

PRODUCTION SIMULATION HYDROGEN GAS FROM HEAVY FUEL OIL GASIFICATION AND LIFE CYCLE ASSESSMENT (LCA) USING UNISIM DESIGN R460.1 AND GABI TS SOFTWARE

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Abstract

Heavy fuel oil utilization via combustion leads to negative impacts towards the environment. A cleaner way of heavy fuel oil utilization should be implemented, gasification is one. Gasification process can convert heavy fuel oil feed into valuable gas like hydrogen. Based on the simulation result, hydrogen purity (on dry basis) was obtained at 98,02% (volume). Study on temperature and addition of gasifying agent was also done. At high gasification temperature, more hydrogen tends to be produced. Steam addition also gives positive effect on hydrogen yield. Environmental impacts evaluation using life cycle assessment method has been performed. Based on the simulation, this process significantly contributes to climate change with the score of 2.630 kgCO2eq. Carbon dioxide utilization via enhanced oil recovery can overcome this problem. From economical point of view, annual net income after tax is at Rp 45.956.031.943,16 with the annual return on investment rate of 59,46%, which is economically justified.

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1. Introduction

Global energy sources are currently still dominated by fossil-based hydrocarbon fuels, one of which is heavy fuel oil. Heavy fuel oil (HFO) is a residue from the distillation and cracking of petroleum, consisting of saturated, aromatic and olefinic hydrocarbons with a carbon number range of C9 to C50. This fraction has a boiling point of approximately 160–600°C and contains organometallic compounds, including heavy metals such as vanadium and nickel in low concentrations. [1]. In general, heavy fuel oil contains 85–90% carbon and 8–13% hydrogen, with small amounts of sulphur, nitrogen and oxygen. [2]. The sulphur and heavy metal content means that direct combustion of heavy fuel oil produces significant pollutant emissions and has the potential to increase the environmental burden. With increasing energy demands and the need to reduce emissions, cleaner HFO utilisation technologies are required.

Gasification is a thermochemical conversion technology capable of converting heavy fuel oil into synthesis gas (syngas) containing hydrogen (H₂), carbon monoxide (CO), carbon dioxide (CO₂), and methane (CH₄). [3]. The main reactions in gasification include partial oxidation, steam reforming, water-gas shift, and cracking[4] heavy hydrocarbon compounds affected by temperature, gasification agent ratio, and feed characteristics. Heavy oil gasification has been studied under various operating conditions—for example, increasing the temperature has been shown to increase hydrocarbon conversion and hydrogen yield, while adding water vapour increases the H₂/CO ratio through the water-gas shift reaction [5]. Hydrogen produced by gasification is very important in the petroleum industry, especially for hydrotreating and hydrocracking processes.

Modelling using process simulation software, such as UniSim Design R460.1, provides the ability to comprehensively study gasification phenomena without the need for large-scale experiments. Simulation

enables process sensitivity evaluation, mass–energy balance calculations, hydrogen purity analysis, and optimisation of operating parameters based on relevant thermodynamic and kinetic conditions, as has been done by [6], [7], [8]. In addition to technical analysis, a quantitative assessment of the environmental impacts arising throughout the process life cycle is required. The Life Cycle Assessment (LCA) method is used to assess the contribution of impact categories such as climate change, acidification, eutrophication, and resource use in accordance with the ISO 14040 standard. [9]. The GaBi software is used to calculate the environmental impact of each stage of the system, from feed preparation, gasification, hydrogen purification, to process emissions. On the other hand, economic feasibility must also be reviewed, given that the sustainability of the process is largely determined by profitability and return on investment.

Therefore, this study was conducted to provide a comprehensive understanding of the utilisation of heavy fuel oil through gasification technology. This study includes the development of a simulation model for the gasification-based hydrogen production process using UniSim Design R460.1, evaluation of environmental impacts through a Life Cycle Assessment (LCA) approach with the help of GaBi software, and economic feasibility analysis based on investment estimates, operating costs, and profitability parameters. The results of this study are expected to provide a scientific basis for the development of cleaner and more sustainable HFO utilisation technology.

2. Method

This research method consists of three main stages, namely simulation of the heavy fuel oil gasification process for hydrogen production using UniSim Design R460.1, environmental impact analysis through Life Cycle Assessment (LCA) with GaBi software, and economic feasibility analysis based on investment parameters and profitability. The general flow diagram of the research includes feed characterisation, process modelling, environmental evaluation, and economic analysis.

A. Process Simulation Using UniSim Design

1) Feed Characterization

This research method consists of three main stages, namely simulation of the heavy fuel oil gasification process for hydrogen production using UniSim Design R460.1, environmental impact analysis through Life Cycle Assessment (LCA) with GaBi software, and economic feasibility analysis based on investment and profit parameters. The general flow chart of the research includes raw material characterisation, process modelling, environmental evaluation, and economic analysis.

