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Hydrogen Production from Flare Gas via Steam Methane Reforming: A Simulation-Based Approach

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Abstract

Hydrogen gas is receiving significant attention as a versatile and alternative energy carrier with the possibility of being used for different purposes in industries, including power or energy generation, chemical production, transportation, and iron and steel production, with minimal environmental impacts and concerns when produced from renewable and alternative sources. This study investigated hydrogen production from flare gas via Steam Methane Reforming (SMR) using a simulation-based approach. With Nigeria experiencing significant gas flaring challenges, the research explores converting flare gas into a valuable energy resource. Using DWSIM as the simulation tool, the SMR process was modelled under varying conditions of temperature, pressure, and steam-to-carbon (S/C) ratio. Results showed that Nigerian flare gas can achieve hydrogen yields of up to 72.9 mol% and methane conversion efficiencies exceeding 92% under optimal conditions (950°C, 5 bar, S/C = 4.0). The baseline case (850°C, 15 bar, S/C = 3.0) achieved a hydrogen yield of 68.7 mol% with 85.4% methane conversion, validating flare gas as a suitable feedstock for hydrogen production. Sensitivity analysis revealed that higher temperatures and lower pressures favoured hydrogen yield, while the optimal S/C ratio was between 2.5 and 3.5. Environmental impact analysis indicated a potential 27% reduction in CO_2 emissions compared to direct flaring, alongside elimination of unburned hydrocarbons and particulates. These findings demonstrate that flare-to-hydrogen conversion is technically feasible and environmentally beneficial, offering Nigeria a dual pathway to reduce flaring while advancing its clean energy transition.

Keywords: *Hydrogen production; Flare gas; Steam methane reforming; DWSIM simulation; Gas flaring.*

1.0 Introduction

The global energy landscape is changing rapidly, with countries worldwide moving toward cleaner, more sustainable energy sources. Hydrogen has emerged as one of the most promising energy carriers because of its high energy density, versatility, and ability to serve as a clean fuel when used in fuel cells, producing only water as a by-product [1]. Meanwhile, the oil and gas industry, especially in developing countries like Nigeria, continues to struggle with the persistent challenge of gas flaring [2-4]

Gas flaring, which is the controlled burning of associated natural gas during crude oil production, has been a long-standing environmental and economic problem in Nigeria. Despite government policies and international pressure to reduce emissions, Nigeria remains one of the world's highest gas-flaring nations [5]. Reports show that billions of cubic feet of gas are flared annually, resulting in significant financial losses, wasted energy, and environmental damage from the release of greenhouse gases such as carbon dioxide (CO_2) and methane (CH_4). The Niger Delta has particularly suffered from this practice, with local communities experiencing negative health impacts, ecosystem damage, and declining agricultural productivity [6-8].

Converting flare gas into valuable products like hydrogen offers a dual opportunity: reducing environmental harm while contributing to the energy transition agenda. Among the various hydrogen production methods, Steam Methane Reforming (SMR) remains the most commercially viable and widely used process, accounting for over 70% of global hydrogen production [9]. SMR involves the catalytic reaction of methane with steam to produce hydrogen and carbon monoxide, followed by a water-gas shift reaction to maximize hydrogen yield.

Globally, hydrogen plays a critical industrial role in petroleum refining, ammonia and fertilizer production, methanol synthesis, and food processing. Its use in fuel cells has expanded hydrogen's relevance to transportation, while countries such as Japan, Germany, and the United States are investing heavily in hydrogen-based power systems [10-12]. According to the International Energy Agency, global hydrogen demand reached 95 million tonnes in 2022, with projections exceeding 130 million tonnes by 2030 under current energy transition scenarios. The market value is expected to surpass USD 300 billion by 2030, driven by decarbonization targets and the shift towards clean fuels [3, 13-14]

In Nigeria's context, where billions of cubic meters of gas are flared annually, hydrogen production from flare gas presents a dual advantage: reducing emissions while supplying a commodity with growing international demand. Integrating flare gas into SMR has the potential to reduce waste and strengthen Nigeria's position in the emerging global hydrogen economy [15-17]. Modern process simulation tools like DWSIM provide an effective

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platform for modelling these processes, allowing researchers to assess the technical feasibility, efficiency, and environmental impact of flare-to-hydrogen conversion under different operating conditions.

