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Simulation and Evaluation of Hydro-processing for Jet Fuel Quality Improvement Using Aspen HYSYS: A Case Study

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Abstract

This study focuses on improving jet fuel quality by removing sulfur compounds, represented by the Thiophene compound, and enhancing its physical and chemical properties using thermal treatment, based on simulation. The Plug Flow Reactor (PFR) was operated at 400 °C and 2500 kPa to treat the feedstock, targeting the removal of Thiophene as the primary sulfur compound. The sulfur content decreased from 7.0 x_i in the initial mixture (Feed-Stream) to approximately 0.0085 x_i in the product stream (Treated-Feed) after treatment by HDS-Reactor, this achieves a removal efficiency of approximately 98.79%. After the reactor, the three-phase separation unit was operated at a temperature of 145.3 °C and a pressure of 897.7 kPa, where it successfully transferred most of the H_2S (0.0716 x_i) produced by the desulfurization process to the gas phase, reducing its concentration in the liquid hydrocarbon phase (Final-Product) to about 0.0080 x_i , which greatly reduced the solubility of acid gases in the final product. On the other hand, a mixing unit was also applied to add performance-enhancing materials, namely C_2=GC_4EthrAc and 1-Dodecanol. These additions contributed to improving density, viscosity, and freezing point without affecting the basic hydrocarbon structure. The final analysis results showed that most of the properties met the requirements of ASTM D1655 specifications for jet fuel, with a density of 740.5 kg/m³, a viscosity reduced to 0.56 cP, and the fuel's low heat value (LHV) was approximately 43,640 kJ/kg, while its high heat value (HHV) was approximately 46,464 kJ/kg. Therefore, these results show an effective methodology for producing high-quality jet fuel the process to meet international specifications.

Keywords: Thiophene, Feed-Stream, Aspen HYSYS, Component Lists, Plug Flow Reactor.

1. Introduction

In the oil refining sector, basic procedures cover separation, conversion, enhancement, and purifying. In order to achieve high-quality products that satisfy transportation, environmental, and human requirements, these procedures are required. A certain kind of separation is catalytic cracking, which involves reducing the molecular weight of hydrocarbons. The modification of this process into hydrocracking, which results in a variety of advantages over the conventional approach that has been used traditionally, is accomplished by injecting hydrogen gas throughout the catalytic cracking process. Fast expansion, enhanced catalytic activity, lower operating temperatures, and more selectivity are all benefits of hydrogen. The use of hydrogen makes the effects of coke deposition and catalyst deactivation almost nonexistent [1]. Hydrodesulphurization (HDS) is a chemical process that uses a catalyst to obtain eliminated of impurities, mostly sulfur-containing compounds, from hydrocarbon-based substances including gasoline, jet fuel, kerosene, diesel fuel, and fuel oils. Sulfur, nitrogen, as well as oxygen are essentially found in petroleum products, while its unsaturated elements are formed via refineries [2]. The primary objective for getting eliminated of impurities, especially sulfur, is to lower the amount of sulfur dioxide (SO_2) that comes out when we utilize those fuels in automobiles, aircraft, trains, ships, gas or oil burning power plants, home and commercial furnaces, and other types of fuel combustion. An HDS unit is sometimes called a hydrotreater [3][4]. On the other hand, Airlines for commercial use continue to be employing increasing quantities of aviation fuels created from fossil fuels every year. Aviation is responsible for around 2.8% of the total emissions of greenhouse gases around the world. To decarbonize the aviation industry and cut net greenhouse gas emissions, it will be important to make environmentally friendly aviation fuels [5][6]. Furthermore, in the last few years, technological developments and international politics have moved closer to allowing the utilization of Sustainable Aviation Fuel (SAF). The European Union's "Fit for 55" package requires that the amount of SAF blended into gasoline rise about 2% in 2025 to 70% by 2050. The United States, on the other hand, wants to make 3 billion gallons of SAF every year by 2030 as part of the SAF Grand Challenge Roadmap. The ICAO CORSIA framework and the

IATA net-zero roadmap make the global commitment to SAF growth even stronger. Recent technological breakthroughs include high-selectivity isomerization approaches for HEFA fuels, hybrid catalytic systems, and new techniques to turn trash into fuel, like catalytic hydro-thermolysis and SAF made from plastic. Over 450,000 commercial flights throughout the world have utilized SAF mixes as of 2024. This shows that the technology has advanced from testing to scalability [7]. The main ingredients of jet fuel, which is a catch-all term to describe the aviation fuels utilized by gas-turbine fueled aircraft, are cycloalkanes and linear and branched alkanes having carbon chain lengths ranging from C8 to C18, with C_8 to C_{16} being the optimal carbon chain length [8][9]. In addition, a lot of investigations were carried out in the past several years about developing jet fuel or other fractions via hydrocracking and isomerization reactions with hydrocarbons from n-C_{15} to n-C_{18} as a model for hydrotreated fat or FT wax [10]. There are different accredited techniques for producing jet fuel. Gas-to-jet (GTJ) procedures include Fischer-Tropsch synthesis (FTS), oil-to-jet (OTJ) methods involve hydrotreated renewable jet (HRJ), alcohol-to-jet (ATJ) processes consist of ethanol-to-jet or butanol-to-jet, and sugar-to-jet (STG) techniques involve catalytic enhancement of sugar to jet [11][12]. Simulating processes using Aspen HYSYS software offers tangible scientific and practical benefits. It is an advanced tool for simulating chemical and petroleum processes, contributing to the analysis and design of jet fuel catalytic processing units and determining optimal operating conditions for quality improvement. It also provides accurate material and energy balancing and estimates the properties of the resulting fuel in accordance with international standards. Moreover, its use is characterized by being much faster than laboratory experiments, less risky and less costly, making it an effective means of reducing development time and supporting technical and economic decision-making in the design and improvement phases [13]. Therefore, this study aims to analyze the effect of sulfur compounds, particularly thiophene, on jet fuel quality, in addition to simulating its removal using catalytic reactors in the Aspen HYSYS environment. It also aims to evaluate the impact of these treatment processes on the fuel's physical and chemical properties, ensuring its compliance with international standards such as ASTM D1655.

2. Methodology

This section will cover the steps for building a simulation model in Aspen HYSYS V10 to fulfill the project requirements (analysis and simulation of desulfurization and jet fuel quality improvement using catalytic reactors in an Aspen HYSYS environment), starting with inputting the components (Component Lists) that will be involved in the chemical reactions, whether as reactants, products, or catalysts, and the mole fraction of each. In addition to designing the optimization and processing system, which consists of feed-stream currents, mixer, separator, HDS-reactor, cooler, heater, and the final-product current.

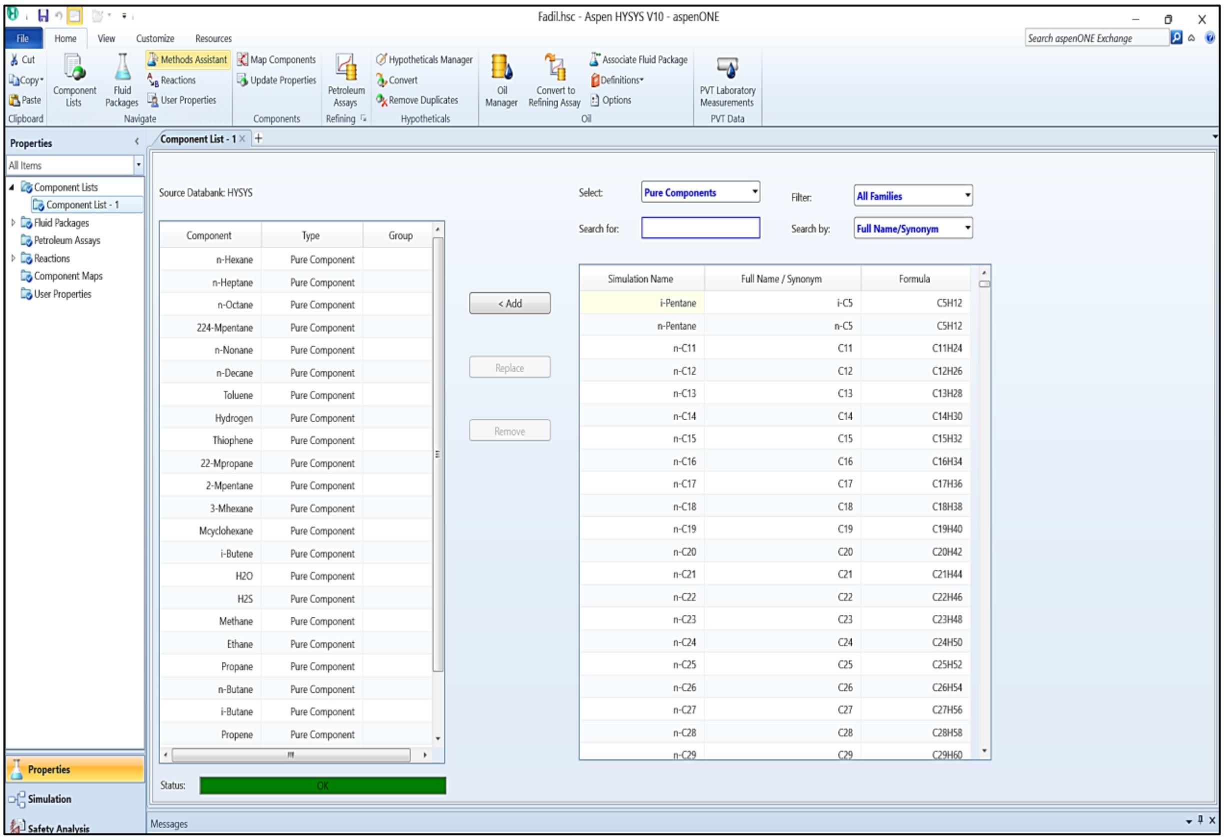
2.1. Component Lists:

The step of selecting the chemical components involved in the simulation (whether they are reactants, products, catalysts, or even by-products) is one of the essential factors that affect the quality of the model and its accuracy in representing reality. In this study, the feedstock components were selected based on the characteristics of the raw jet fuel (As shown in Figure 1 and Table 1), which consisted of a mixture of hydrocarbon and sulfur compounds that negatively affect fuel quality and cause harmful emissions when burned. This mixture represents a realistic blend of naphtha and kerosene, containing both light and heavy components, as well as sulfur compounds that must be removed and additives used for treatment. The presence of hydrogen is essential for the hydrogenation reaction to take place within the reactor. These components were used as a starting point for constructing the feed flows and subsequently forming the reaction model in the simulation.

