iConclusions https://iconclusions.com/ Conclusions in Engineering

Production of Green Hydrogen: A Sustainable Pathway Toward Clean Energy

Baha I. Elzaki,[1, 2, a)] **Neida Abdallah Abdelgawi**,[2] and **Badraldeen Gaffar Sulfab**[2]

[1)] *School of New Energy and Intelligent Networked Vehicle, University of Sanya, China*

[2)] *Chemical Engineering Department, College of Engineering, Karary University, Sudan*

ABSTRACT: The production of green hydrogen is a promising sustainable pathway toward clean energy, offering a carbon-free alternative to conventional fuels. This study utilizes Aspen HYSYS simulation to analyze the mass and energy balance, entropy changes, and the effects of key process variables on the efficiency of hydrogen production via electrolysis. The simulation results demonstrate the impact of temperature on entropy, revealing that higher temperatures lead to increased entropy and energy losses. Additionally, the molar flow of reactants significantly influences reactor efficiency and hydrogen yield. The molar concentration of potassium hydroxide (KOH), used as an electrolyte, enhanced hydrogen production by improving conductivity, although it also affects the system's entropy. The findings underscore the importance of optimizing operating parameters, such as temperature and KOH concentration, to achieve maximum hydrogen production efficiency with minimal energy losses. This study affirms the viability of green hydrogen as a clean energy solution through process optimization and highlights its role in advancing sustainable energy technologies.

Received: 02 March 2025
Accepted: 05 Dec. 2025
DOI: https://doi.org/10.71107/xxwy7x08

I. INTRODUCTION

There has been a severe development in energy demand in recent decades, introducing increasing pressure on the energy field[1,2]. Carbon-rich fuels such as oil, gas, and coal have met with success because several advantages distinguish them: the large number of areas of their uses, the high rate of energy they produce, and the ease of storage and transportation[3–5]. Green hydrogen is produced from clean or renewable energy, and hydrogen is considered one of the most efficient fuels[6–8]. Recently, there has been renewed interest in the issue of global climate change, produced by the emission of a considerable amount of greenhouse gases (GHGs)[9]. The main challenge faced by many researchers is producing green hydrogen in an environmentally friendly method, using renewable and clean energy sources[6,10].Production of green hydrogen has been studied by many researchers using different methods of production such as electrolyzed cell, alkaline electrolysis, and polymer electrolyzes, flow sheet of production process showed in figure fig. 1[11,12]. Green hydrogen can play an essential role in addressing the issue of climate change by reducing the emission of greenhouse gases[13,14].

Recently, there has been renewed interest in Nanotechnologies used in the production of green hydrogen to improve quality, efficiency, and economic cost. The key important factor of hydrogen production is the hydrogen economy. Hydrogen production technologies are commercially available, while some are still under development. In 2017, Gaoqiang Yang et al. manufactured the SS 316L bipolar plate with parallel flow channels using SLM technology. This study used electrodes (anode and cathode) in the electrolysis cell and showed high results in terms of operating voltage of up to 1.779 V at 2 amperes /cm2. The results show that the weight percentages of the elements deviate only slightly from those in the raw powder, with minimal oxidation. The study did not show the analysis conditions nor the amount

---

[a)] Electronic mail: bahaelzaki@sanya.edu.cn of hydrogen produced[13]. In 2020, Chennm Ting Lee, et al, developed a new catalyst for the photocatalytic cell, MgTiP titanium phosphate treated with magnesium salt, with the use of seawater. After adjusting the pH and photocatalysis of a cell, hydrogen was produced at a rate of up to 629.3μ mol$\cdot$ g$\cdot$cat$^{-1}\cdot$ h^{-1}. The study did not mention the amount or intensity of the beam nor the amount of water used in the cell[14]. The study presented here is one of the investigations to explore producing green hydrogen by using an electrolyzed cell in modeling software (Aspen Hysys). The simulation's energy source was solar energy, as an important renewable energy.

II. METHODOLOGY

Green hydrogen, produced by the electrolysis of water using renewable energy, represents a critical step in the transition to clean energy. Using the commercial process simulator Aspen HYSYS® (Version 10, Aspen Technology Inc., USA), an end-to-end steady-state model of the process is developed. fig. 1 shows the process flow-sheet for hydrogen production from water.

A. Process Flow Setup

The primary chemical reaction for green hydrogen production via electrolysis is the splitting of water into hydrogen (H_2) and oxygen (O_2). This reaction is powered by renewable energy sources (wind energy). The stoichiometric reaction is as follows:

$$2H_2O \rightarrow 2H_{2(g)} + O_{2(g)} \quad (1)$$

B. Component Selection

The key components, namely water (H_2O), hydrogen (H_2), and oxygen (O_2), are selected from the Aspen HYSYS component library.

C. Electrolyzer Modeling

Aspen HYSYS lacks a built-in electrolyzer model; a Stoichiometric reactor can simulate the electrolysis process. The electrolysis reaction is defined based on the conversion of water into hydrogen and oxygen, and the conditions of the reactor are shown in Table I.