Several studies have investigated hydrogen production, gas flaring reduction, and the role of simulation in process optimization. A comparative study was conducted on the thermodynamic simulations of SMR using DWSIM, COCO, and analytical methods, finding that DWSIM produces hydrogen results within 9% deviation from analytical benchmarks, validating its reliability [18]. A techno-economic study of flare gas-to-hydrogen conversion in Nigeria was conducted using Aspen HYSYS, emphasizing economic feasibility but not addressing DWSIM-based simulation [19]. Optimization of SMR parameters using a genetic algorithm, achieving a methane conversion of 67% under conditions of approximately 736 K, 20 bar, and S/C = 7.96, was also conducted, demonstrating the importance of parameter optimization [20].

However, few studies have focused specifically on flare gas as a feedstock using DWSIM, which defines the gap addressed in this research. This work explores the potential of converting Nigerian flare gas into hydrogen through SMR using an accessible, open-source simulation platform, evaluating the effects of key operating parameters on process performance.

This study investigates hydrogen production from flare gas via steam methane reforming using a simulation-based approach with specific objectives of analysing typical flare gas compositions in Nigeria, developing a simulation model of SMR using flare gas feedstock in DWSIM, and evaluating the effect of operating parameters (temperature, pressure, and steam-to-carbon ratio) on hydrogen yield.

2.0 Experimental Section

2.1 Research Design

This research was designed as a simulation-based study aimed at evaluating the technical feasibility of producing hydrogen from flare gas through Steam Methane Reforming (SMR). The study adopts a quantitative research design, making use of computational modelling and process simulation to analyze performance under different operating conditions. The advantage of this design lies in its ability to replicate real process behaviour without requiring costly laboratory equipment or pilot plants.

The research workflow begins with a review of typical flare gas compositions reported in the Nigerian oil and gas industry, followed by the selection of an appropriate thermodynamic model within DWSIM. A sensitivity analysis was incorporated into the design to examine the effect of varying temperature, pressure, and steam-to-carbon (S/C) ratio on hydrogen production. This approach allows the study to identify operating windows that maximize hydrogen yield while minimizing emissions.

2.2 Flare Gas Composition Data

The flare gas composition used in this study is based on data reported from Nigerian oilfields, particularly in the Niger Delta region, where gas flaring remains widespread. Flare gas is not a pure stream but a complex mixture of light hydrocarbons, non-hydrocarbon gases, and impurities. Its composition varies depending on the crude oil source, production conditions, and the efficiency of gas-oil separation facilities.

For the purpose of this research, a representative flare gas composition was adopted from published reports and industry data [2, 9]. The baseline molar composition assumed in the simulation includes: Methane (CH_4): 75%, Ethane (C_2H_6): 7%, Propane (C_3H_8): 4%, Carbon dioxide (CO_2): 6%, Nitrogen (N_2): 5%, Hydrogen sulfide (H_2S): 1%, and traces of higher hydrocarbons (<2%).

This composition reflects a typical Nigerian flare stream dominated by methane, with minor amounts of heavier hydrocarbons and non-combustible gases. Methane serves as the primary feedstock for hydrogen production, while the presence of CO_2 and H_2S introduces challenges related to process efficiency and potential catalyst poisoning in real-world applications.

2.3 Simulation Setup (DWSIM)

The simulation was conducted in DWSIM using the following setup: Peng-Robinson equation of state as the thermodynamic package, Gibbs Reactor for SMR, Equilibrium Reactor for water-gas shift (WGS), and a separator block to model Pressure Swing Adsorption (PSA) for hydrogen purification. The parameters varied included: Temperature (700-1000°C), Pressure (3-25 bar), and Steam-to-Carbon ratio (2-4).

The Peng-Robinson equation of state was selected due to its reliability for hydrocarbon systems at moderate pressures and elevated temperatures. This model accurately predicts phase behaviour and reaction equilibria under reforming conditions while handling both light hydrocarbons and polar compounds like water and carbon dioxide.

2.4 Process Flow Configuration

The process flow diagram consists of a flare gas feed, steam generator, reformer, water-gas shift reactor, separator (PSA), and hydrogen product stream. The initial mixer unit operation combined the flare gas feed stream with superheated steam at the specified steam-to-carbon ratio. The primary reforming reactor was modelled using

DWSIM's Gibbs reactor, which calculates equilibrium compositions by minimizing Gibbs free energy. The WGS reactor was modelled using an equilibrium reactor operating at 400°C to convert carbon monoxide and steam into hydrogen and carbon dioxide.

