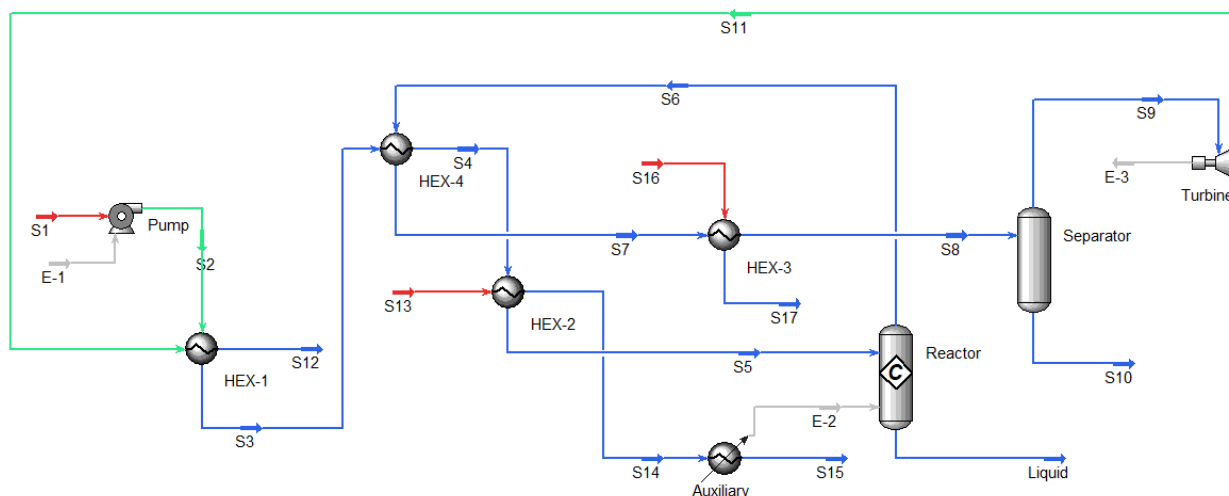**Figure 3.** Optimization strategy #1 of the dehydrogenation system.

Figure 4. Optimization strategy #2 of the dehydrogenation system.

3. Results

The first part of this study is focused on the optimization of the weight fraction of platinum on an alumina catalyst for the dehydrogenation system under suitable conditions. The analysis shows that for 0.5 wt.% Pt/Al_2O_3 catalyst, a maximum of 40% degree of dehydrogenation is obtained at a temperature of 270 °C, while for 5 wt.% Pt/Al_2O_3 catalyst, 51.3% degree of dehydrogenation is obtained, which makes 0.5 wt.% Pt/Al_2O_3 catalyst unfavorable for the system. At the highest temperature of 320 °C, the degree of dehydrogenation obtained for 5 wt. %, 1 wt. %, and 2 wt.% Pt/Al_2O_3 catalysts are 81.3, 90, and 96%, respectively, which shows that 2 wt.% Pt/Al_2O_3 catalyst is the most suitable catalyst for the dehydrogenation of perhydro-dibenzyl-toluene. The analysis shows an increase in metal loading (platinum) from 0.5 to 2 wt.% has led to an increase in the value of DoD, however, the further increase has led to a decrease in the degree of dehydrogenation, as shown for 5 wt.% catalyst. This is in agreement with the study by Palma et al. [43], i.e., for the metal loading of 2 wt. %, there is a fine dispersion on the base surface with the least agglomeration, while the increase in metal loading from 2 to 5 wt.% has led to a comparative increase in the agglomeration, reduced dispersion, reduced metallic surface area, and reduced number of reducible species, thereby leading to reduced catalytic activity. For the study presented so far, the pressure is taken as 1 bar. Since the dehydrogenation process is endothermic, so the value of DoD is found to be decreasing with the increase in pressure up to 3 bar. However, for the real-time operation of the system, 1 bar pressure is not sufficient. Since pressure drops are considered in the heat exchangers (in accordance with the real-time operation), therefore, for the real-time operation of the system, the followings conditions are selected:

