Modelling Production of Renewable Energy from Water Splitting High Thermal Electrolysis Processes

Osaretin N.I. Ebuehi, Kingsley Abhulimen, and Daniel O. Adebisin

Abstract — Recently, fuel gas from water has become the center of attention because it is a renewable source of energy and eco-friendly. In this study, the hydrogen gas simulated was obtained from the high-temperature water splitting electrolysis model, because it is more efficient than the low-temperature water splitting electrolysis process. It also releases oxygen as a byproduct. The high-temperature electrolysis model is made up of three loops: primary high-temperature helium loop, secondary helium loop, and high-temperature electrolysis loop. Hydrogen gave a temperature of 27.2°C, a pressure of 49.5 bars, and a molar flow of 84.02MMSCFD. The hydrogen gas from a high-temperature electrolysis model is simulated with a CO₂ gas stream to produce methane and water, also releasing unreacted carbon dioxide and hydrogen. Key parameters such as molar entropy, molar enthalpy, heat flow, and cost flow were evaluated by Aspen HYSYS V8.8. The simulation model used for this work is the Sabatier Process Model. In this model, Continuous stirred tank, Converter, Equilibrium, Gibbs, Plug flow reactors were used to generate methane. The Converter reactor gave the highest yield of methane gas with a mole fraction of 0.2390. Key benchmarks, including temperature, heat flow, cost flow, cost factor were varied to see how they can affect methane gas and other products.

Index Terms — Electrolysis, environment, fuel gas, hydrogen, renewable energy, simulation model, temperature.

I. INTRODUCTION

Renewable energy is the energy obtained from renewable resources, which are naturally renewed during a human period, such as sunlight, rain, wind, tides, waves, and geothermal heat [1]. Renewable energy delivers energy in four vital areas, namely electricity generation, air, water heating/cooling, and transportation [2], [3].

Photovoltaic systems are a renewable energy source that serves as a platform for building an environmental, energy economy [4]-[6]. The power generated from Photovoltaic systems is dependent on climatic conditions. However, the power generated cannot be produced steadily due to changes in weather conditions [7], [8]. A photovoltaic system uses solar panels to convert water into hydrogen and oxygen for electricity generation (Fig.1). Varieties of methods exist for solar hydrogen production, which is electrolysis of water utilizing a solar cell, reforming of biomass, photocatalytic water splitting [9], [10]. Modelling of a water fusion photocatalytic system is bound to use electrolysis in zeolite/aluminum catalyst and Nickel/Cobalt at high

temperatures to aid the water-splitting process with no detrimental effect on the environment. The first step towards photocatalytic water splitting involves the absorption of photons to form electron-hole pairs. A photocatalytic reaction proceeds on semiconductor materials [11], [12]. The highest photochemical stable semiconductors in aqueous solution are oxides, but their band gaps are grand for effective light absorption [13], [14].

Fig. 1. Photocatalytic reactions ensue on semiconductor materials [6], [7].

Semiconductors maintain band structures that distinguish the conduction band from the valence band by a bandgap known which must have an appropriate width. Suppose the energy of incident light is exceeding the bandgap, electrons together with holes arise in the conduction and valence bands respectively [15], [16]. Photo-generated electrons and holes form redox reactions which are analogous to electrolysis. The coal Gasification process provides distinctive and branded technology processes for the water fuel production process of conversion of coal/ waste of products and remediation of coal/waste polluted sites. Gasification deals with the transformation of materials composed of carbon, namely coal, petroleum, biomass, coke into carbon monoxide and hydrogen [15], [17].

The gaseous products generated are used as an energy basis or production of liquid fuels, the choice of gasification technology employed depends on several elements, but coal type is the minimum supply factor, and the choice of gasification technology depends on the coal to be handled [17]. Gasifiers can be divided into three categories depending on the type of reactor bed in which the coal is gasified which are fixed bed, fluidized bed, and entrained flow gasifiers. To determine the optimal gasification process, factors such as feedstock features, standard requirements for clean gas, condition of waste products, operating features, and environmental codification are to be reviewed.