2.5 Governing Reactions

The key reactions modelled in this study include:

Steam Methane Reforming: $CH_4 + H_2O \rightarrow CO + 3H_2$ ($\Delta H° = +206$ kJ/mol)

Water-Gas Shift Reaction: $CO + H_2O \rightarrow CO_2 + H_2$ ($\Delta H° = -41$ kJ/mol)

Higher hydrocarbons (ethane, propane) present in flare gas undergo analogous reforming reactions producing hydrogen and carbon oxides. The endothermic nature of SMR reactions requires high temperatures for favourable equilibrium, while the exothermic WGS reaction operates effectively at lower temperatures.

2.6 Validation Approach

Validation of simulation results is critical to ensure the reliability of the findings. In this study, the validation approach is based on comparison with published literature and theoretical expectations. The hydrogen yields, methane conversion rates, and CO_2 emissions obtained from the simulation were compared with values as reported in literature [18, 21]. The results were also cross-checked against the predictions of Le Chatelier's principle and established equilibrium behaviour.

DWSIM has been validated in prior studies as a reliable tool for simulating SMR and other chemical processes [6]. By triangulating simulation outputs with theoretical expectations and published data, this study ensures that its results are credible and reflective of real-world process behaviour, despite the absence of laboratory or industrial validation.

3.0 Results and Discussion

3.1 Baseline Simulation Performance

The DWSIM simulation successfully modelled the conversion of a representative Nigerian flare gas composition into a hydrogen-rich product stream. The baseline simulation, conducted at 850°C, 15 bar, and a steam-to-carbon ratio of 3.0, achieved promising results that validate the concept of flare-to-hydrogen conversion. Under these conditions, the integrated SMR-WGS system achieved a hydrogen yield of 68.7 mol% with a methane conversion efficiency of 85.4%. Table 1 presents the complete baseline simulation results.

Table 1: Baseline Simulation Results

Parameter	Value	Unit
Feed Temperature	25	°C
Reformer Temperature	850	°C
WGS Reactor Temperature	400	°C
System Pressure	15	Bar
Steam-to-Carbon Ratio	3.0	-
Methane Conversion	85.4	%
Hydrogen Yield	68.7	mol%
Carbon Monoxide Content	12.3	mol%
Carbon Dioxide Content	15.2	mol%
Unreacted Methane	3.8	mol%

These results demonstrate that flare gas can serve as a viable feedstock for hydrogen production, with performance comparable to conventional natural gas streams as reported in literature (10, 19 & 22). The baseline methane conversion of 85.4% significantly exceeds the 67% due to higher operating temperature and water-gas shift integration [22]. This conversion rate falls within the 80-95% range typical of industrial SMR+WGS systems, validating the simulation's performance prediction capabilities.

3.2 Simulation Validation and Benchmarking

To ensure the reliability of the DWSIM simulation results, a comprehensive validation was conducted by comparing key performance indicators with published literature on complete steam methane reforming processes with water-gas shift integration. The hydrogen yield of 68.7 mol% obtained in the baseline case compares favourably with conventional SMR processes. Literature reports for complete SMR+WGS systems typically achieve 65-75% hydrogen content [19], placing the current results in the middle of this range. Table 2 presents the comprehensive literature comparison.

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Table 2: Literature Comparison and Validation

Parameter	This Study	Literature Range	Reference	Deviation (%)
Methane Conversion (%)	85.4	80-95	[1, 23]	Within range
Hydrogen yield (mol%)	68.7	65-75	[18]	Within range
CO Content (mol%)	12.3	8-15	[21]	Within range
Optimal Temperature (°C)	850-900	800-900	[23]	Within range
Optimal S/C Ratio	2.5-3.5	2.5-3.5	[19]	Exact match

The relatively low CO content of 12.3 mol% in the product stream demonstrated effective water-gas shift performance. Industrial SMR+WGS systems typically reduce CO content to 8-15% before final purification, confirming that the simulation accurately represents integrated reforming and shift operations. All simulation results demonstrate thermodynamic consistency with established equilibrium behaviour for integrated SMR+WGS systems.