- Catalyst: 2 wt.% Pt/Al_2O_3 catalyst
- Temperature: 320 °C
- Pressure: 2 bar

The second part of the study is focused on the exergy analysis of the overall system. The exergy analysis of the system is presented in Figure 5. The analysis shows that the reactor and heat exchangers #1 and 3 are responsible for major exergy destruction in the process. Further improvement in the reactor conditions or further decrease in exergy destruction rate is not possible since reaction conditions cannot be changed. However, for heat exchangers #1 and 3, the improvement is still possible, which has been considered during the optimization study, using the concepts of process integration.
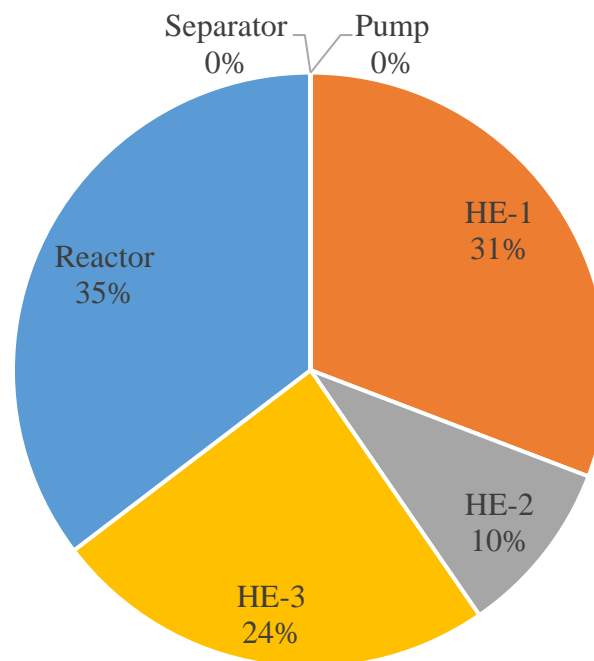
Figure 5. Contribution of different equipment in total exergy destruction rate—base case (%).

The third part of this study is focused on optimization of the system, based on results obtained from exergy analysis. Two strategies are developed for improving the overall efficiency of the system (presented in the methodology). The overall results of the strategies are presented as follows:

- *Strategy #1*: hot utility consumption is reduced by 47.06%, while cold utility consumption is reduced by 30%, with an overall reduction in utility consumption rate by 37.84%. The electricity is produced in the system, i.e., the turbine is producing a power of 485 kW, an important aspect missing in the base case, and therefore an improvement in the overall system. The % exergy destruction rate of strategy #1 is presented in Figure 6. The % exergy destruction in heat exchanger #1 is reduced from 31 (base-case) to 27%, while in heat exchanger #3, it is reduced from 24 (base-case) to 19%. The overall exergy destruction rate is reduced by 9.01% in comparison to the base case.

- *Strategy #2*: hot utility consumption is reduced by 70.59%, while cold utility consumption is reduced by 30%, with an overall reduction in utility consumption by 48.65%, at an expense of installation of one extra heat exchanger. In this case, the turbine is comparatively producing lesser power, i.e., 359 kW in the system, because the product of the reactor (S7) is exchanging heat with feed stream (S3); therefore, comparatively lesser heat is available for electricity generation. However, in this strategy, the % exergy destruction rate is reduced by 14.28% in comparison to the base case. The % exergy destruction rate in heat exchanger #1 is reduced from 31 (base-case) to 14%, in heat exchanger #2, it is reduced from 10 (base-case) to 3%, and in exchanger #3, it is reduced from 24 (base-case) to 18%, as presented in Figure 7.
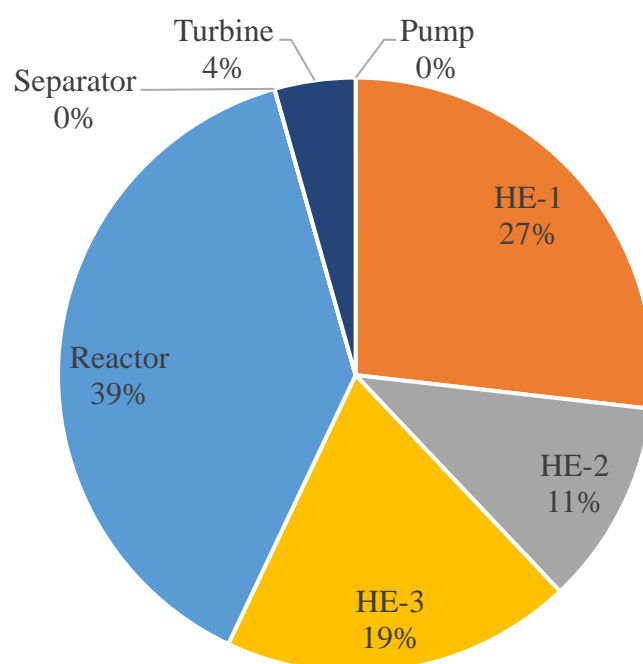
Figure 6. Contribution of different equipment in total exergy destruction rate—strategy #1 (%).
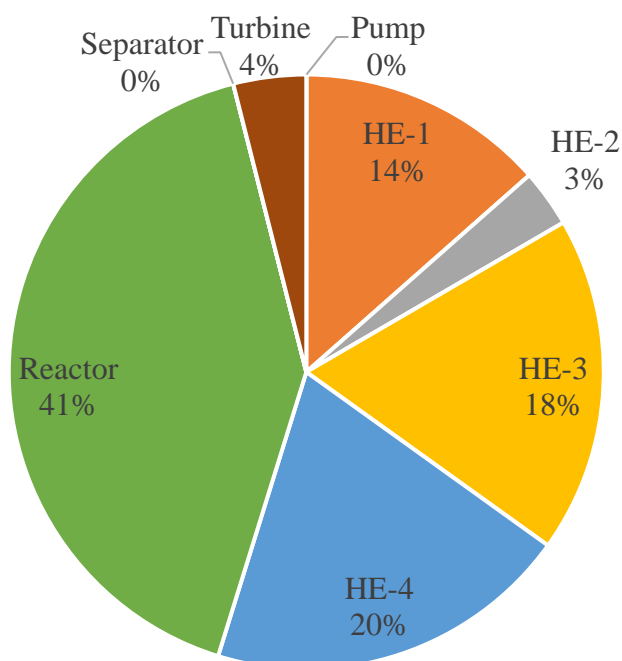