Table (1): Simulation Name and chemical formulas, and status of all components included in the simulation model

NO.	Simulation Name	Chemical Formula	Status
1	n-Hexane	C_6H_{14}	Feed – Naphtha
2	n-Heptane	C_7H_{16}	Feed – Kerosene
3	n-Octane	C_8H_{18}	Feed – Kerosene
4	224-Mpentane or i-Octane	C_8H_{18} (i)	Feed – Kerosene
5	n-Nonane	C_9H_{20}	Feed – Kerosene
6	n-Decane	$C_{10}H_{22}$	Feed – Kerosene
7	Toluene	C_7H_8	Feed – Aromatics

NO.	Simulation Name	Chemical Formula	Status
8	Hydrogen	H_2	Reactant
9	Thiophene	C_4H_4S	Reactant
10	22-Mpropane or Iso-Paraffins	C_5H_{12} (i)	Product - Isomerization
11	2-Mpentane or Iso-Paraffins	C_6H_{14} (i)	Product - Isomerization
12	3-Mhexane or Iso-Paraffins	C_7H_{16} (i)	Product - Isomerization
13	Mcyclohexane	C_7H_{14}	Product - Cyclization
14	i-Butene	C_4H_8	Product – Cracking
15	Water	H_2O	Byproduct - Reaction
16	Hydrogen Sulfide	H_2S	Byproduct - Reaction
17	Methane	CH_4	Byproduct - Light gas
18	Ethane	C_2H_6	Byproduct - Light gas
19	Propane	C_3H_8	Byproduct - Light gas
20	n-Butane	C_4H_{10}	Byproduct - Light gas
21	i-Butane	C_4H_{10}	Byproduct - Light gas
22	Propene	C_3H_6	Product – Cracking
23	1-Butene	C_4H_8	Product – Cracking
24	C_2=GC$_4$EthrAc or FSII Additive	$C_8H_{16}O_3$	Additive - Anti-icing
25	1-Dodecanol or Lubricity Improver	$C_{12}H_{26}O$	Additive - Lubricity improver



Source Databank: HYSYS

Component	Type	Group
n-Hexane	Pure Component	
n-Heptane	Pure Component	
n-Octane	Pure Component	
224-Mpentane	Pure Component	
n-Nonane	Pure Component	
n-Decane	Pure Component	
Toluene	Pure Component	
Hydrogen	Pure Component	
Thiophene	Pure Component	
22-Mpropane	Pure Component	
2-Mpentane	Pure Component	
3-Mhexane	Pure Component	
Mcyclohexane	Pure Component	
i-Butene	Pure Component	
H2O	Pure Component	
H2S	Pure Component	
Methane	Pure Component	
Ethane	Pure Component	
Propane	Pure Component	
n-Butane	Pure Component	
i-Butane	Pure Component	
Propene	Pure Component	

Status: OK

Select: Pure Components
Filter: All Families
Search for:
Search by: Full Name/Synonym

Simulation Name	Full Name / Synonym	Formula
i-Pentane	i-C5	C5H12
n-Pentane	n-C5	C5H12
n-C11	C11	C11H24
n-C12	C12	C12H26
n-C13	C13	C13H28
n-C14	C14	C14H30
n-C15	C15	C15H32
n-C16	C16	C16H34
n-C17	C17	C17H36
n-C18	C18	C18H38
n-C19	C19	C19H40
n-C20	C20	C20H42
n-C21	C21	C21H44
n-C22	C22	C22H46
n-C23	C23	C23H48
n-C24	C24	C24H50
n-C25	C25	C25H52
n-C26	C26	C26H54
n-C27	C27	C27H56
n-C28	C28	C28H58
n-C29	C29	C29H60

Figure (1): The chemical compounds utilized in the construction of the simulation model

2.2. Fluid Package:

The Peng –Robinson –Stryjek -Vera (PRSV) thermal model was chosen for its accuracy in representing the physical and thermodynamic properties of hydrocarbon and sulfur compounds, especially under high operating conditions of pressure and temperature. It is suitable for kinetic reactions, where the reaction rates (Plug Flow Reactor (PFR)) occurring within the kinetic reactions reactor and the efficiency of the chemical transformation depend on the accuracy of calculating the equilibrium parameters and phase properties. It has been used to ensure accurate calculations of the equilibrium between the gas and liquid phases, and to ensure the reliability of results related to desulfurization and fuel property enhancement.

2.3. Mole Fraction:

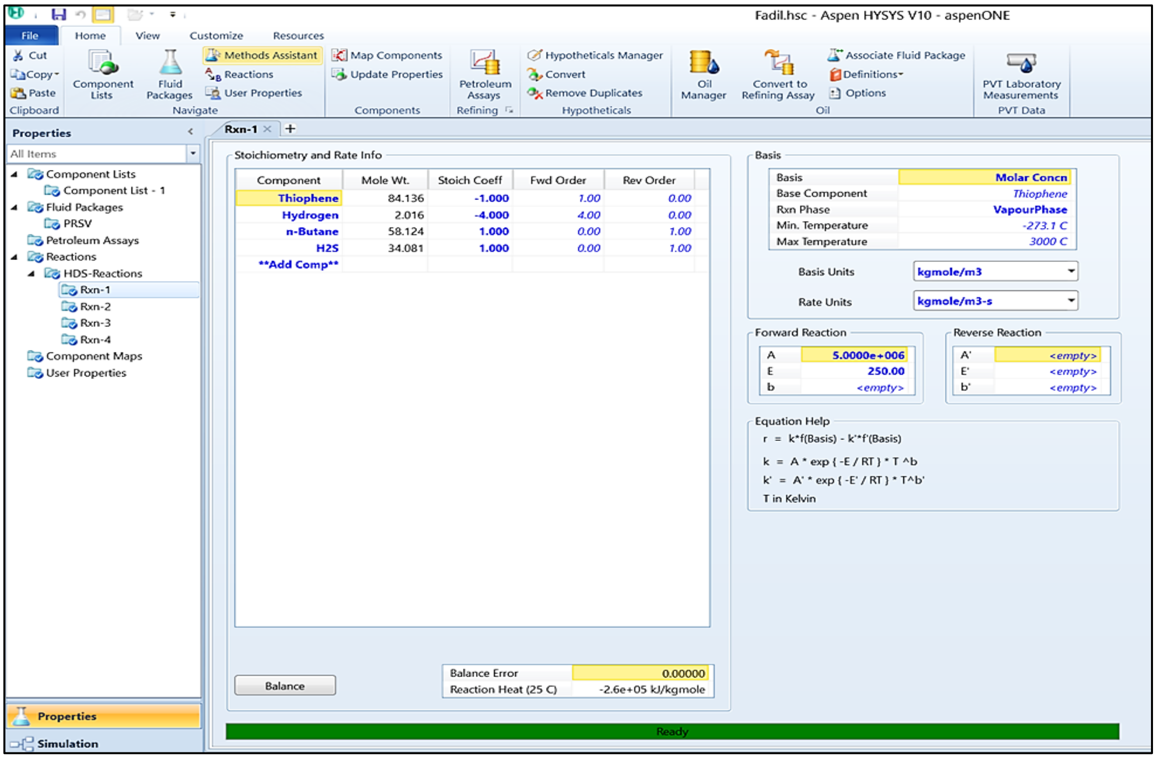
The feedstock composition was determined based on the mole fraction of the main components in the kerosene, naphtha, and sulfur compounds mixture. The proportions were adjusted to reflect the true composition of the crude oil before processing. As shown in Appendix A, the sum of the mole fractions was verified to be 1, ensuring the accuracy of the simulation in the Aspen HYSYS software.

2.4. Type of Reaction and Chemical Reactions:

In this study, the removal of sulfur process relies on catalytic hydrogenation reactions (Plug Flow Reactor), which are carried out inside a tubular Hydrodesulfurization (HDS) reactor (PFR) using a kinetic reaction model. This type of reaction was chosen because of its accuracy in representing the chemical transformations that occur on the surface of the catalyst at high temperatures and pressures. The primary reaction aims to remove thiophene (C_4H_4S) by reacting it with hydrogen gas (H_2) to produce hydrogen sulfide gas (H_2S) and saturated or unsaturated hydrocarbons. These reactions were defined using the Arrhenius Equation, where frequency coefficients (A) and activation energies (E) were introduced for each reaction individually, ensuring an accurate representation of the reaction behavior within the reactor. Table 2 and Figure 2 illustrate all the chemical reactions (4 reactions), activation energy values, and frequency coefficients, in addition to the explanation in Appendix A. These reactions form the basis of the HDS process, which is responsible for effectively removing sulfur from the hydrocarbon mix, thus improving the quality of jet fuel and reducing harmful sulfur emissions.