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Methane steam reforming involves the reaction of methane and steam at high temperatures between 700-1100 °C bolstered with nickel-catalyst to yield a mixture of H₂, CO, CO₂, and CH₄. This process is carried out in a reformer. The reformer which consists of steam and methane is widely used in the manufacturing of hydrogen from natural gas [18].

$\text{CH}_4 + \text{H}_2\text{O} \rightleftharpoons \text{CO} + 3\text{H}_2$ Nickel catalyst was used

Nickel is known to possess a high surface- area to volume ratio because of diffusion hindrances due to the effect of operating at intense temperatures between 700-1100 °C. The reaction between methane and steam is endothermic and the change in heat of the reaction is about 206 kJ/mole [18].

Further Hydrogen can be produced through the reaction of carbon monoxide with water through a water-gas shift reaction.

The above reaction is slightly exothermic and the change in heat of the reaction is about -41 kJ/Mol. Steam reforming of gaseous hydrocarbons is perceived as an efficient method to supply fuel for fuel cells. However, it is costlier to assemble, a well-rounded steam methane reforming can generate hydrogen cost-efficiently than auto thermal reforming [19], [20]. The demerits of steam reforming are it decreases carbon dioxide emanations, eradicates carbon monoxide emissions in contrast to flaring of conventional fuels because of amplified efficiency as well as fuel cell features and it may be exorbitant at lesser proportions required for fuel cells [18].

In methane steam reforming, the catalytic fixed bed reaction is introduced with a gas mixture of CH₄ and CH₄O in a molar ratio from 1:3 to 1:4. The industrial reactor is poised with vertical tubes within 10 and 900 with inner widths 7 to 16 cm and dimensions from 6 to 12 m introduced into the radiant furnace compartment. The entrance reactor temperature is 600 °C and pressures vary from 1.5 to 3.0 MPa [17], [18]. The next generation of future energy will be water-based fuel combustion engines, pilot turbine processes, and electric generators.

Therefore, water as an alternative fuel resource would not pollute the air like power plants that burn fossil fuels, and it would allow countries to produce their energy. In this study, we seek to model a water fuel production plant and develop energy-efficient systems that produce energy without being depleted. We seek to model an empirical laboratory-scale water fuel production plant using ASPEN HYSYS V8.8, to measure the compositions of hydrogen, oxygen, methane, carbon dioxide, and water produced, simulate the proposed arrangement of water splitting high thermal electrolysis process and Sabatier process plant systems. We are especially interested in determining the temperature, pressure, and molar flow of hydrogen produced along with other byproducts which were produced.

II. LITERATURE REVIEW

Voitic *et al.* [19] debated the need to use hydrogen as a fuel for transport and power generation. They established

new technologies for efficient production of hydrogen, removal of impurities, and separation processes. Postulates of steam reforming, partial and auto thermal oxidation, and gasification, as well as electrolysis, were dispensed which are required for the production of hydrogen for use in fuel cells.

Armaroli and Balzani [3] proposed the use of hydrogen as a source of fuel for forthcoming decades. They deduced that the transition from fossil fuels to a hydrogen system will require countless scientific and technological problems which will take a large period to realize. They presumed that water splitting by artificial photosynthesis, photobiological methods centered on algae, and grand temperatures via solar power plants are encouraging temperatures, but nowhere near empirical implementation.

Zhou *et al.* [20] supported the idea of splitting water into hydrogen and oxygen by electrolysis using electricity obtained from waste heat, wind, and solar energy. The dissociation of water into hydrogen and oxygen was aided by a stable oxygen evolution reaction catalyst made of amorphous interwoven Ni/Fe (Oxy) hydroxide nanowire array was constructed at room temperatures by an easy technique.

Ellabban *et al.* [1] studied the importance of renewable energy resources as well as the application of renewable energy resources, the findings to enhance renewable research-based energy, upcoming possibilities, and implementation. They mooted on the environmental pollution problems due to release from industrial plants, vehicle exhaust fumes, fossil fuels, natural means and came to an agreement that these practices are not sustainable in the long run as exposure to high concentrations of air pollutants could lead to health impacts like respiratory infections.