Figure 7. Contribution of different equipment in total exergy destruction rate—strategy #2 (%).

The performance analysis of the strategies developed for the dehydrogenation system is summarized in Table 5.

Table 5. Performance analysis of strategies developed for the dehydrogenation system.

Equipment	Base-Case	Strategy #1	Strategy #2
Exergy Efficiency (%)			
Pump	72.21	72.21	72.21
Heat Exchanger-1	99.84	99.92	99.94
Heat Exchanger-2	99.95	99.94	99.98
Heat Exchanger-3	99.86	99.90	99.91
Heat Exchanger-4	-	-	99.95
Reactor	61.73	61.73	61.73
Separator	100.00	100.00	100.00
Turbine	-	84.64	99.93
Overall (%)	84.61	91.06	94.86
Exergy Destruction (kW)			
Overall (kW)	2183.83	2002.48	1872.07

The analyses reveal that strategy #2 is the most suitable option for the dehydrogenation system, because for various reasons:

- Although an extra heat exchanger is required which contributes to the higher fixed cost of the system in strategy #2, however, the benefit associated with this strategy is the reduction in the utility consumption rate by 48.65%, thereby, reducing the operational cost of the system. In comparison, the utility consumption rate is reduced by 37.84% in strategy #1, which can lead to the higher operational cost of the system. Therefore, considering the trade-off between operational and capital cost, strategy #2 appears to be the most suitable for the dehydrogenation system.
- In comparison to the base case, the exergy destruction rate is reduced by 14.28% in strategy #2, while in strategy #1 is reduced by 9.01%. The overall exergy efficiency of the base case is 84.61%. In comparison, the overall exergy efficiency in the case of strategy #1 and strategy #2 is 91.06 and 94.86%, respectively, thus favoring strategy #2 for the system.

4. Conclusions

The performance of the PDBT dehydrogenation system was analyzed based on various parameters, i.e., selection of optimum operational conditions, exergy analysis of the process, and development of optimization strategies for the system to identify the most suitable configuration. The analysis showed that the most suitable catalyst for the system was 2 wt.% Pt/Al_2O_3 with optimum temperature and pressure condition as 320 °C, and 2 bar, respectively. The exergy analysis of the base-case showed that reactor and heat exchanger-2 had caused a comparatively higher exergy destruction rate. The exergy analysis and process integration helped in the optimization of the system, i.e., two design strategies were developed for the system. The optimization increased the overall exergy efficiency of the overall system up to 7.08 and 10.81% with the exergy destruction rate reduced by 9.01 and 14.28% for strategy #1 and strategy #2, respectively. Therefore, strategy 2 is the most suitable option for the dehydrogenation system.

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Nomenclature

$E_{d:k}$	Exergy destruction (kW)
Ex_q	Exergy supplied through heat flow (kW) = $Q(1 - T_o/T)$ [44]
Ex_{in}	Exergy of inlet stream (kW)
Ex_{out}	Exergy of outlet stream (kW)
E_{phy}	Physical exergy (kW)
E_{chem}	Chemical exergy (kW)
P_o	Reference pressure (bar)
R	Ideal gas constant
T_o	Reference temperature (°C)
W	Work required by pump/Work generated by the turbine (kW)
x_i	Mole fraction of component, i
ΔP	Pressure drop (bar)
Greek Letters	
ε_k	Exergy efficiency (%)
$\varepsilon_{che,\,i}$	Standard chemical exergy of component, i (kJ/mol)
Abbreviations	
DoD	Degree of dehydrogenation
DBT	Dibenzyl toluene
HHV	Higher heating value
HEX	Heat exchanger
PDBT	Perhydro-dibenzyl-toluene

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