Table (2): The chemical reactions, activation energy, and frequency factor

NO.	Chemical reactions	Activation energy	Frequency factor
1	$C_4H_4S + 4H_2 \rightarrow$ n-Butane + H_2S	5.00E+06	250
2	$C_4H_4S + 3H_2 \rightarrow$ i-Butene + H_2S	3.00E+06	300
3	$C_4H_4S + 3H_2 \rightarrow$ 1-Butene + H_2S	1.00E+06	280
4	$C_4H_4S + 3H_2 \rightarrow$ Propene + H_2S+CH_4	6.00E+06	650



Stoichiometry and Rate Info

Component	Mole Wt.	Stoich Coeff	Fwd Order	Rev Order
Thiophene	84.136	-1.000	1.00	0.00
Hydrogen	2.016	-4.000	4.00	0.00
n-Butane	58.124	1.000	0.00	1.00
H2S	34.081	1.000	0.00	1.00
Add Comp				

Balance Error	0.00000
Reaction Heat (25 C)	-2.6e+05 kJ/kgmole

Basis

Basis	Molar Concn
Base Component	Thiophene
Rxn Phase	VapourPhase
Min. Temperature	-273.1 C
Max Temperature	3000 C

Basis Units: kgmole/m3

Rate Units: kgmole/m3-s

Forward Reaction

A	5.0000e+006
E	250.00
b	<empty>

Reverse Reaction

A'	<empty>
E'	<empty>
b'	<empty>

Equation Help
r = k*f(Basis) - k'*f'(Basis)
k = A * exp { -E / RT } * T ^b
k' = A' * exp { -E' / RT } * T^b'
T in Kelvin

Figure (2): Chemical reactions, activation energy, and frequency coefficient in a simulated environment

2.5. Design of the Treatment System:

In this study, an integrated system was designed (as shown in Figure 3) to improve the properties of jet fuel by removing sulfur compounds and enhancing performance characteristics through the addition of additives. The system begins by feeding a hydrocarbon mixture (Feed-Stream) at a flow rate of 25,000 kg/hr, at a temperature of 25°C and a pressure of 2500 kPa. This stream contains carefully selected hydrocarbon and sulfur components to simulate low-quality fuel. Then, the feed current is heated by a heater to an operating temperature of 400°C, while maintaining an operating pressure about 2500 kPa, in preparation for its introduction into a reactor (HDS-Reactor) with a volume of 3 m³. After the reaction inside the reactor, the production stream is cooled via a cooler to a temperature of 145°C, then passed to a three-phase separator which separates the stream into three phases: the aqueous phase, the gas phase (Which in turn goes to another processing unit to concentrate the hydrocarbons along with the impurities), and the liquid (hydrocarbon) phase (Liquid-Hydrocarbons), which in turn is transferred to a mixer and final processing unit. In the final processing unit, two feed streams are combined with the separator output (Liquid-Hydrocarbons), with these streams containing fuel performance-enhancing additives. All operating conditions (flow rate, reactor volume, density, temperature, and pressure) for all units are shown in Appendix A, which provides a visual representation of all processes within the system.

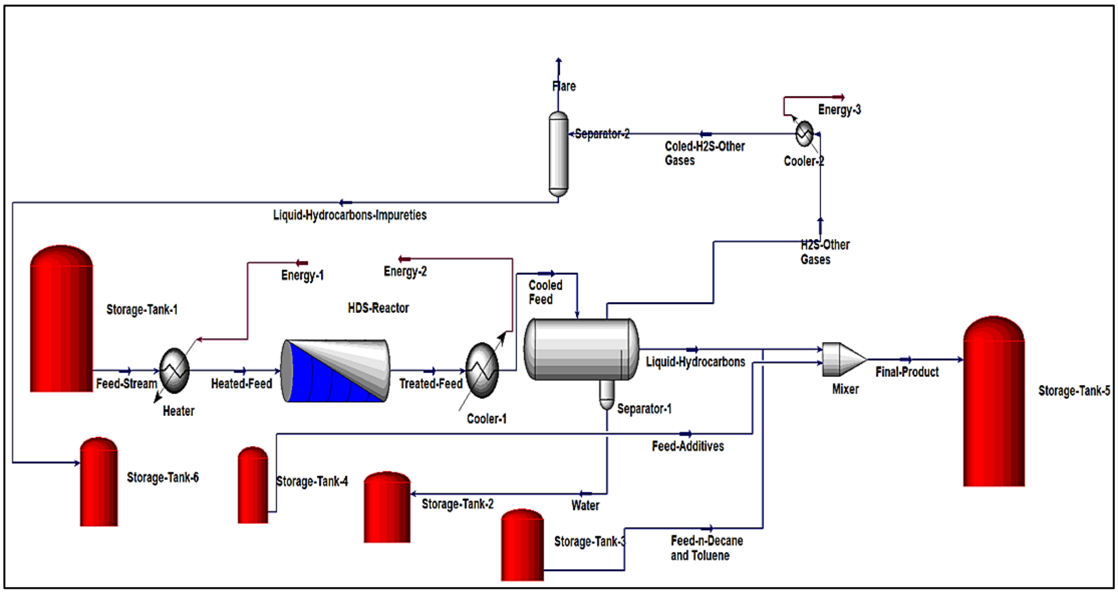


Figure (3): A jet fuel properties treatment system

3. Results and Dissuasions

This section aims to present and analyze the results obtained from a study on desulfurization and fuel quality improvement using catalytic reactions, which was carried out within a simulation environment. The presentation of results in this section is organized in a way that includes quantitative tables and illustrative graphs showing the changes in the chemical composition and physical properties of the fuel, before and after catalytic treatment and final additives.

3.1. HDS-Reactor:

The results, as shown in Table 3 and Appendix B, indicate that the HDS desulfurization process was highly effective in reducing the concentration of Thiophene (C_4H_4S) from 0.070 mole fraction in the initial mixture (Feed-Stream) to approximately 0.0085 mole fraction in the product stream (Treated-Feed) after treatment, this achieves a removal efficiency of approximately 98.79%, which was calculated by the equation shown below. This significant decrease indicates the success of the catalytic reaction that carried out in the HDS-Reactor in breaking down the complex sulfur compound (Thiophene) and converting them into hydrogen sulfide (H_2S), which is reflected in the increased concentration of H_2S in the Treated-Feed (approximately to 0.0716 mole fraction). In contrast, a relative increase was observed in most of the major hydrocarbon components such as n-Hexane, n-Heptane and Toluene, due to a reduction in the concentration of sulfur compounds that occupied part of the molecular space, in addition to the possibility of some secondary reactions that may lead to a redistribution of the components. The decrease in hydrogen from 0.19 to 0.0016 mole fraction after treatment is evidence of hydrogen consumption during the catalytic reaction, where it plays a key role in desulfurization (hydrogenation). These results indicate that the operating conditions at 400°C and 2500 kPa (Appendix B) were suitable for achieving a high thiophene removal rate while preserving the composition of the basic hydrocarbon components. The estimated desulfurization efficiency also reflects the system's ability to produce high-purity jet fuel, minimizing sulfur contamination and meeting international standards. On the other hand, the reason for the increase in temperature inside the reactor from 400°C to approximately 440°C as well as decrease the pressure to 2398 kPa is due to the exothermic reactions generated during the desulfurization process. These reactions naturally raise the temperature of the reaction mixture as it passes through the reactor [14].

Table (3): The results of components after HDS-Reactor

NO.	Components	Feed-Stream, x_i	Treated-Feed, x_i
1	n-Hexane	0.1100	0.1258
2	n-Heptane	0.1000	0.1144
3	n-Octane	0.0800	0.0915
4	224-Mpentane or i-Octane	0.0700	0.0801
5	n-Nonane	0.1100	0.1258
6	n-Decane	0.1000	0.1144
7	Toluene	0.1700	0.1945
8	Hydrogen	0.1900	0.0017
9	Thiophene	0.0700	0.0085
10	22-Mpropane or Iso-Paraffins	0.0000	0.0000
11	2-Mpentane or Iso-Paraffins	0.0000	0.0000
12	3-Mhexane or Iso-Paraffins	0.0000	0.0000
13	Mcyclohexane	0.0000	0.0000
14	i-Butene	0.0000	0.0530
15	Water	0.0000	0.0000
16	Hydrogen Sulfide	0.0000	0.0716
17	Methane	0.0000	0.0000
18	Ethane	0.0000	0.0000
19	Propane	0.0000	0.0000
20	n-Butane	0.0000	0.0009
21	i-Butane	0.0000	0.0000
22	Propene	0.0000	0.0000
23	1-Butene	0.0000	0.0177
24	C2=GC4EthrAc or FSII Additive	0.0000	0.0000
25	1-Dodecanol or Lubricity Improver	0.0000	0.0000

3.1.1. Calculation of Thiophene Removal Efficiency:

$$Removal\ Efficiency\ \% = \frac{0.070 - \ 0.0085}{0.070} * 100\% = 98.79\%$$

That is, approximately 98.79% of the Thiophene compound was removed during the catalytic process, indicating the high efficiency of the HDS unit in desulfurization.

3.1.2. Calculating Residence Time:

The residence time in a reactor is a crucial factor in determining the effectiveness of a catalytic reaction in removing sulfur compounds, such as Thiophene, from jet fuel. Residence time is defined as the time the mixture spends within the available reactor volume for the reaction, and is calculated by the following relationship [15]:

$$Residence\ Time = \frac{V}{Q}$$

Where V is the volume of the reactor (30 m^3 in this study), and Q is the volumetric flow rate of the mixture under operating conditions.