Kudo and Miseki [9] examined the ground of photocatalytic water splitting, laboratory findings, or deductions and reviewed heterogeneous photocatalyst materials for water dissociation into H₂ or O₂ development via aqueous solution involving a prepared reagent. It was observed that the quantity of photocatalyst available was very sufficient and the familiar light-driven photocatalysts were CdS and WO₃ for H₂ and O₂ development.

Terada *et al.* [15] succeeded in the sampling of water from Yugama Crater Lake at Kusatsu- Shirane volcano, Japan with the aid of a drone. They successfully tested 250ml of water from Yugama Crater Lake during tranquil weather in Kusatsu-Shirane volcano. They contrasted the lake water obtained via the drone to that obtained by, hand close to where basic sampling had been performed. It was observed that the chemical concentrations and unvarying isotope ratios were coherent amid the two methods.

Adeli *et al.* [4] focused on the optimization of thermal and electrical proficiency of solar photovoltaic thermal collectors. They constructed a laboratory framework of an archetypal PV/T air collector to determine thermal and electrical values. It was concluded that there is excellent accordance between simulated and experimental results.

III. METHODOLOGY

The study method used in modelling water fuel production plant using high-temperature electrolysis as per the method of [18]. The research was carried out with the aim of

modelling and simulating a water-splitting process using high-temperature electrolysis and simulation of the production of methane by employing the Sabatier Process [20].

A. Equipment and Operating Conditions for Research Flow Loops

Tables I-IV and Fig. 2 illustrated the operating conditions of the three loops (primary, high-temperature helium loop, secondary helium loop as well as high-temperature electrolysis process loop) employed in this study. Temperatures, pressures, and flows of the primary loop used in the study are illustrated in Table I.

TABLE I: THE TEMPERATURES, PRESSURES, AND FLOWS OF THE PRIMARY LOOP

Stream	Temperature (°C)	Pressure (MPa)	Flow (kg/s)
1 – Reactor Outlet	590	7.07	321
2 – Turbine Inlet	950	7	279
3 – Pre-cooler Inlet	129	2.77	279
4 – Pre-cooler Outlet	26	2.74	279
5 – Turbine Outlet	600	2.8	279
6 – Low-Pressure Outlet	93	4.31	279
7 – Intermediate Heat Exchanger Outlet	950	7	42
8 – High-Pressure Recuperator Outlet	575	7.07	279
9 – High-Pressure Compressor Inlet	26	4.27	279
10 – High-Pressure Compressor Outlet	104	7.14	279
11 – Reactor Inlet	590	7.07	321
12 – Primary Side Circulator Outlet	689	7.07	42
13 – Intermediate Heat Exchanger Inlet	679	6.93	42

The power and heat flows of the primary loop used in the study are illustrated in Table II.

TABLE II: THE POWER AND HEAT FLOW OF THE PRIMARY LOOP

Stream	Temperature (°C)	Pressure (MPa)	Flow (kg/s)
14 – Intermediate Heat Exchanger Inlet	292	6	18.1
15 – Intermediate Heat Exchanger Outlet	917	5.94	18.1
22 – HX4 Outlet	854	5.88	18.1
23 – HX2 Outlet	280	5.76	18.1
27 – HX3 Outlet	530	5.82	18.1

The power and heat flow of the secondary helium loop is presented in Table III.

TABLE III: THE POWER AND HEAT FLOW OF THE SECONDARY HELIUM LOOP

Component	Power or Heat Flow (kW)
Reactor, Heat	600,000
Turbine Power	510,215
High-pressure Compressor Power	114,959
Low-pressure Compressor Power	98,676
Primary Side Circulator Power	2,224
Recuperator Duty	683,261
Pre-cooler Cooling	149,424
Intercooler Cooling	97,489
Intermediate Heat Exchanger Duty	58,730
Secondary Side Circulator Power	1,154
Intermediate Heat Exchanger Duty	58,730
HX2 Duty	23,473
HX3 Duty	30,440
HX4 Duty	5,971

The proposed arrangement for the Water Splitting Process Model used for the study is schematically illustrated in Fig. 2 and Fig. 3.