2) Fluid Package

Heavy fuel oil (HFO) is modelled as an assay using atmospheric distillation data and available physical properties. Pseudo-components are generated according to the boiling point range of heavy fuel oil fractions. The selection of thermodynamic models can be accessed in the Simulation Basis Manager menu. In this simulation, two types of thermodynamic models are used, namely Peng-Robinson (PR) and Amine Package.

3) Process Simulation

This simulation process consists of five main stages, namely:

- **Feed preheating**, namely heating heavy fuel oil and oxygen using steam through a heat exchanger until it reaches the gasifier operating temperature.
- **Gasification**, represented using a Gasifier block, where partial oxidation, pyrolysis, and subsequent reactions take place. At this stage, the HFO feed is reacted with air and steam under specific operating conditions. The operating variables set include:
 - Gasification temperature with a temperature range of 1000-2000°C
 - Steam-to-feed ratio (S/F) with the ratio of steam mass flow rate to feed (Steam/Feed) varying from 0.2-2.0.

This model produces an initial syngas composition of H₂, CO, CO₂, CH₄, H₂O, and other minor gases. The hot gas produced is then fed into a waste-heat boiler to generate utility steam.

- **Quenching**, performed using an absorption column that brings hot gas into contact with water, thereby lowering the temperature and separating suspended carbon particles.
- **CO conversion**, modelled using an equilibrium reactor to represent the water-gas shift reaction isothermally at low temperatures.
- **Gas purification/gas sweetening**, using an MEA absorption-desorption system to remove CO₂ and H₂S, with the amount of MEA used based on the process. [10], sehingga dihasilkan gas hidrogen dengan kemurnian minimal 98% volume sesuai standar ISO 14687.

B. Life Cycle Assessment (LCA)

This LCA study was conducted entirely with the assistance of GaBi ts software.

1) Goal and Scope Definition

The LCA study conducted in this research was evaluated using a gate-to-gate approach, where observations began from the point of entry of raw materials into the product system to the point where hydrogen gas was produced by the system. The impact assessment method used was the ReCiPe 2016 v1.1 Midpoint method. The category selected was midpoint, where the impact focused only on several environmental impacts caused by the product system. The boundaries of the product system can be illustrated as follows

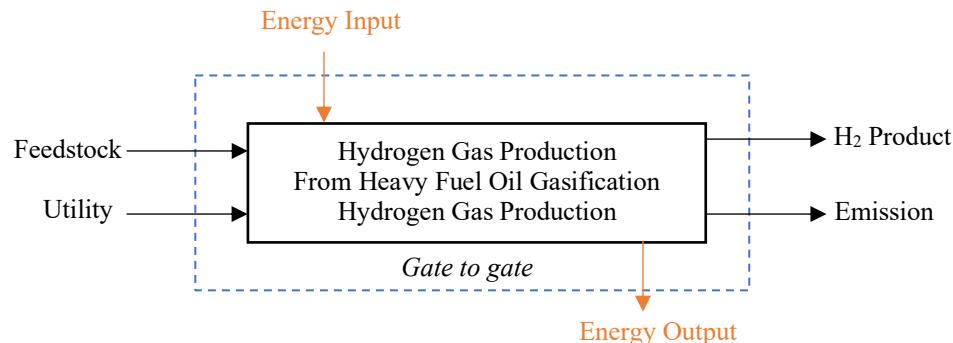


Figure 1. Product System Boundary

2) Life Cycle Inventory (LCI)

This process is carried out by inventorying all inflows and outflows from the system based on UniSim simulation data. The data recorded includes flows of raw materials, utilities, energy, main products, by-products, and emissions released into the environment. The inventory is carried out based on an operating basis of 1000 kg/hour of heavy fuel oil as feed, in accordance with the capacity design specified in the simulation. The data is then entered into the inventory table in GaBi for use in the impact assessment stage.

3) Impact Assessment

The third stage is the phase in which inventory data is translated into environmental impact values through a process of classification, characterisation, normalisation and weighting. This procedure follows the Life Cycle Impact Assessment (LCIA) flow as stipulated in the British Standards, which served as a reference in the previous simulation process. During the characterisation stage, each emission stream is converted into an equivalent impact value, such as CO₂ equivalents for the global warming category. The ReCiPe 2016 method is used for mapping and assessing impact categories. *Economic Feasibility Analysis*

An economic analysis method was used to assess the financial feasibility of hydrogen production from heavy fuel oil gasification. Calculations were made taking into account the initial investment costs, annual operating costs, and revenue from hydrogen sales. Cost components included the main equipment requirements, utilities, raw materials, and maintenance. Economic assessment was carried out using the net present value (NPV), payback period, and return on investment (ROI) parameters to determine the overall profitability and feasibility of the project.