The volumetric flow rate was calculated based on simulation data using Aspen HYSYS software, assuming a mass flow rate of 25,000 kg/hr, an operating temperature of 400°C, and a pressure of 2500 kPa. The average molar mass of the mixture was calculated as approximately 86.91 kg/mol based on the mass and molar flow rates. Using the ideal gas law, the mixture density was estimated to be approximately 31.46 kg/m^3, resulting in a volumetric flow rate of approximately 795 m^3/h. Consequently, the calculated residence time of the mixture in the reactor was approximately 135.6 s. The short residence time is due to the predominance of the vapor phase and the low density of the mixture under the reactor operating conditions (400°C, 2500 kPa). It is indicate that the removal of the thiophene compound takes place during a relatively limited contact period, which requires a good ability to catalytically accelerate the reaction to achieve a removal rate of approximately 98.79%, as observed from the simulation results. Therefore, the relatively short residence time indicates that the reactor designed in this study operates well under the specified operating conditions, supporting the achievement of the goals of improving jet fuel quality while maintaining operational efficiency and productivity. However, it should be noted that the residence time here is calculated based on the assumption of near-ideal gas and no major change in the properties of the mixture during the reaction, which may result in slight variations in reality due to changes in pressure, temperature, and compositional properties along the reactor.

3.2. Separation Unit:

The three-phase separation unit (separartor-1) was operated at a temperature of 145 °C and a pressure of 898 kPa, conditions (That is, a cooler was added after Treated-Feed) that were carefully chosen based on previous results that showed the presence of high amounts of hydrogen sulfide (H_2S) in the mixture produced from the catalytic desulfurization unit (HDS-Reactor), both in the gaseous state and dissolved within the hydrocarbon phase. The purpose of choosing these relatively low values of pressure and temperature compared to the reactor conditions (400°C and 2500 kPa) was to achieve the highest possible efficiency in separating H_2S from the hydrocarbon product. When the pressure is reduced, the solubility of gases in liquids decreases according to Henry's law, which causes the acid gas to transition from the liquid phase to the gas phase. Also, reducing the temperature contributes to the condensation of hydrocarbons and their separation from the acid gases, which enhances the release process [16]. The analysis results indicate that the gas phase exiting the separation unit contained approximately 0.4486 mole fraction of H_2S, reflecting the process's success in releasing most of the acid gas from the product. Conversely, a small percentage 0.0488 mole fraction of H_2S remained dissolved in the hydrocarbon phase, an amount that can be managed in subsequent processing stages if necessary. Operationally, this precise pressure and temperature control has contributed to:

A. Reducing the H_2S content in the liquid phase to acceptable levels, thus approaching ASTM D1655 specifications for jet fuel.
B. Concentrating most of the H_2S in the gas phase, facilitating its treatment or disposal in dedicated sour gas treatment units.

Therefore, the selection of these operating conditions was aimed at efficiently removing sour gas from both its gas and hydrocarbon-dissolved states, ensuring the quality of the fuel. On the other hand, the data also indicate that the water content (H_2O) in all phases is zero, which means that the reactor process and the separation unit did not produce free or dissolved water in measurable quantities. This can be explained by several factors, including that the catalytic reactions used did not involve oxidation reactions that produce water, in addition to the fact that any trace amounts of water vapor may have been separated or removed in the previous treatment stages, or dissolved completely into the hydrocarbon and gaseous phase without forming a separate aqueous phase. This indicates that the operating conditions and feedstock configuration do not support the formation of a free aqueous phase at this stage of the process. Table 4 compares the molecular fraction composition of the process outputs before and after entering the three-phase separation unit for both the gas and hydrocarbon phases.

Table (4): The results of the three-phase separation unit

NO.	Components	Cooled Feed, x_i	Liquid-Hydrocarbons, x_i	H_2S-Other Gases
1	n-Hexane	0.1258	0.1273	0.1016
2	n-Heptane	0.1144	0.1182	0.0520
3	n-Octane	0.0915	0.0956	0.0235
4	224-Mpentane	0.0801	0.0828	0.0348
5	n-Nonane	0.1258	0.1324	0.0179
6	n-Decane	0.1144	0.1208	0.0094
7	Toluene	0.1945	0.2017	0.0760
8	Hydrogen	0.0017	0.0003	0.0259
9	Thiophene	0.0085	0.0086	0.0061
10	22-Mpropane	0.0000	0.0000	0.0000
11	2-Mpentane	0.0000	0.0000	0.0000
12	3-Mhexane	0.0000	0.0000	0.0000
13	Mcyclohexane	0.0000	0.0000	0.0000
14	i-Butene	0.0530	0.0470	0.1518
15	Water	0.0000	0.0000	0.0000
16	Hydrogen Sulfide	0.0716	0.0488	0.4486
17	Methane	0.0000	0.0000	0.0000
18	Ethane	0.0000	0.0000	0.0000
19	Propane	0.0000	0.0000	0.0000
20	n-Butane	0.0009	0.0008	0.0022
21	i-Butane	0.0000	0.0000	0.0000
22	Propene	0.0000	0.0000	0.0000
23	1-Butene	0.0177	0.0158	0.0501
24	C2=GC4EthrAc	0.0000	0.0000	0.0000
25	1-Dodecanol	0.0000	0.0000	0.0000

Furthermore, Figures Appendix B show the results of the three-phase separation unit through a graphical representation of the transition of components between the gaseous and hydrocarbon (liquid) phases after the desulfurization process. Appendix A also details the numerical values and detailed operating conditions for this stage, including temperatures, pressures, and flow rates, which supports performance analysis and a comprehensive understanding of the separation mechanism. On other hand, gas phase (H_2S-Other Gases), it was cooled from its high operating temperature to about 40°C at a pressure of approximately 400 kPa, with the aim of condensing the heavy hydrocarbon fractions and enhancing the separation of the two phases. When the cooled mixture was introduced into the separator-2, two distinct phases were formed: a liquid phase rich in heavy and aromatic compounds that condensed as a result of the thermal reduction, and a gaseous phase containing the lighter components and the greater part of the acidic gas, in particular hydrogen sulfide (H_2S). The liquid phase produced at this stage is not ready for use due to the presence of acidic compounds and impurities. Therefore, it is treated and then recycled within the process to utilize the hydrocarbons and minimize losses. The gas phase, however, contains a high concentration of H_2S and is an acidic gas requiring special treatment in amine units. The treatment of this gas will be discussed in detail in subsequent studies within this project.

3.3. Final-Product:

The results of the mixing of the incoming stream to the mixer, Liquid-Hydrocarbons coming out of the separator-1, indicate a composition close to the required specifications, but final adjustments and further improvements are still needed to ensure that the jet fuel accurately conforms to ASTM D1655 standards. It also requires the introduction of special processing components and improvements to enhance the physical and chemical properties of the fuel, such as density, freezing point, and oxidation resistance, to ensure high performance and stability under different operating conditions. Therefore, at this stage of the process, the base fuel mixture consisting of n-Decane and Toluene was introduced at a total flow rate of 1,500 kg/hr, which represents only 7.82% of the base feed fuel weight, where n-Decane constitutes about 65%, while Toluene constitutes about 35% of the total additive weight. This distribution reflects a balanced formulation designed to improve the physical and chemical properties of the fuel, such as density, boiling point, and chemical stability. Additionally, processing components were added at a rate of 150 kg/hr, representing only 0.78% of the base feedstock weight. These additives are distributed equally between C_2=GC_4EthrAc and 1-Dodecanol, each comprising 50% of the total additive weight. These additives contribute to improved fuel properties; C_2=GC_4EthrAc lowers the freezing point and improves flow characteristics, while 1-Dodecanol enhances viscosity and surface properties, thus improving overall fuel performance under various operating conditions without altering the fuel's basic composition. These materials were added under moderate operating conditions to ensure homogeneous mixing and stable performance within the crusher, while maintaining appropriate thermal and pressure balance for the process. Table 5, along with Figures in Appendix B, shows the results of the final product after completion of all processing and improvement stages. It is also include detailed illustrations of the operating conditions and measured results, contributing to a comprehensive and accurate understanding of the final fuel performance and its physical and chemical properties under different operating conditions.

The final results showed that the product coming out of the mixer was a 100% fully liquid hydrocarbon mixture in terms of the phase fraction, at an operating temperature of 44.9°C and a pressure of approximately 101.3 kPa, demonstrating excellent physical stability of the product under these conditions. The results showed a significant decrease in the sulfur content, with a very low mole fraction of Thiophene (about 0.0011 x_i), as shown in figure 4. A small percentage of H_2S was also observed (about 0.0014 x_i) in the final product, indicating the high efficiency of the HDS unit in reducing sulfur pollutants and limiting their environmental impacts and negative effects on engine performance. The product recorded a high flow rate of 174,308 kg/hr and a mass density of approximately 740.5 kg/m³, a value that falls within the acceptable range for jet fuel specifications according to ASTM D1655 standards. Fuel performance-enhancing additives such as C_2=GC_4EthrAc and 1-Dodecanol were also noted at a trace amount of 0.03% mole fraction each. Thermally, the fuel's low heat value (LHV) was approximately 43,640 kJ/kg, while its high heat value (HHV) was approximately 46,464 kJ/kg. These are excellent values indicating combustion efficiency perfectly suited for jet engines. The viscosity was approximately 0.56 cP under current conditions, a low value that allows for good fuel flow within injection systems. Watson's K = 11.99 indicates a favorable balance between paraffinic, naphthenic, and aromatic compounds, reflecting a product with stable and efficient distillation properties. The surface tension was also recorded at 22.22 dyne/cm, a value that supports the atomization and evaporation process within the combustion chamber.