Fig. 2. The proposed arrangement of the Water Splitting Process Model.

Fig. 3. The proposed arrangement of the Water Splitting Process Model.

For this study, a high-temperature electrolysis (HTE) plant integrated with a high-temperature helium reactor was constructed using Aspen HYSYS V8.8 process modelling software. The process set up in the model comprises three loops namely: a primary high-temperature helium loop, a secondary helium loop, and a high-temperature electrolysis process loop.

The primary loop contained helium, which passed through the reactor and provided cooling for the high-temperature reactor fuel by taking away 600 MW of thermal power from the reactor center. High-temperature helium exiting the reactor is then divided into two streams, with a little amount of the proceed (13%) distributed to an intermediary heat exchanger which serves as a medium for providing heat to the high-temperature electrolysis process streams and bulk of the flow stream transiting to the Brayton- cycle gas turbine which produces electrical power. Then the major flow stream was cooled down with the use of a recuperator along with a circulating pre-cooler heat exchanger. The vapor was compressed to maximum pressure as it passed through the high-pressure compressor. Heating took place when it passed through the recuperator.

The final streamlet was commingled alongside the exit flow of the intermediate heat exchanger before getting into the reactor. The second proceeds passed through an intermediary heat exchanger where the amount of warmth was moved to the secondary helium loop, during which the flow was constructed through the primary side circulator.

Tables I and II showed the markers derived in the primary loop.

The secondary helium loop made up on the edge of the

intermediate heat exchanger consisted of a unit of three supplementary process heat exchangers. The two other heat exchangers served as a source of warmth to the hydrogen edge of the high-temperature electrolysis process and the leftover heat exchanger stimulated vapor which was utilized to brush oxygen from the electrolysis process.

Tables III and IV explained the conditions calculated for this loop. The last loop was the high-temperature electrolysis process. A special type of make – up water was forced to the electrolysis pressure in the liquid phase and was connected to the reused water. The Adam's ale was raised to a point where phase changes occurred by the heat exchanger employed (1). The heat from the heat exchanger (2) heated the residual liquid during which the reused hydrogen was introduced to the streamlet. The constituents of the stream following hydrogen addition were 10% hydrogen and 90%, steam via mole grounds and this was paramount to ensure equilibrium in lower conditions.

Heat exchanger HX3 increased the temperature of hydrogen electrodes of the electrolysis cells. It also increased the temperature of the vapor mixture to the appropriate temperature electrolysis. A high-Temperature Heater supplied additional heat for the electrolysis process. The hydrogen streamlet exiting the electrolysis process is 90% hydrogen and 10% vapor on a mole ground. The water from the hydrogen exiting the electrolysis process was condensed using the heat exchanger HX1 and the hydrogen stream was divided into two different streams. The first steam obtained contained hydrogen product and the second stream obtained was reused hydrogen added before the start of the electrolysis process.

The sweep gas was generated by tapping water to the electrolysis pressure. The water was heated and superheated in the heat exchanger HX5. The steam was additionally heated in a heat exchanger HX4 to the electrolysis temperature by supplying heat from the helium secondary loop. Modular Helium reactor functioned with a coolant vent temperature of 950 °C, the vapor was chilled in heat exchanger HX5 to a point where changes in the phase began

to occur. The water was discharged at a high-pressure H₂O/O₂ knockout Tank and then increased through a turbine to atmospheric pressure. The stream was additionally chilled in the low-pressure H₂O/O₂ knockout tank to the ambient temperature and water was discharged from the stream.

The proposed arrangement for the Sabatier Process Model is presented in Fig. 4.

Fig. 4. The proposed arrangement of the Sabatier Process Model [20].