3. Result and Discussion

A. Process Simulation

The results of simulations of hydrogen production through heavy fuel oil gasification show that the process configuration built in UniSim Design R460.1 is capable of producing a hydrogen flow with a purity of 98.02% vol, in accordance with the ISO 14687 standard for Grade A hydrogen, with the following details:

Table 1. Key Product Specifications Based on
 Simulation Results (Dry Basis)

Component	Value	Unit
H2	98,02%	%vol.
CO	0,00%	%vol.
CO2	0,00%	%vol.
H2S	0,8891	ppm
CH4	0,04%	%vol.
N2	1,87%	%vol.

With the overall mass balance showing a total inflow and outflow of 8,634.70 kg/hour, this indicates that the model has achieved good stability and convergence, as follows:

Table 2. Mass Balance of Simulation Results

Input		Output	
Stream	Mass Flowrate (kg/jam)	Stream	Mass Flowrate (kg/hour)
Feed	1000,00	Steam	2424,00
Oxygen	1160,00	Quench Water	2814,95
Steam	750,00	WGSR Bottom	251,48
CW Gasifier	300,70	Produk Utama (Sweet Gas)	299,80
BFW	2424,00	Sour Gas	2697,40
Quench Water	3000,00	Slag	147,07
Total	8634,70	Total	8634,70

- Syngas Production

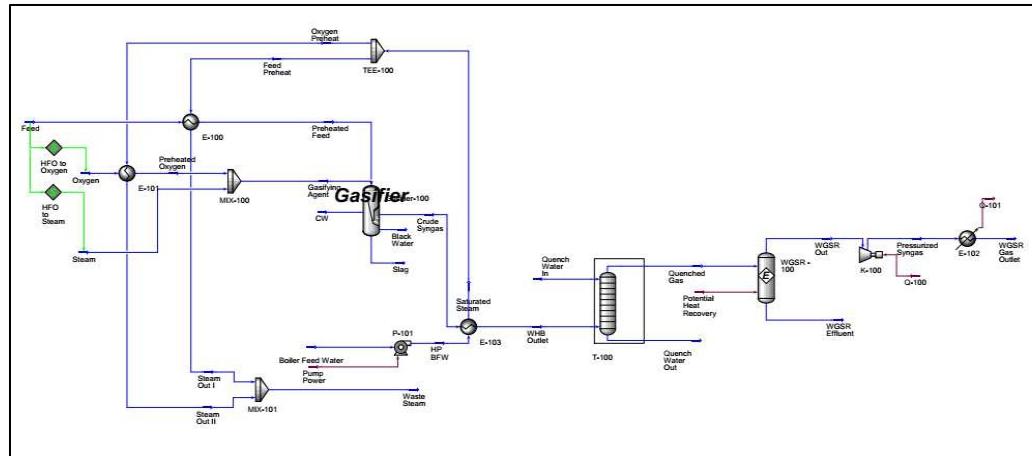


Figure 2. Process Flow Diagram of the Syngas Production Simulation Stage

The image shows the complete configuration of the syngas production simulation process built using UniSim Design R460.1. In the syngas production process using the heavy fuel oil gasification method, various process equipment is used in accordance with the operating conditions applied in this simulation, including the following:

Table 3. List of Equipment for Heavy Fuel Oil Gasification Process Simulation

No	Equipment	Operation Condition		Description
		Temp. (°C)	Pressure (kPa)	
1.	Heat Exchanger, E-100 (<i>Feed steam preheater</i>)	200	308,2	Heating Heavy Fuel Oil Feed ΔP: 20 kPa
2.	Heat Exchanger, E-101 (<i>Oxygen steam preheater</i>)	210	4238	Oxygen Warming ΔP: 20 kPa
3.	Mixer, MIX-100	-	-	Mixing of Gasification Agents
4.	Gasifier, Gasifier-100	1680	307,2	-
5.	Heat Exchanger, E-103 (Waste-heat boiler)	250	101,3	ΔP: 20 kPa
6.	Quench Tower, T-100	50,56	30 (<i>Top Stage Pressure</i>)	-
7.	Reactor, WGSR-100	25	30	Isotermik
8.	Compressor, K-100	164,7	100	Efficiency (adiabatic), 75%
9.	Cooler, E-102	25	100	-

As can be seen in the composition of the gasification product stream, a molar ratio of H₂ to CO of 0.98 and a volume ratio of 0.80 were obtained. When compared to the results of experiments on a research scale conducted by Ashizawa, Hara, Kidoguchi, & Inumaru [5] The H₂/CO volume ratio obtained was 1.01, so using this value as a reference, the absolute error percentage was 21%. This shows that the gasification model in UniSim is capable of representing the reaction phenomena that occur, particularly pyrolysis, partial oxidation, and gasification reactions that take place at a temperature of 1680 °C.