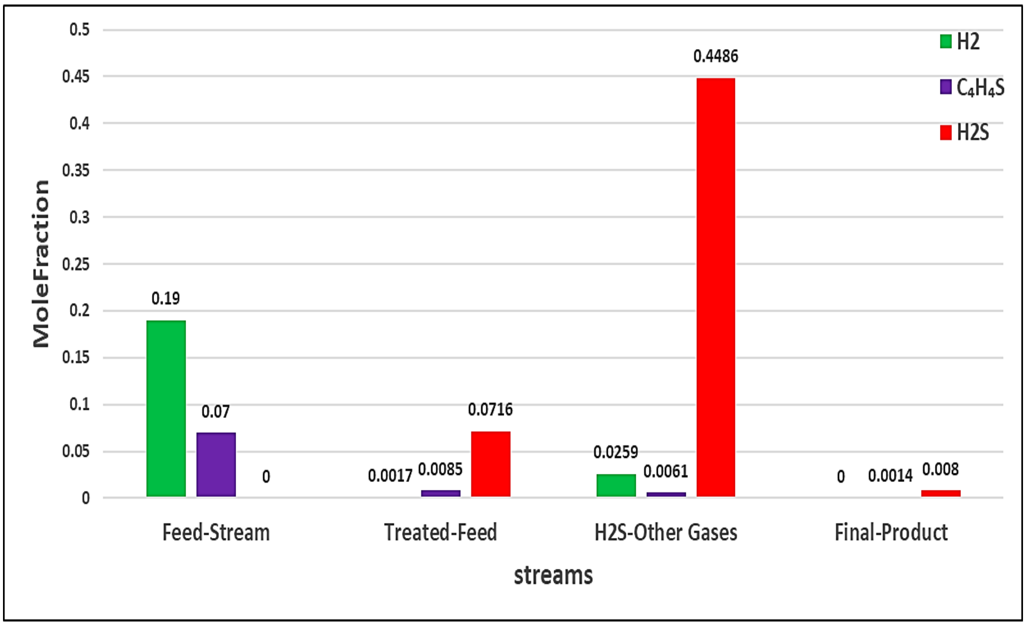


Figure (4): The mole fractions of H_2, C_4H_4S, and H_2S during treatment system

Table (5): The results of the components Feed-Stream in and Final-Product

NO.	Components	Feed-Stream, x_i	Final-Product, x_i
1	n-Hexane	0.1100	0.0139
2	n-Heptane	0.1000	0.0154
3	n-Octane	0.0800	0.0140
4	224-Mpentane	0.0700	0.0109
5	n-Nonane	0.1100	0.0208
6	n-Decane	0.1000	0.5861
7	Toluene	0.1700	0.3322
8	Hydrogen	0.1900	0.0000
9	Thiophene	0.0700	0.0011
10	22-Mpropane	0.0000	0.0000
11	2-Mpentane	0.0000	0.0000
12	3-Mhexane	0.0000	0.0000
13	Mcyclohexane	0.0000	0.0000
14	i-Butene	0.0000	0.0025
15	Water	0.0000	0.0000
16	Hydrogen Sulfide	0.0000	0.0014
17	Methane	0.0000	0.0000
18	Ethane	0.0000	0.0000

NO.	Components	Feed-Stream, x_i	Final-Product, x_i
19	Propane	0.0000	0.0000
20	n-Butane	0.0000	0.0001
21	i-Butane	0.0000	0.0000
22	Propene	0.0000	0.0000
23	1-Butene	0.0000	0.0000
24	C2=GC4EthrAc	0.0000	0.0003
25	1-Dodecanol	0.0000	0.0003

4. Conclusion

In this study, we conclude that the catalytic reactor, which was operated at a temperature of 400°C and a pressure of 2500 kPa, achieved a significant reduction in the concentration of the Thiophene compound, indicating the success of the desulfurization processes and the improvement of fuel quality. furthermore, the process of separating acid gas H_2S using a three-phase separation unit at a temperature of 145.3 °C and a pressure of 897.7 kPa was very effective, as these conditions contributed to reducing the solubility of acid gases in the liquid phases and transferring a large proportion of them to the gaseous phase. It can also be concluded that the final product, after the completion of the processing and improvement operations, which included the separation of phases and the addition of the treated compounds, reached specifications close to the international standards ASTM D1655. Based on these final study results, it can be concluded that the methodology followed and the selected operating conditions provide a practical and effective framework for improving the quality of jet fuel while taking into economic and environmental aspects, especially through precise control of temperatures and pressures in the reactor and separation unit to ensure optimal disposal of dissolved gases.

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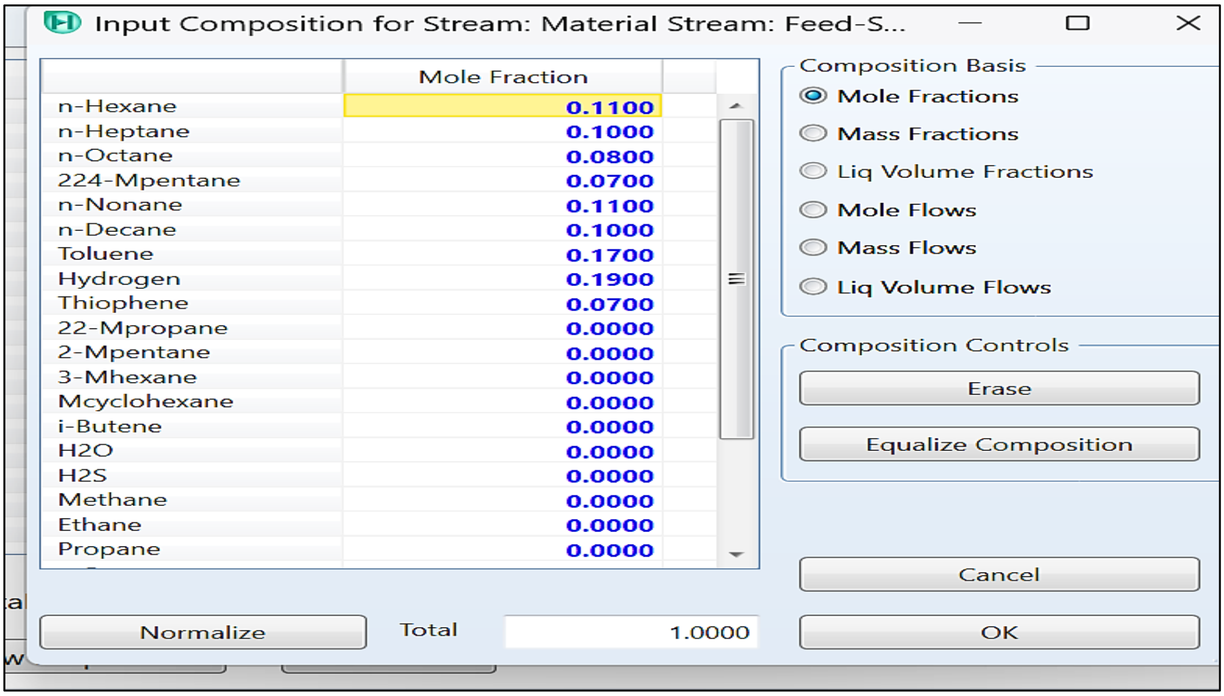
Appendix A

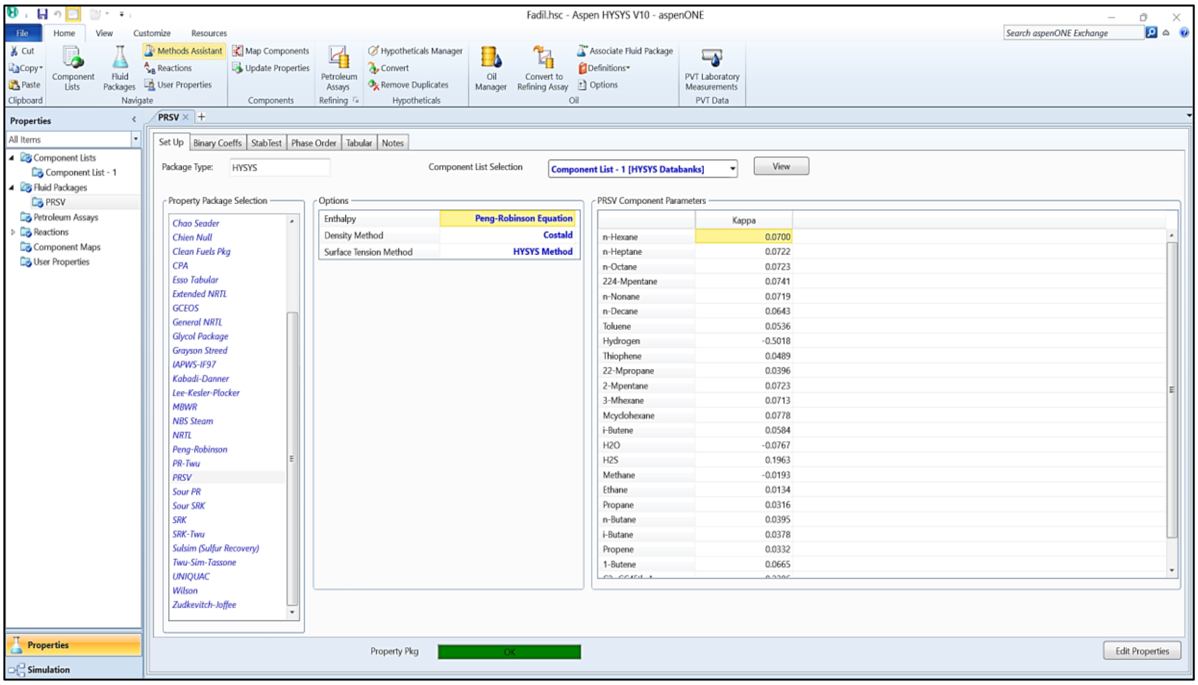

Input Composition for Stream: Material Stream: Feed-S...