IV. RESULT

These were the results obtained from the water-splitting simulation and Sabatier process simulation. The simulations were carried out using Aspen HYSYS V8.8. High-temperature electrolysis involved the dissociation of steam into hydrogen and oxygen at elevated temperatures. These were the results of process analyses performed to evaluate the temperature, pressure, the molar flow of hydrogen product which were 27.20 °C, 49.50 bars, and 84.02MMSCFD for n High-temperature electrolysis plant attached to a 600 MW Modular Helium Reactor that gives both the electricity and process heat desired to operate the process. The sweep gas or oxygen out was 862 °C, with a pressure of about 50 bars, 65.73MMSCFD. The hydrogen product obtained from the water-splitting process simulation was used to create the Sabatier process simulation. It was reacted with carbon dioxide to produce methane and water. The mole fractions of carbon dioxide, methane, hydrogen, and water were determined to fully know the amount of methane produced.

The types of reactors used, and compositions of methane generated are presented in Table IV.

TABLE IV: THE TYPES OF REACTORS USED AND COMPOSITIONS OF METHANE GENERATED

Reactors used	Mole fraction of methane generated
Equilibrium Reactor	0.1283
Converter Reactor	0.2390
Continuous Stirred Tank Reactor	0
Gibbs Flow Reactor	0.1282

Plug Flow Reactor 0

A. Operating Parameters of Methane Generated

The operating parameters of methane generated include Actual gas flow (ACT_m3/hr.), Temperature (°C), cost factor (cost/kg mole), cost flow, heat flow (kJ/h), molar enthalpy (kJ/kg mole), and molar entropy (kJ/kg mole-C) which had a significant effect on the methane produced and were evaluated to obtain the best product yield.

Fig. 5. The temperature against the actual gas flow for methane and other products.

Fig. 6. Combined Graph of actual gas flow against pressure, and temperature against pressure for methane and other products.

Fig. 10. Graph of actual gas flow against molar entropy of methane and other products.

V. DISCUSSION

Throughout the reaction, the Steam/Hydrogen out of the heat exchanger three with a temperature of 772 °C and a pressure of 50.50 bars and a molar flow of 95.89MMSCFD was monitored before going into the high-temperature heater at a ΔT of 55 °C and 50.0 kPa. The high-temperature electrolysis process was carried out at a temperature of 827 °C and 50.0 bars for the steam to be split into hydrogen and oxygen. The energy stream for the electrolysis heat inflow was -2.408×10^9 kJ/h while the energy stream for the electrolysis power was 2.920×10^5 kW.

Fig. 2 and Fig. 2.1 showed the proposed arrangement of a water-splitting plant, and also showed the dissociation of steam into hydrogen and oxygen at elevated temperatures. The hydrogen gas product produced a molar flow of 84.02MMSCFD at a temperature of 27.20 °C and 49.50 bars.

The hydrogen gas generated was reacted with carbon dioxide at a temperature of 300 °C, at a pressure of 30 bars, with a molar flow of 4700MMSCFD to produce methane gas and water. Various reactors were used to find out the best production of methane gas. An equilibrium reactor produced a mole fraction of 0.1283 methane gas, a converter reactor produced a mole fraction of 0.2390 methane gas, a continuous stirred tank reactor produced mole fraction of 0.0000 methane gas, a Gibbs flow reactor produced a mole fraction of 0.1282 methane gas, and a plug flow reactor produced a mole fraction of 0.0000 methane gas.

It can be deduced that a converter reactor is an ideal reactor for the high production of methane gas with a mole fraction of 0.2390. The vessel temperature and pressure were 1039 °C and 120 bars. It was deduced to be accompanied by an exothermic reaction with a ΔE of -165.0 kJ/Mol.

Fig. 5 showed the plot of temperature against the actual gas flow of methane generated using Aspen HYSYS. We deduced that as the temperature of the product stream increased, the actual gas flow decreased. This relationship is inversely proportional in the sense that when the temperature of CH_4 , CO_2 , H_2 , and H_2O decreased the actual gas flow of CH_4 , CO_2 , H_2 , and H_2O increased.

Fig. 6 showed a plot of actual gas flow against the pressure of methane generated using Aspen HYSYS. We denoted that when the actual gas flow increased, a notable decrease in pressure was observed. This relationship is inversely proportional meaning that a decrease in the flow of CH_4 ,

Fig. 7. Combined graph of actual gas flow against cost factor, and cost flow against cost factor for methane and other products.