Within the gasifier, the process takes place in three zones—pyrolysis, gasification and quench—each of which contributes to the formation of char, devolatilisation and syngas production. In the pyrolysis zone, drying and thermal cracking (devolatilisation) occur, significantly reducing the volatile components in the heavy fuel oil feed from 41,530 kgmol/hour to 3,0017 kgmol/hour.

Name	Pyrolysis Feed	Pyrolysis Prod
Temperature [C]	990.7434	800.0000
Pressure [kPa]	308.1682	307.1682
Total Molar Flow [kgmole/h]	173.6735	157.1969

Figure 3. Operating Conditions Between Feed and Pyrolysis Zone Products

Name	Pyrolysis Feed	Pyrolysis Prod
Coal [kgmole/h]	95.6062	55.9674
Fixed C [kgmole/h]	51.3771	51.3771
Volatile [kgmole/h]	41.530	3.0017
Ash [kgmole/h]	1.5886	1.5886
Moisture [kgmole/h]	1.1102	0.00000

Figure 4. Proximate Content of Feed and Pyrolysis Zone Products

At a temperature of 800°C [11], All feedstock is converted into char and volatile substances, where char serves as fuel to provide heat energy when reacting with oxygen and steam. Simulation results show that the pyrolysis zone output stream contains CO₂ from char combustion and H₂S formed as a result of the reaction of sulphur in the feedstock with hydrogen released during pyrolysis.

Component	Inlet Mole Flow [kgmole/h]	Outlet Mole Flow [kgmole/h]
Hydrogen	0.00000	0.00000
CO	0.00000	0.00000
CO ₂	0.00000	8.2611
H ₂ O	41.632	84.874
H ₂ S	0.00000	0.98595
Methane	0.00000	0.00000
Nitrogen	1.4892	1.4892
Oxygen	34.946	5.6192
Heavy Fuel Oil*	95.606	55.967

Figure 5. Proximate Content of Feed and Pyrolysis Zone Products

In the gasification zone, syngas begins to form when the temperature reaches 800°C. Based on simulation results, this zone extends 6.592 m inside the gasifier vessel. Gasification occurs as indicated by a decrease in the fixed carbon fraction in the product compared to the feed, as a result of the water-gas and Boudouard reactions. In the water-gas reaction, carbon reacts with steam to form an equimolar mixture of H₂ and CO, while the Boudouard reaction produces CO through the interaction of carbon with CO₂.

Length [m]	Coal [kgmole/h]	Fixed Carbon [kgmole/h]	Volatile [kgmole/h]	Ash [kgmole/h]	Moisture [kgmole/h]
0.0000	55.967	51.377	3.0017	1.5886	0.00000
6.592	4.7488	0.15857	3.0017	1.5886	0.00000

Figure 6. Proximate Composition of Feedstock and Gasification Zone Products

Further steam consumption confirms the ongoing gasification process, primarily through water-gas and water-gas shift reactions, in which CO reacts again with steam to produce H₂ and CO₂. This is evident from the increase in the number of moles of CO₂ at the end of the gasification zone. Hydrogenation reactions with carbon also occur, as indicated by the formation of methane (CH₄) at the outlet of this zone.

Length [m]	Hydrogen [kgmole/h]	CO [kgmole/h]	CO ₂ [kgmole/h]	H ₂ O [kgmole/h]	H ₂ S [kgmole/h]	Methane [kgmole/h]	Nitrogen [kgmole/h]	Oxygen [kgmole/h]	Heavy Fuel Oil* [kgmole/h]
0.0000	0.00000	0.00000	8.2611	84.874	0.98595	0.00000	1.4892	5.6192	55.967
6.592	45.153	45.991	13.486	39.680	0.98595	2.6332e-002	1.4892	0.00000	4.7488

Figure 7. Flow Rate of Feedstock and Product Components in the Gasification Zone

In the quench zone, based on simulation results, hot gas is brought into contact with cooling water so that the outlet temperature drops to around 1300°C. This quench process produces 4.7488 kgmol/hour of slag, while the cooling water evaporates and is carried away with the gas flow, as evidenced by the absence of water content in the slag that comes out. Slag is a solid residue left over from the gasification process. The simulation results also show that hydrogen gas exits the gasifier at a rate of 45.153 kmol/hour, formed through a series of reactions inside the gasifier. To determine the contribution of each reaction to hydrogen production, a more in-depth study of reaction kinetics is required.