3.3 Effect of Temperature on Hydrogen Yield

Temperature emerged as the most influential parameter affecting hydrogen production from flare gas. As the reformer temperature increased from 700°C to 950°C, there was a marked improvement in both methane conversion and hydrogen yield. At the lower end of this range, around 700°C, the hydrogen content in the product stream remained at 58.2 mol%, indicating incomplete conversion of the methane-rich flare gas. However, as temperatures approached 850-900°C, hydrogen yields improved dramatically, reaching 72.9 mol% at 950°C. Table 3 shows the detailed temperature sensitivity analysis results.

Table 3: Temperature Sensitivity Analysis Results

Temperature (°C)	Methane Conversion (%)	Hydrogen Yield (mol%)
700	65.8	58.2
750	72.4	62.1
800	78.9	65.7
850	85.4	68.7
900	89.7	71.2
950	92.1	72.9

This behaviour aligns well with the endothermic nature of the steam reforming reaction, where higher temperatures drive the equilibrium toward product formation. The simulation results confirm what Le Chatelier's principle predicts: increasing temperature favors the forward reaction, leading to greater methane conversion and hydrogen production. Interestingly, the rate of improvement as seen in Table 3 on an average of 3% yield increase began to plateau beyond 900°C, suggesting that extremely high temperatures may not justify the additional energy costs in practical applications. This finding is consistent with industrial practice, where most commercial SMR units operate in the 800-900°C range to balance conversion efficiency with economic considerations.

The strong influence of temperature on hydrogen yield observed in this study is consistent with thermodynamic expectations and agrees with the findings [22], who optimized SMR parameters and reported significant increases in methane conversion at elevated temperatures. Similarly, the observed plateauing of hydrogen yield above 900°C [21] emphasized the diminishing benefits of excessively high reforming temperatures due to energy penalties.

3.4 Effect of Pressure on Hydrogen Yield

The pressure analysis revealed an inverse relationship between system pressure and hydrogen production efficiency. When the reformer pressure was varied from 5 to 25 bar, the simulation showed that lower pressures consistently favoured higher hydrogen yields. At 5-10 bar, hydrogen concentrations reached their peak, while pressures above 20 bar resulted in yields dropping significantly. Table 4 presents the pressure sensitivity analysis results.

Table 4: Pressure Sensitivity Analysis Results

Pressure (bar)	Methane Conversion (%)	Hydrogen Yield (mol%)	CO Content (mol%)
5	91.8	74.3	8.9
10	88.2	71.5	10.6
15	85.4	68.7	12.3
20	82.1	65.9	14.1
25	78.8	63.2	15.8

This trend reflects the fundamental thermodynamics of the reforming reaction, where one mole of methane and one mole of steam produce four moles of products (three moles of hydrogen and one mole of carbon monoxide). According to Le Chatelier's principle, reactions that increase the total number of moles are favoured at lower pressures, explaining why the simulation showed improved performance under these conditions.

The pressure-dependent behaviour of the system, where lower pressures favoured higher hydrogen yields, echoes the results in [18], who demonstrated through thermodynamic modelling that equilibrium limitations reduce hydrogen recovery at elevated pressures. However, while their work focused on purified methane streams, this study shows that the same trend applies to more complex Nigerian flare gas compositions, thereby extending the applicability of their findings.

From a practical standpoint, these results suggest that flare gas reforming systems should be designed to operate at moderate pressures to maximize hydrogen recovery. However, it's worth noting that extremely low pressures might create challenges for downstream processing and hydrogen compression, indicating the need for optimization studies to find the ideal operating window.

3.5 Effect of Steam-to-Carbon Ratio

The steam-to-carbon ratio investigation revealed an optimization curve typical of reforming processes. Starting with an S/C ratio of 2.0, the hydrogen yield was 62.4 mol%, indicating that insufficient steam was available for complete conversion of the carbon-containing compounds in the flare gas. As the ratio increased to 3.0, there was a noticeable improvement, with hydrogen yields reaching 68.7 mol%. This explains the effect of increase in Steam to carbon ration enhanced good combustion minimizing coke formation which is responsible for catalyst deactivation. Table 5 presents the steam-to-carbon ratio analysis results.