Accordingly, we have introduced the appropriate conditions for the process and made some improvements to raise the efficiency of hydrogen production and reduce energy consumption, and this is shown in the following table II

III. RESULTS AND DISCUSSION

A. Materials Balance

In this study, the water (H_2O) is the primary feedstock. Electricity: Energy is supplied to split water molecules. We can perform a basic material balance based on stoichiometry as shown in question (1) for water electrolysis. Every mole of water, 2 moles of hydrogen gas, and 1 mole of oxygen gas are produced. The results of the materials balance are shown in table III, with the purity of hydrogen from electrolysis being very high at 99.8%.

B. Energy Balance

The energy required for electrolysis is significant. The energy balance for water electrolysis is shown in Table IV below. This energy requirement can be met through renewable energy sources, ensuring that the hydrogen produced is considered "green" hydrogen. The energy balance of the hydrogen production process indicates that significant energy is stored in the hydrogen product, far exceeding the stated 6529 kJ/h. However, in typical electrolysis processes, the energy input is higher, and efficiencies are around 75%.

C. Effect of Temperature

The results in Figure 2 showed that the case study in Aspen HYSYS simulation has provided the entropy values and the change in entropy of the hydrogen system as the temperature rises from 50°C to 90°C. This is consistent with the expected behaviour, as an increase in temperature typically leads to an increase in molecular disorder, and thus, an increase in entropy.

D. Effect of Reactor Efficiency

The molar flow rate of reactants (water in electrolysis) can significantly impact the reactor's performance. Higher molar flow rates generally increase the throughput, but they can also lower residence time in the reactor, which could reduce conversion efficiency if not optimized. Simulation in Aspen HYSYS the molar flow rates are specified in the material streams feeding into the reactor as shown in fig. 3a. By altering the molar flow rate, you can observe changes in conversion efficiency, reaction rates, and overall hydrogen production. Balance the flow rates with operating conditions (temperature, pressure) to maintain reactor efficiency has been adjusted by Aspen simulation. In fig. 3b, the effect of entropy changes on the reactor efficiency is calculated in HYSYS using built-in thermodynamic packages. The results showed that monitoring entropy generation across each unit operation and optimizing for

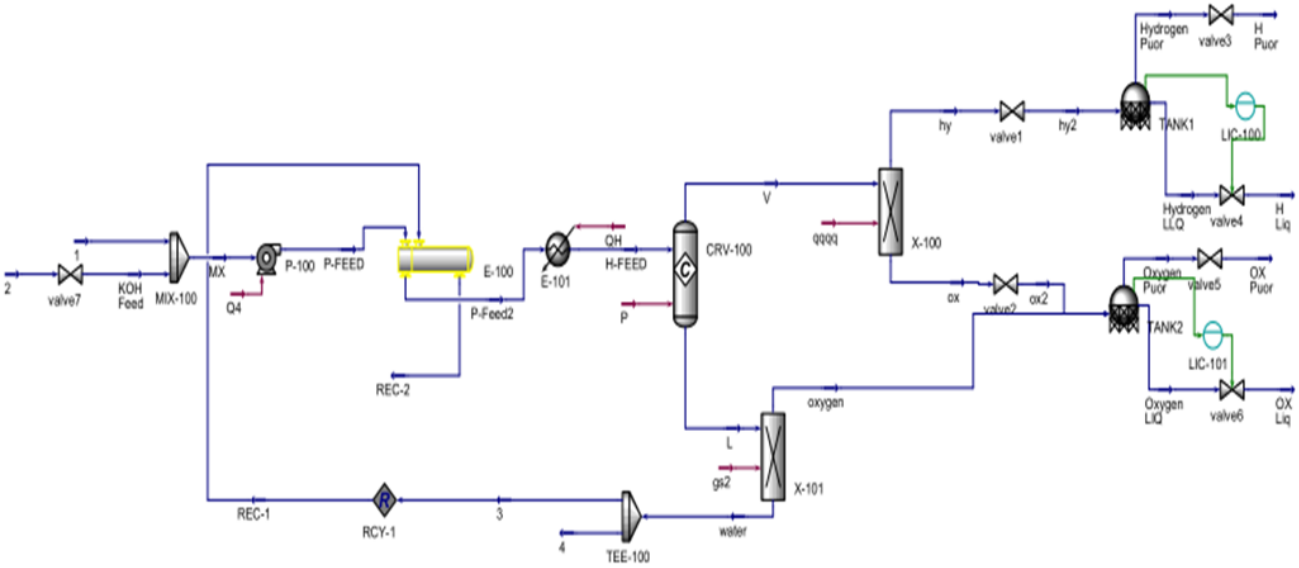


FIG. 1: Process flow sheet for green hydrogen production.

TABLE I: Reaction conditions in the mixer (MIX-100).