Name	Temperature [C]	Pressure [kPa]	Molar Flow [kgmole/h]
Cooling Feed	25.0000	101.3250	27.7545
Internal Feed	1680.3365	307.1682	151.5598
Vap Prod	1299.8809	101.3250	174.5655
Liq Prod	1299.8809	101.3250	0.0000
Slag Prod	1299.8809	101.3250	4.7488

Figure 8. Operating Conditions of the Quench Zone

And for the water-gas shift reactor, which functions to increase hydrogen yield through the conversion of carbon monoxide (CO). Based on the simulation results, CO conversion reached 99.99%, indicating that almost all CO in the inlet stream reacted with steam to produce hydrogen and CO₂. The isothermal reaction conditions provide a high equilibrium constant so that the reaction shift is strongly directed towards product formation. Since CO is used as the base component, the amount of H₂ and CO₂ formed follows the amount of CO entering the reactor. This conversion value is in line with Callaghan's findings[12], which shows that equilibrium conversion can reach around 99%.

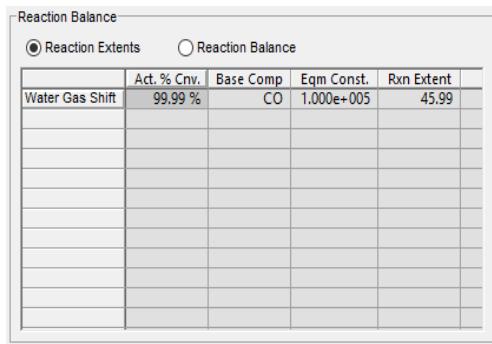


Figure 10. Water Gas Shift Reaction Performance

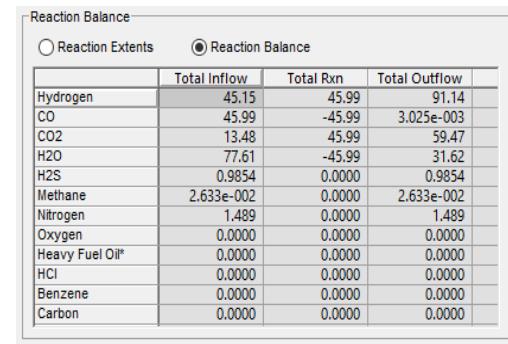


Figure 9. Flow of Mol Entering and Leaving the Reactor

- Purification

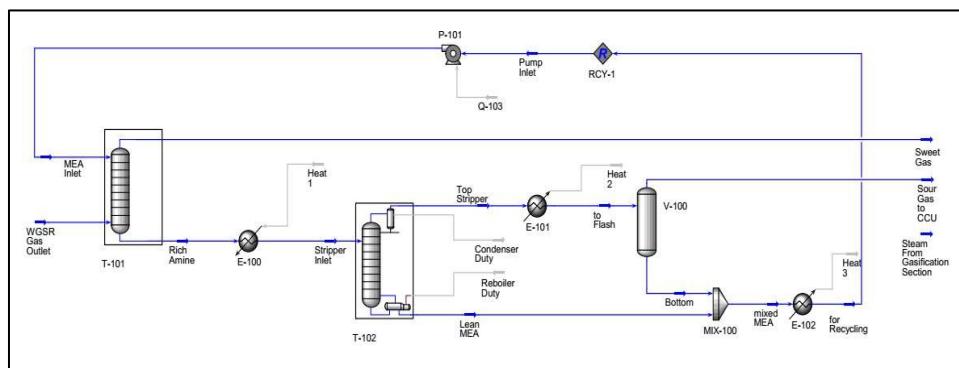


Figure 11. Process Flow Diagram of Purification

The image shows the complete configuration of the purification resistance simulation process built using UniSim Design R460.1. In this process, various process equipment is used in accordance with the operating conditions applied in this simulation, including the following:

Table 4. List of Equipment for Gasification Product Purification Process Simulation

No	Equipment	Operation Condition		Description
		Temp. (°C)	Pressure (kPa)	
1.	Absoprtion Column, T-101	25	100	-
2.	Heater, E-100	50	90	No difference in pressure
3.	Desorption Column (Stripper), T-101	50	90	-
4.	Cooler, E-101	25	80	No difference in pressure
5.	Separator, V-100	25	80	-
6.	Mixer, M-100	-	-	Mixing of liquid product from the separator with the bottom product of the desorption column
7.	Pump, P-101	25	100	-
8.	Cooler, E-102	25	-	No difference in pressure

- Study of Variable Effect

The study of variable effects in this research was conducted with the help of the case studies feature in the UniSim Design R460.1 software. Case studies can be accessed in the Databook menu option, Tools tab of the UniSim Design R460.1 software.