Table 5: Steam-to-carbon Ratio Analysis Results

S/C Ratio	Methane Conversion (%)	Hydrogen Yield (mol%)	CO Content (mol%)
2.0	81.2	62.4	18.7
2.5	83.7	65.8	15.2
3.0	85.4	68.7	12.3
3.5	86.8	70.9	10.1
4.0	87.2	71.8	9.2

This improvement occurs because additional steam drives the reforming reaction forward and helps suppress carbon formation, which can deactivate catalysts in real-world applications. Beyond an S/C ratio of 3.5, however, the benefits became marginal, with yields plateauing around 71.8 mol%. This diminishing return pattern suggests that excessive steam primarily increases the energy requirements for steam generation without providing proportional benefits in hydrogen production. The simulation results indicate that an optimal S/C ratio lies between 2.5 and 3.5, balancing conversion efficiency with energy economics.

The importance of the steam-to-carbon (S/C) ratio in maximizing hydrogen yield and minimizing carbon formation was also highlighted in this research, with an optimal range of 2.5-3.5 identified. This outcome is in agreement with the results [10] who demonstrated that higher steam ratios enhance hydrogen yield but at the cost of higher energy requirements for steam generation.

3.6 Carbon Emissions and Environmental Impact

One of the notable aspects of the simulation results was the carbon monoxide and carbon dioxide emissions profile. With the Water Gas Shift reaction converting CO into additional hydrogen and CO_2, the carbon monoxide levels in the product stream were reduced to 12.3 mol% under baseline conditions, representing effective but not complete CO conversion. The remaining CO content reflects equilibrium limitations at the 400°C WGS operating temperature, where complete conversion is thermodynamically constrained.

The simulation also showed moderate CO_2 generation, primarily from the decomposition reactions of heavier hydrocarbons present in the flare gas. While this represents a reduction compared to direct flaring of the gas, the overall carbon intensity could be further improved through integration with carbon capture technologies.

Based on simulation results, each cubic meter of flare gas processed produces 1.1 cubic meters of hydrogen while generating 0.8 cubic meters of CO_2. Direct flaring would produce 1.1 cubic meters of CO_2, representing a 27% reduction in carbon emissions when accounting for the valuable hydrogen product displacement of fossil fuels (that is the ratio of the converted flare gas to yield CO_2 and H_2 gas. The conversion process eliminates release of unburned hydrocarbons, NOx, and particulate matter associated with open flaring. For Nigeria's annual flare volume, this represents elimination of approximately 15.6 million standard cubic feet of NOx and 2,380 standard cubic feet of particulate emissions annually.

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The 68.7% hydrogen yield represents recovery of approximately 85% of the chemical energy content in the original flare gas, significantly higher than the 35-45% thermal efficiency typical of direct flaring for energy recovery. Lifecycle carbon intensity of the flare-derived hydrogen is estimated at 8-12 kg CO_2/kg H_2, substantially lower than conventional SMR from purchased natural gas (9-15 kg CO_2/kg H_2) due to the avoided upstream emissions from gas production and transport.

In terms of environmental implications, this study estimated a 27% reduction in CO_2 emissions compared to direct flaring, which complements the work of [22], who performed a life-cycle assessment and reported significant emission reduction potentials when flare gas is harnessed for hydrogen production. By confirming these environmental benefits through simulation, this research provides further evidence of the sustainability value of flare-to-hydrogen pathways.

4.0 Conclusion

This study successfully demonstrated that hydrogen can be produced from Nigerian flare gas through Steam Methane Reforming using DWSIM process simulation. Representative Nigerian flare gas composition (75% methane, 7% ethane, 4% propane) achieved hydrogen yields of 68.7 mol% under baseline conditions and up to 72.9 mol% under optimal conditions, proving flare gas performs comparably to conventional natural gas feedstocks. A comprehensive simulation model using Peng-Robinson equation of state, Gibbs reactor for SMR, and equilibrium reactor for water-gas shift reactions was developed. The simulation results showed good agreement with literature values. Optimal operating conditions were identified through systematic analysis: temperature range of 850-900°C, pressure range of 5-15 bar, and steam-to-carbon ratio of 2.5-3.5, with maximum methane conversion efficiency of 92.1% achieved at 950°C. Environmental impact analysis indicated 27% reduction in CO_2 emissions compared to direct flaring, alongside the elimination of unburned hydrocarbons and particulate emissions. The process achieved 85% energy recovery from flare gas compared to 35-45% from direct flaring, demonstrating significant sustainability advantages. Overall, the results presented in this study are consistent with literature trends, while also filling a research gap by applying DWSIM, an open-source simulation platform, to model hydrogen production from Nigerian flare gas.

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