Fig. 8. Graph of heat flow against the actual gas flow for methane and other products.

Fig. 9. Graph of heat flow against molar enthalpy of methane and other products.

CO₂, H₂, and H₂O will lead to an increase in pressures of CH₄, CO₂, H₂, and H₂O.

Fig. 7 represented the graph of actual gas flow against cost factor and cost flow against cost factor for methane and other products. The graph of cost flow against the cost factor was constant all through the process.

Fig. 8 illustrated the graph of heat flow against the actual gas flow of methane generated using Aspen HYSYS. Using arbitrary values from the Aspen HYSYS V8.8, when the heat flow was increased from -1.550e+010 kJ/h to -1.660e+010 kJ/h for CH₄, CO₂, H₂, H₂O, the actual gas flow increased from 2.500e+005 (ACT_m³/h) to 2.700e+005 (ACT_m³/h). We denoted that heat flow increased, the actual gas flow also increased.

Fig. 9 showed a plot of heat flow against molar enthalpy using Aspen HYSYS. As the heat flow increased, the molar enthalpy increased. Heat flow is proportionate to the molar entropy. When the heat flow of CH₄, CO₂, H₂, and H₂O increased from -2.030e+010 kJ/h to -1.950e+010 kJ/h, the molar enthalpy increased from -1.200e+005 kJ/kg mole to -1.150e+005 kJ/kg mole.

Fig. 10 represented the graph of Actual Gas Flow against molar entropy using Aspen HYSYS. With the use of arbitrary values, as the gas flow decreased from 8000e+005 (ACT_m³/h) to 6000e+005 (ACT_m³/h), the molar entropy increased from 165.0 bar to 168.0 bar. Therefore, the actual gas flow was inversely proportional to molar entropy.

VI. CONCLUSION

Consumption of petrol as a source of energy is a serious environmental issue. Production of hydrogen gas from water fusion processes can be viewed as one of the strategic studies to overcome this problem. The major benefit of high-temperature electrolysis over conventional low-temperature electrolysis is that considerably higher hydrogen production efficiencies can be achieved. Performing the electrolysis process at elevated temperatures gives the effect of an encouraging process at elevated temperatures, which generates appreciative thermodynamics for electrolysis, more effective generation of electricity.

In this study, the water-splitting electrolysis process at high temperature was simulated using Aspen HYSYS gave a hydrogen gas at a temperature of 27.20 °C, a pressure of 49.50 bars, and a molar flow of 84.02MMSCFD. Simulation of hydrogen gas produced in conjunction with carbon dioxide gas stream reacts in a reactor at a temperature of 300 °C and a pressure of 30 bars for the Sabatier process model to run. The reaction is exothermic with a change in enthalpy of -165 kJ/Mol.

It can be concluded that after making use of the following reactors, which were the equilibrium reactor, converter reactor, Gibbs flow reactor, plug flow reactor, and continuous stirred tank reactor, the converter reactor was the best reactor to use because its production of methane generated was higher than other reactors with the mole fraction of 0.2390 of methane gas. It can also be concluded that the vessel temperature was 1039 °C and a vessel pressure of 120 bar. It can be denoted that methane and water were the products while hydrogen and carbon dioxide were the unreacted by-products.

It can be inferred that the temperature was inversely proportional to the actual gas flow, the actual gas flow was inversely proportional to pressure, heat flow was directly proportional to cost flow, and the temperature was directly proportional to the pressure of the product.

It can also be inferred that heat flow was proportionate to actual gas flow, the temperature was also proportionate to pressure, heat flow was directly proportional to the molar entropy, and actual gas flow was inversely proportional to the molar entropy of the product.

It can be concluded that the splitting of water into hydrogen and oxygen by high thermal electrolysis was an uncomplicated and uncluttered technique for the production of hydrogen and an economical way to conserve large amounts of electrical energy.

AUTHOR'S CONTRIBUTION

The manuscript was written with contributions from all authors, and they all gave their approval of the final version of the manuscript.

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