- a. The Effect of Gasification Temperature on the Volumetric Composition of H₂ and CO Gases

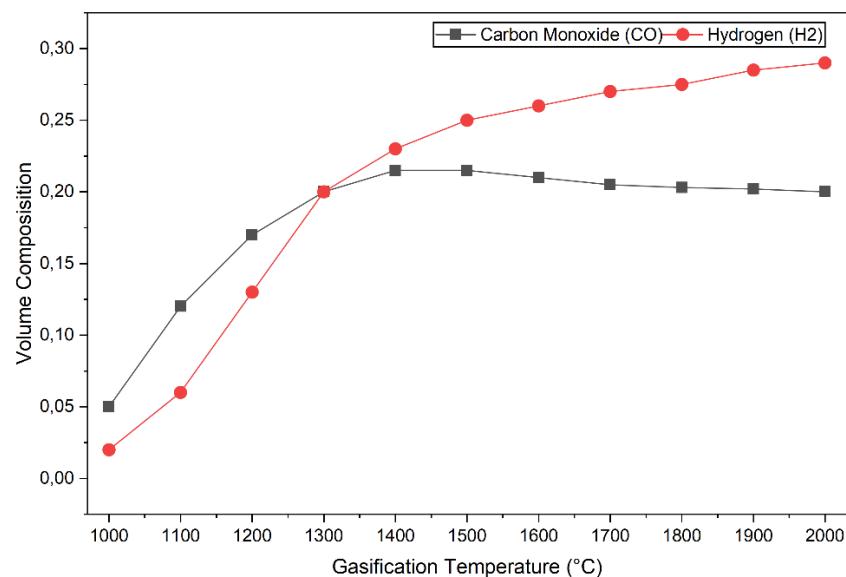


Figure 12. Graph of the Effect of Gasification Temperature on H₂ and CO Composition

Gasification temperature variations were conducted to observe the volume composition profiles of the two main gasification products, namely hydrogen and carbon monoxide. Using a gasification temperature range of 1000-2000°C, hydrogen formation tended to increase continuously. Meanwhile, carbon monoxide formation appears to be constant above a gasification temperature of 1500°C. This is due to the limited availability of oxygen used in the gasifier, which also limits the rate of CO formation. More hydrogen is obtained when gasification is carried out at high temperatures. This is because high temperatures can aid in the cracking process of heavy fractions found in fuel oil. Efek Temperatur Gasifikasi Terhadap Komposisi Volum Gas H₂ dan CO

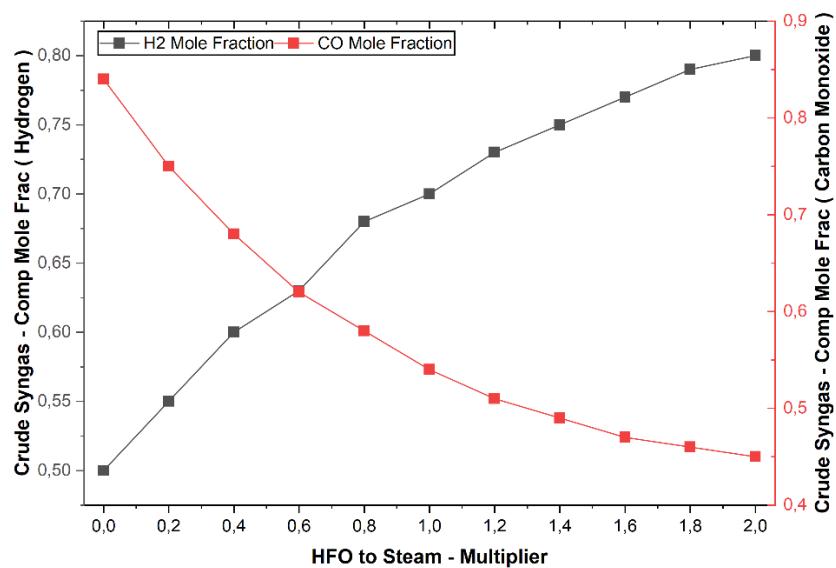


Figure 13. Graph showing the effect of steam volume on the composition of H₂ and CO

In this study, the oxygen mass flow rate to feed ratio (O₂ /Feed) was kept constant to observe the effect of steam on the gasification product. The steam mass flow rate to feed ratio (Steam/Feed) was varied from 0.2 to 2.0. Based on the results graph below, the addition of steam will increase the hydrogen gas composition and suppress the carbon monoxide composition. Thus, the presence of steam can increase the effectiveness of the gasification process by increasing the H₂ /CO ratio.