	Mole Fraction
n-Hexane	0.1100
n-Heptane	0.1000
n-Octane	0.0800
224-Mpentane	0.0700
n-Nonane	0.1100
n-Decane	0.1000
Toluene	0.1700
Hydrogen	0.1900
Thiophene	0.0700
22-Mpropane	0.0000
2-Mpentane	0.0000
3-Mhexane	0.0000
Mcyclohexane	0.0000
i-Butene	0.0000
H2O	0.0000
H2S	0.0000
Methane	0.0000
Ethane	0.0000
Propane	0.0000

Composition Basis
● Mole Fractions
○ Mass Fractions
○ Liq Volume Fractions
○ Mole Flows
○ Mass Flows
○ Liq Volume Flows

Total 1.0000

Figure (5): The mole fractions of the components in Feed-Stream


Fadil.hsc - Aspen HYSYS V10 - aspenONE

PRSV

Package Type: HYSYS

Component List Selection: Component List - 1 [HYSYS Databanks]

Options

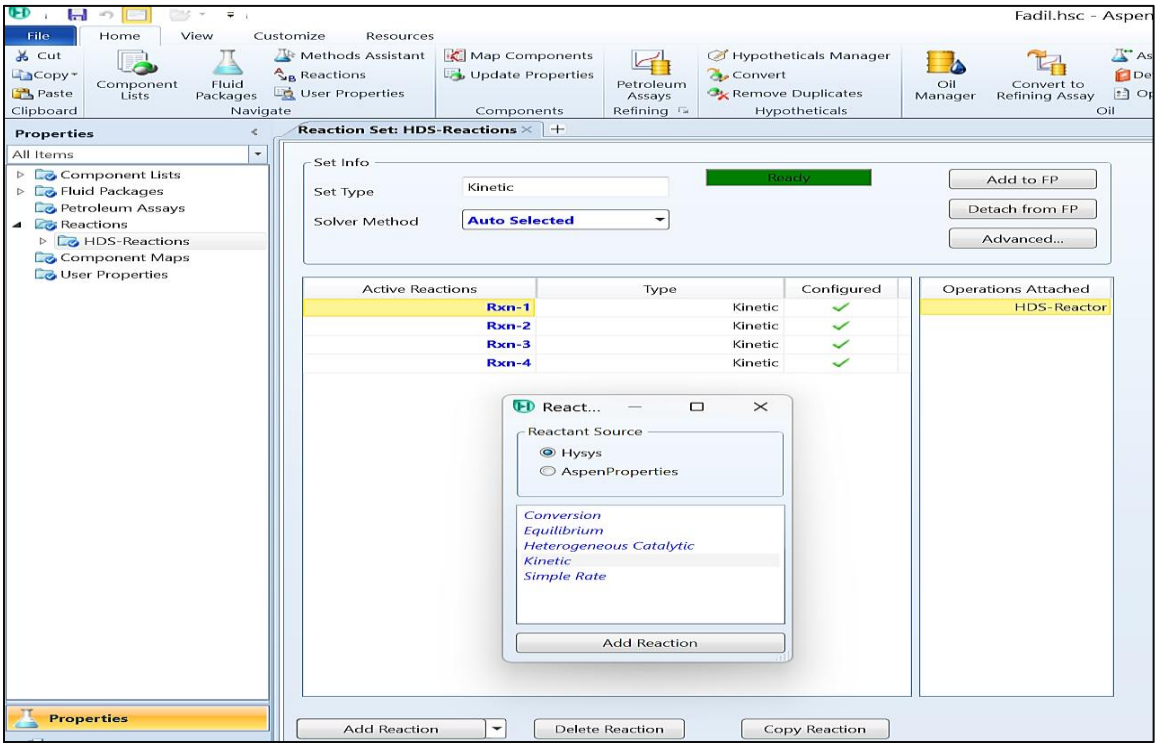
Enthalpy	Peng-Robinson Equation
Density Method	Costald
Surface Tension Method	HYSYS Method

PRSV Component Parameters

	Kappa
n-Hexane	0.0700
n-Heptane	0.0722
n-Octane	0.0723
224-Mpentane	0.0741
n-Nonane	0.0719
n-Decane	0.0643
Toluene	0.0536
Hydrogen	-0.5018
Thiophene	0.0489
22-Mpropane	0.0396
2-Mpentane	0.0723
3-Mhexane	0.0713
Mcyclohexane	0.0778
i-Butene	0.0584
H2O	-0.0767
H2S	0.1963
Methane	-0.0193
Ethane	0.0134
Propane	0.0316
n-Butane	0.0395
i-Butane	0.0378
Propene	0.0332
1-Butene	0.0665

Property Pkg OK

Figure (6): Fluid Package selected for the simulation model



Set Info
Set Type: Kinetic
Solver Method: Auto Selected
Ready

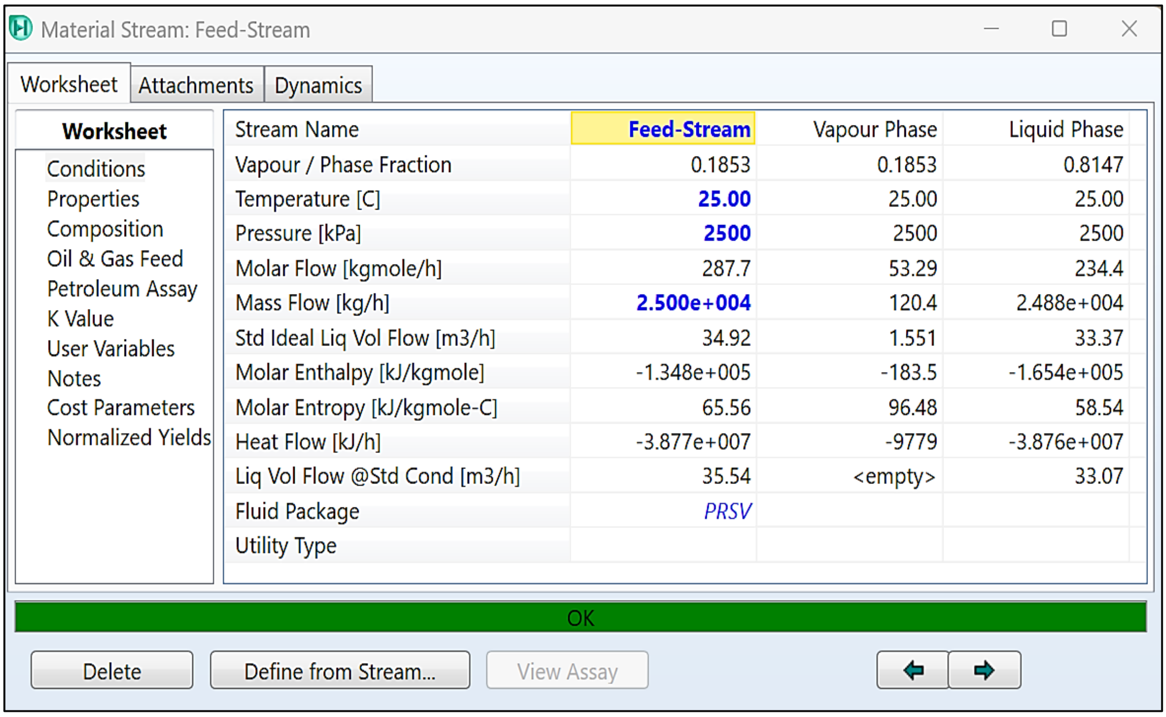
Active Reactions	Type	Configured
Rxn-1	Kinetic	✓
Rxn-2	Kinetic	✓
Rxn-3	Kinetic	✓
Rxn-4	Kinetic	✓

Operations Attached
HDS-Reactor

Reactant Source
● Hysys
○ AspenProperties

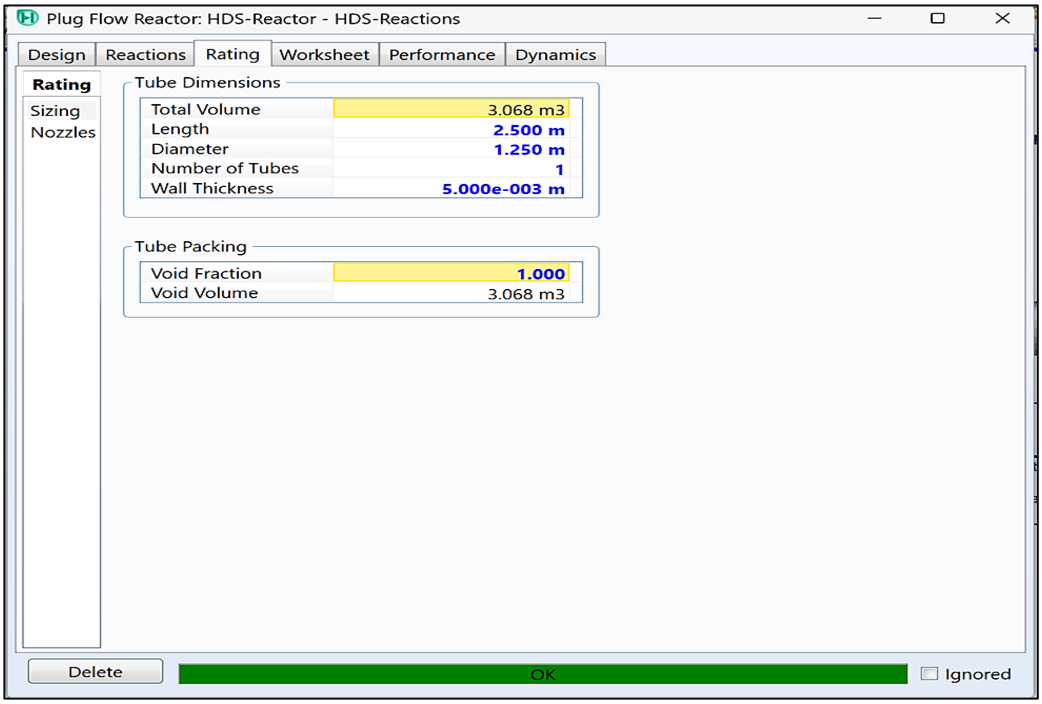
Conversion
Equilibrium
Heterogeneous Catalytic
Kinetic
Simple Rate