B. Life Cycle Assessment (LCA)

After entering all flow data from the process simulation results into the GaBi ts software, several environmental impacts resulting from hydrogen production through heavy fuel oil gasification were obtained. There are six categories of impacts, namely:

- Climate Change

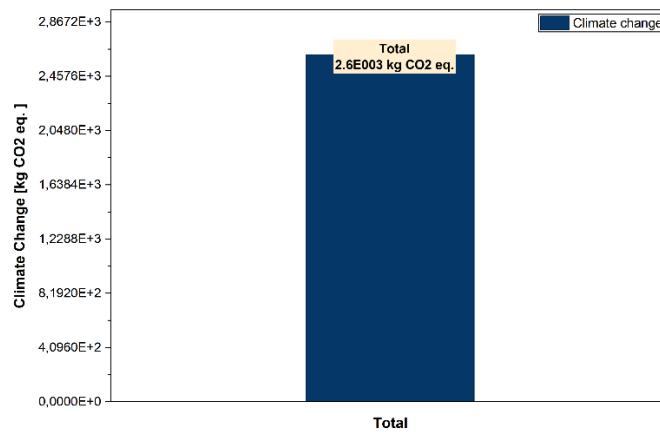


Figure 14. Climate Change

This category describes the impact on climate change expressed in kg CO₂ equivalent. The graph below shows that this hydrogen production process contributes 2,620 kgCO₂ equivalent (per hour) for a process base of 1,000 kg/hour of feed input.

- Freshwater Ecotoxicity

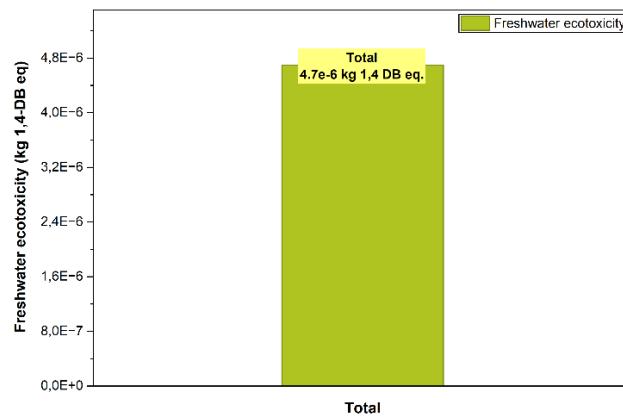


Figure 15. • Freshwater Ecotoxicity

This category describes the impact on water pollution expressed in kg of 1,4-dichlorobenzene equivalent. The graph below shows that this hydrogen production process contributes 4.7×10^{-6} kg of 1,4-dichlorobenzene equivalent (per hour) for a process basis of 1000 kg/hour of feed input.

- Marine Eotoxicity

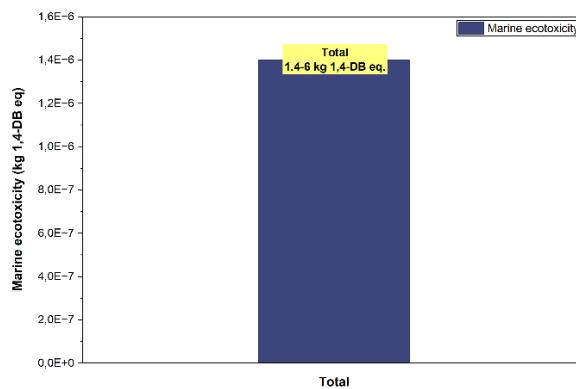


Figure 16. Pencemaran Laut

This category describes the impact on marine pollution expressed in kg of 1,4-dichlorobenzene equivalent. The graph below shows that this hydrogen production process contributes 1.4×10^{-6} kg of 1,4-dichlorobenzene equivalent (per hour) for a process basis of 1000 kg/hour of feed input.

- Marine Eutrophication

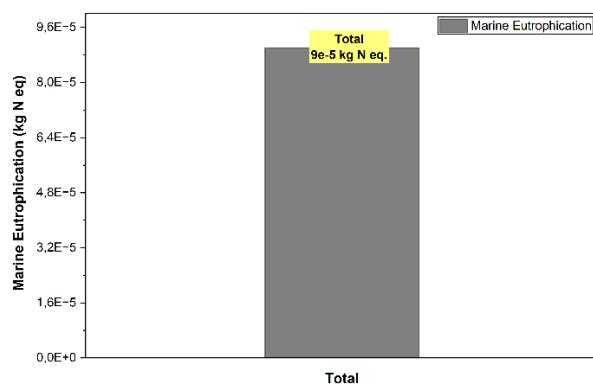


Figure 17. Marine Eutrophication

This category describes the impact on eutrophication of marine ecosystems expressed in kg N equivalent. The graph below shows that this hydrogen production process contributes 9×10^{-5} kg N (per hour) equivalent for a process base of 1000 kg/hour of feed input.