Figure (7): Names and types of reactions in a simulation environment



Stream Name	Feed-Stream	Vapour Phase	Liquid Phase
Vapour / Phase Fraction	0.1853	0.1853	0.8147
Temperature [C]	25.00	25.00	25.00
Pressure [kPa]	2500	2500	2500
Molar Flow [kgmole/h]	287.7	53.29	234.4
Mass Flow [kg/h]	2.500e+004	120.4	2.488e+004
Std Ideal Liq Vol Flow [m3/h]	34.92	1.551	33.37
Molar Enthalpy [kJ/kgmole]	-1.348e+005	-183.5	-1.654e+005
Molar Entropy [kJ/kgmole-C]	65.56	96.48	58.54
Heat Flow [kJ/h]	-3.877e+007	-9779	-3.876e+007
Liq Vol Flow @Std Cond [m3/h]	35.54	<empty>	33.07
Fluid Package	PRSV		
Utility Type			

Figure (8): Operating conditions in the Feed-Stream



Tube Dimensions

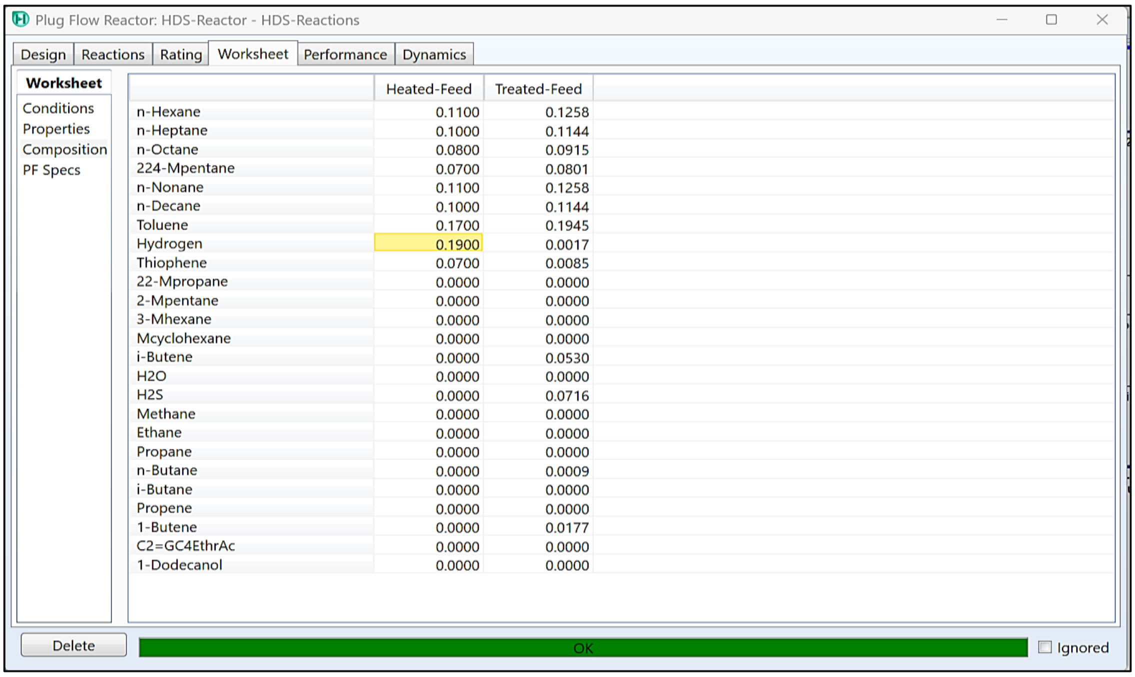
Total Volume	3.068 m3
Length	2.500 m
Diameter	1.250 m
Number of Tubes	1
Wall Thickness	5.000e-003 m

Tube Packing

Void Fraction	1.000
Void Volume	3.068 m3

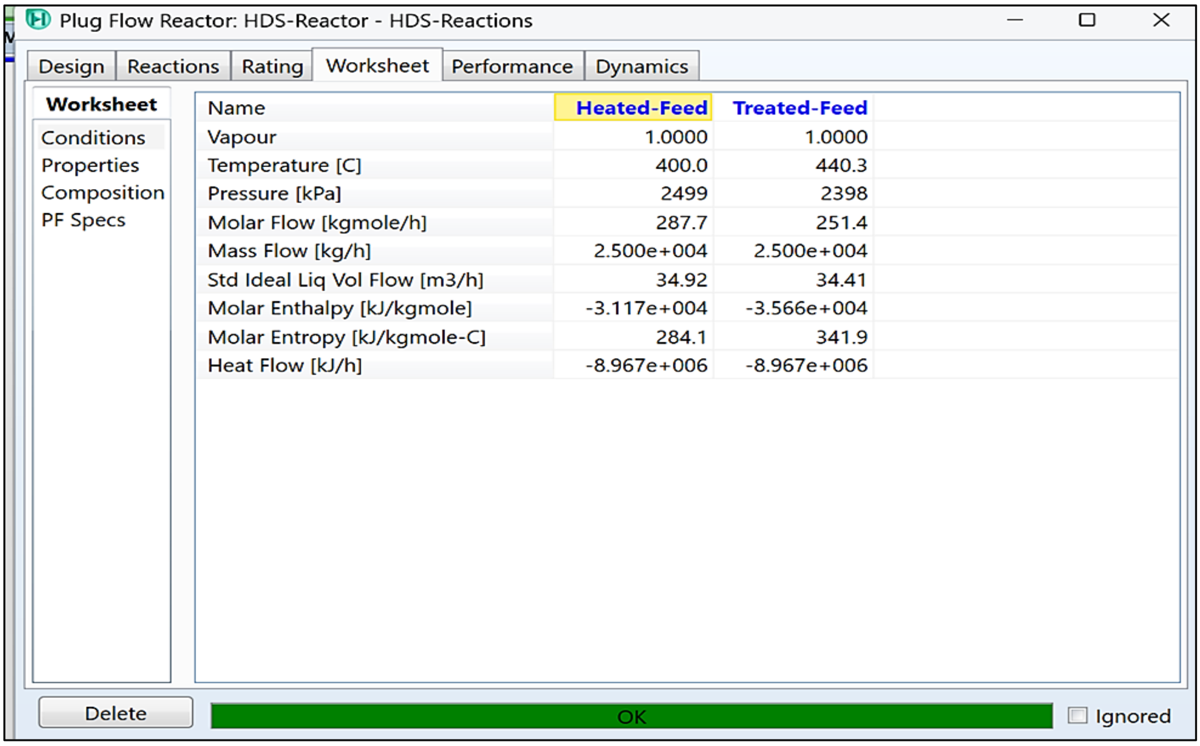
Figure (9): Engineering design of HDS-Reactor

Appendix B



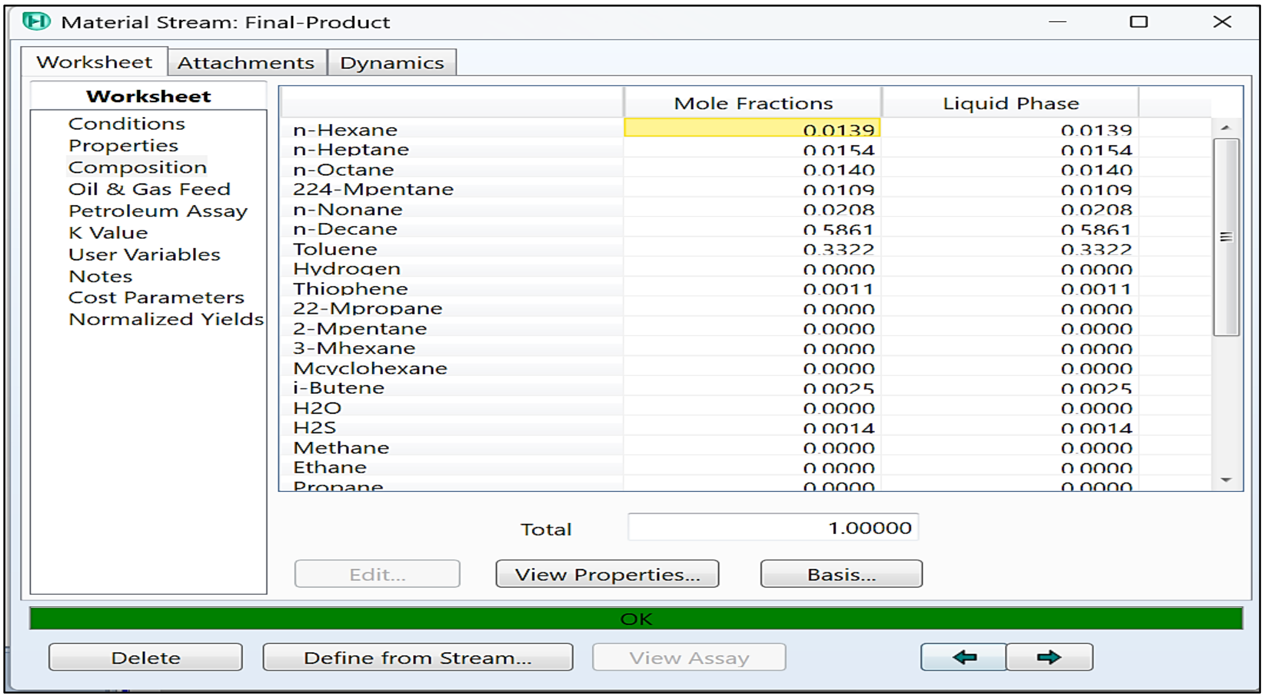
	Heated-Feed	Treated-Feed
n-Hexane	0.1100	0.1258
n-Heptane	0.1000	0.1144
n-Octane	0.0800	0.0915
224-Mpentane	0.0700	0.0801
n-Nonane	0.1100	0.1258
n-Decane	0.1000	0.1144
Toluene	0.1700	0.1945
Hydrogen	0.1900	0.0017
Thiophene	0.0700	0.0085
22-Mpropane	0.0000	0.0000
2-Mpentane	0.0000	0.0000
3-Mhexane	0.0000	0.0000
Mcyclohexane	0.0000	0.0000
i-Butene	0.0000	0.0530
H2O	0.0000	0.0000
H2S	0.0000	0.0716
Methane	0.0000	0.0000
Ethane	0.0000	0.0000
Propane	0.0000	0.0000
n-Butane	0.0000	0.0009
i-Butane	0.0000	0.0000
Propene	0.0000	0.0000
1-Butene	0.0000	0.0177
C2=GC4EthrAc	0.0000	0.0000
1-Dodecanol	0.0000	0.0000

Figure (10): The results of components before and after HDS-Reactor



Name	Heated-Feed	Treated-Feed
Vapour	1.0000	1.0000
Temperature [C]	400.0	440.3
Pressure [kPa]	2499	2398
Molar Flow [kgmole/h]	287.7	251.4
Mass Flow [kg/h]	2.500e+004	2.500e+004
Std Ideal Liq Vol Flow [m3/h]	34.92	34.41
Molar Enthalpy [kJ/kgmole]	-3.117e+004	-3.566e+004
Molar Entropy [kJ/kgmole-C]	284.1	341.9
Heat Flow [kJ/h]	-8.967e+006	-8.967e+006

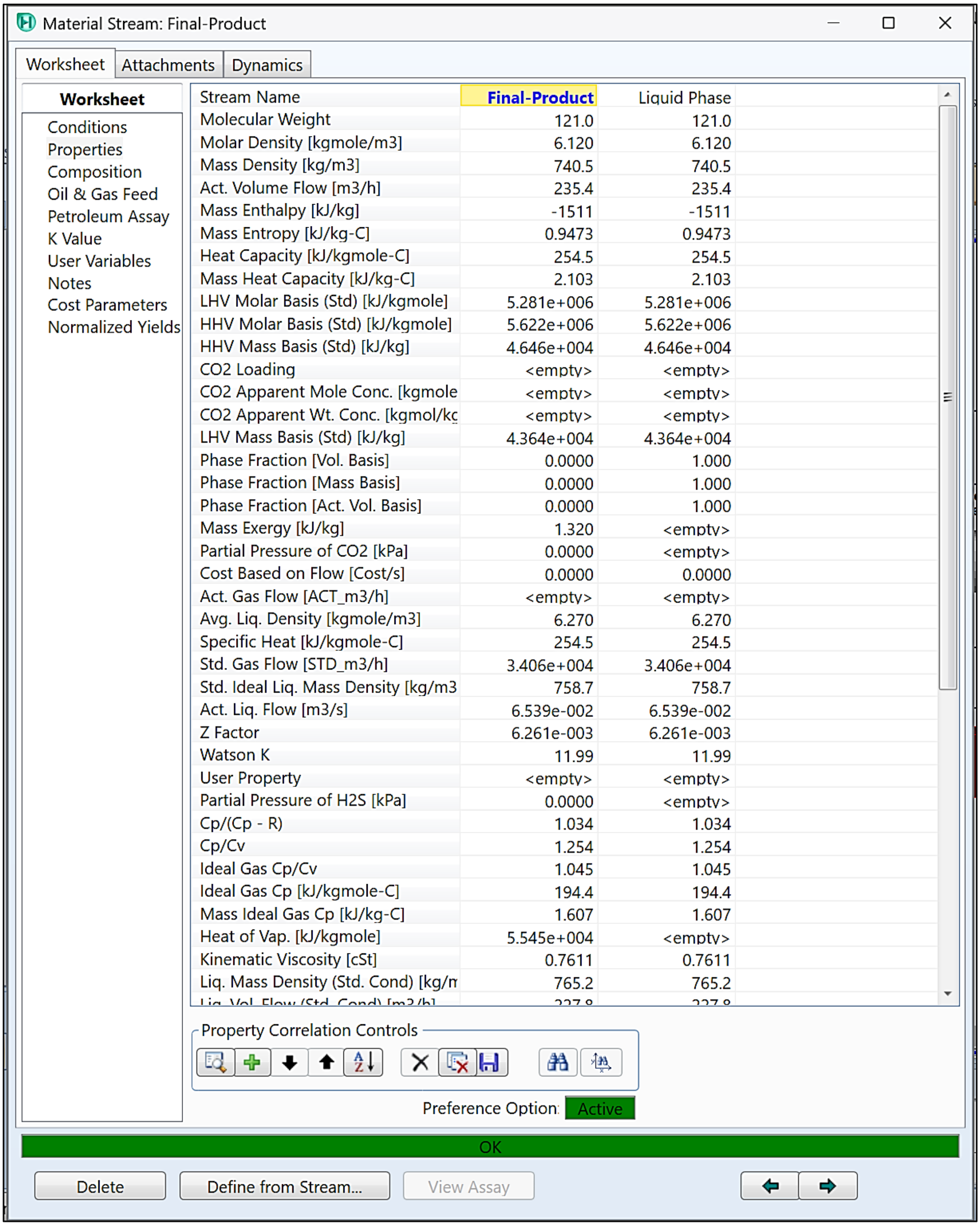
Figure (11): Operating conditions before and after HDS-Reactor



	Mole Fractions	Liquid Phase
n-Hexane	0.0139	0.0139
n-Heptane	0.0154	0.0154
n-Octane	0.0140	0.0140
224-Mpentane	0.0109	0.0109
n-Nonane	0.0208	0.0208
n-Decane	0.5861	0.5861
Toluene	0.3322	0.3322
Hydrogen	0.0000	0.0000
Thiophene	0.0011	0.0011
22-Mpropane	0.0000	0.0000
2-Mpentane	0.0000	0.0000
3-Mhexane	0.0000	0.0000
Mcyclohexane	0.0000	0.0000
i-Butene	0.0025	0.0025
H2O	0.0000	0.0000
H2S	0.0014	0.0014
Methane	0.0000	0.0000
Ethane	0.0000	0.0000
Propane	0.0000	0.0000

Total 1.00000

Figure (12): The mole fractions of the components in final stream (Final-Product)



Stream Name	Final-Product	Liquid Phase
Molecular Weight	121.0	121.0
Molar Density [kgmole/m3]	6.120	6.120
Mass Density [kg/m3]	740.5	740.5
Act. Volume Flow [m3/h]	235.4	235.4
Mass Enthalpy [kJ/kg]	-1511	-1511
Mass Entropy [kJ/kg-C]	0.9473	0.9473
Heat Capacity [kJ/kgmole-C]	254.5	254.5
Mass Heat Capacity [kJ/kg-C]	2.103	2.103
LHV Molar Basis (Std) [kJ/kgmole]	5.281e+006	5.281e+006
HHV Molar Basis (Std) [kJ/kgmole]	5.622e+006	5.622e+006
HHV Mass Basis (Std) [kJ/kg]	4.646e+004	4.646e+004
CO2 Loading	<empty>	<empty>
CO2 Apparent Mole Conc. [kgmole	<empty>	<empty>
CO2 Apparent Wt. Conc. [kgmol/kc	<empty>	<empty>
LHV Mass Basis (Std) [kJ/kg]	4.364e+004	4.364e+004
Phase Fraction [Vol. Basis]	0.0000	1.000
Phase Fraction [Mass Basis]	0.0000	1.000
Phase Fraction [Act. Vol. Basis]	0.0000	1.000
Mass Exergy [kJ/kg]	1.320	<empty>
Partial Pressure of CO2 [kPa]	0.0000	<empty>
Cost Based on Flow [Cost/s]	0.0000	0.0000
Act. Gas Flow [ACT_m3/h]	<empty>	<empty>
Avg. Liq. Density [kgmole/m3]	6.270	6.270
Specific Heat [kJ/kgmole-C]	254.5	254.5
Std. Gas Flow [STD_m3/h]	3.406e+004	3.406e+004
Std. Ideal Liq. Mass Density [kg/m3	758.7	758.7
Act. Liq. Flow [m3/s]	6.539e-002	6.539e-002
Z Factor	6.261e-003	6.261e-003
Watson K	11.99	11.99
User Property	<empty>	<empty>
Partial Pressure of H2S [kPa]	0.0000	<empty>
Cp/(Cp - R)	1.034	1.034
Cp/Cv	1.254	1.254
Ideal Gas Cp/Cv	1.045	1.045
Ideal Gas Cp [kJ/kgmole-C]	194.4	194.4
Mass Ideal Gas Cp [kJ/kg-C]	1.607	1.607
Heat of Vap. [kJ/kgmole]	5.545e+004	<empty>
Kinematic Viscosity [cSt]	0.7611	0.7611
Liq. Mass Density (Std. Cond) [kg/m	765.2	765.2

Figure (13): The properties in final stream (Final-Product)