- Terrestrial Ecotoxicity

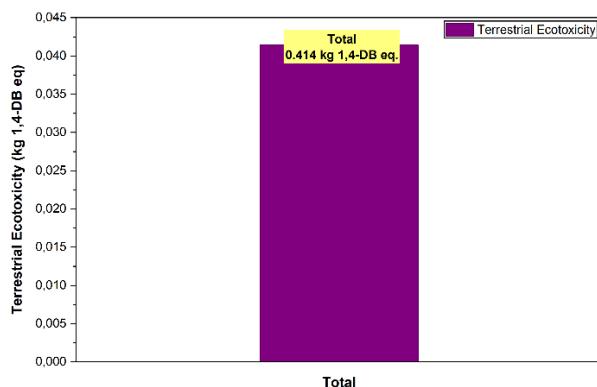


Figure 18. Terrestrial Ecotoxicity

This category describes the impact on soil contamination expressed in kg of 1,4-dichlorobenzene equivalent. The graph below shows that this hydrogen production process contributes 0.0414 kg of 1,4-dichlorobenzene equivalent (per hour) for a process basis of 1000 kg/hour of feed input.

To minimise the environmental impact, there are solutions that can be implemented. The following table recommends several alternatives for utilising CO₂ gas produced by the product system, so that it is not released as emissions into the surrounding environment, based on Hepburn. [13] :

Table 5. Alternatif Utilisasi CO₂

No	Alternative	Potential for CO ₂ Removal (Mt CO ₂ /year)
1	Manufacture of Building Materials Based on CO ₂	100-1400
2	Enhanced Oil Recovery	100-1800
3	Bioenergy with Carbon Capture and Storage	500-5000

Perbandingan dampak lingkungan terhadap penggunaan minyak bakar berat secara konvensional juga dilakukan. Penggunaan minyak bakar berat dengan cara pembakaran 1000 kg/jam umpan menghasilkan emisi sebagai berikut:

Table 6. Heavy Fuel Oil Combustion Emissions

Component	Flowrate	Unit
CO ₂	850	kg/hour
H ₂ O	110	
SO ₂	40	

These emission results are based on the assumption that combustion occurs completely, so that all ultimate components in the feed are oxidised into non-combustible gases in the form of carbon dioxide, water and sulphur dioxide.

The following is a comparison of the environmental impact of the two heavy fuel oil utilisation methods:

Table 7. Comparison of Environmental Impacts of Heavy Fuel Oil Utilisation Methods

Environmental Impacts	Methode	
	Gasification + 80% CO ₂ Sequestration	Burning
Climate Change Potention (kg CO ₂ eq.)	520	850
Acidification Potention (kgSO ₂ eq.)	0	40

Based on the comparison results, it was found that the environmental impact is minimal when using the gasification method accompanied by CO₂ sequestration. It is assumed that the injected carbon dioxide is 80% of the total emissions and the rest is considered to be released back into the atmosphere.

C. Economic Feasibility Analysis

In evaluating a project, information about the project's economic viability is required. According to [14], There are several factors that control the success of a business. These factors are based on the project's ability to generate profits. An economic evaluation is carried out to determine the following aspects:

- Capital Investment

After evaluation, this hydrogen gas production project requires a total investment capital of IDR 121,243,430,694.96 per year, consisting of fixed investment capital of IDR 103,046,693,204.49 per year.

- Production costs

The production costs required for this project amount to Rp47,193,691,710.60 per year.

- Revenue

On the sales side, if all products are successfully sold, the income that will be obtained per year during the project is IDR 108,776,314,080.00 per year. The net profit that can be reaped after tax deductions is IDR 45,956,031,943.16.

- Return Of Investment (ROI)

By knowing the costs required for production and the profit value, the rate of return on capital can also be determined using the return on investment parameter. From the calculations, the pre-tax and post-tax rates of return on investment were obtained as follows: 59.46% and 44.60%. By referring to the following minimum rate of return reference table, this project is declared feasible because it exceeds the minimum threshold. This project is categorised as a high-risk project because it is classified as a new process.

4. Conclusion

Based on the simulation results, the hydrogen gas production process through heavy fuel oil gasification has been successfully carried out with a final hydrogen gas purity of 98.02% (volume) and a production flow rate of 299.8 kg/hour. The production process involves several main stages, namely: gasification, quenching, conversion, and finally gas purification. An environmental impact analysis was also conducted using the life cycle assessment method. In terms of the environmental impact of the process, hydrogen gas production through gasification contributes to several categories of environmental impact. This hydrogen production process contributes to climate change, soil pollution, eutrophication of marine ecosystems, and water pollution. In addition, the economic aspects of the process were also reviewed. With the Return on Investment parameter, the pre-tax rate of return on this project is 59.46%, which exceeds the minimum threshold of 44%.

Acknowledgment

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Biographies of Authors



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