Name	**Conditions**	**KOH feed**	**Mix**
Temperature (°C)	25.00	25.00	34.68
Pressure (kPa)	101.33	101.33	101.33
Molar Flow (kgmole/h)	55.51	9.02	64.53
Mass Flow (kg/h)	1000.0	300.0	1300.0
Molar Enthalpy (kJ/kgmole)	-2.858×10^5	-3.588×10^5	-2.960×10^5
Molar Entropy (kJ/kgmole·°C)	-163.2	-165.3	-159.4
Heat Flow (kJ/h)	-1.587×10^7	-3.237×10^6	-1.910×10^7

TABLE II: The conditions of Materials streams

Conditions	Stream -1		Stream -2	
	Overall	Aqueous phase	Overall	Aqueous phase
Vapour / Phase Fraction	0.00	1.00	0.00	1.00
Temperature (C)	25.00	25.00	25.00	25.00
Pressure (kPa)	101.3	101.3	101.3	101.3
Molar Flow (kgmole/h)	55.51	55.51	9.022	9.022
Mass Flow (kg/h)	1000	1000	300.0	300.0
Std Ideal Liq Vol Flow (m3/h)	1.002	1.002	0.2067	0.2067
Molar Enthalpy (kJ/kgmole)	-2.858e+5	-2.858e+5	-3.588e+5	-3.588e+5
Molar Entropy (kJ/kgmol-C)	-163.2	-163.2	-165.3	-165.3
Heat Flow (kJ/h)	-1.587e+7	-1.587e+7	-3.237e+6	-3.237e+6
Liq Vol Flow @Std Cond (m3/h)	1.001	1.001	0.1753	0.1753

TABLE III: Materials balance in hydrogen production simulation.

Inlet Material	Mass Flow	Outlet Material	Mass Flow
Stream 1	1000 kg/h	Stream 4	120.1 kg/h
Stream 2	300.0 kg/h	H_2 Pure	11.05 kg/h
		O_2 Pure	87.72 kg/h
		REC-2	1081 kg/h
Total Inlet	**1300 kg/h**	**Total Outlet**	**1300 kg/h**

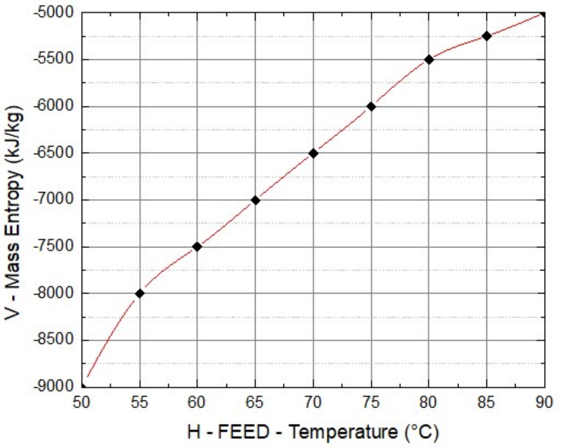
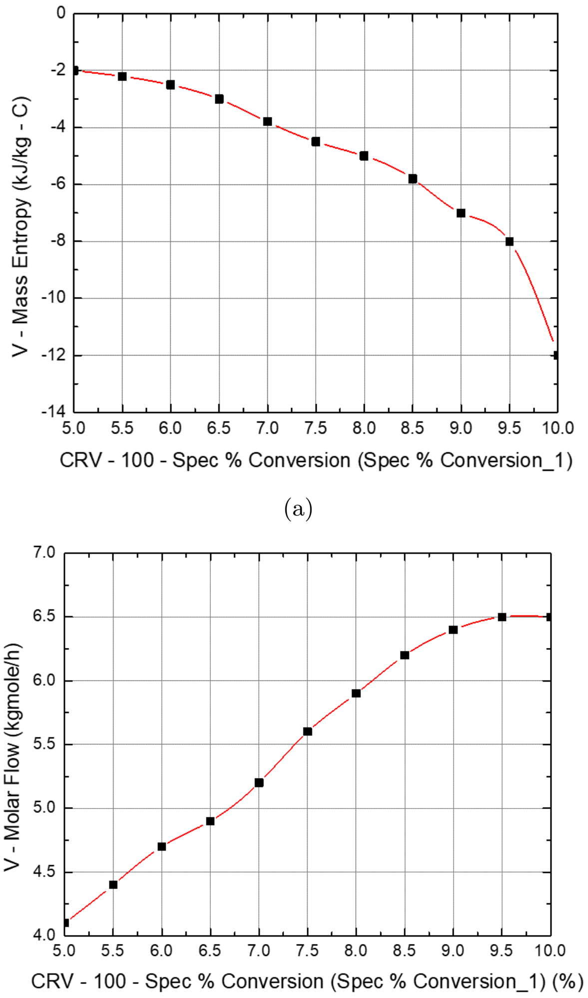


FIG. 2: The change in entropy with changes in temperature.

lower entropy production, thus enhancing system efficiency.

E. Effect of KOH Concentration

Aspen HYSYS simulation for the production of green hydrogen, involving potassium hydroxide (KOH), changes in the molar number of KOH can affect both entropy and the molar properties of the reaction products, such as hydrogen gas. This typically happens through a series of complex interactions between the chemical species, their thermodynamic properties, and the energy balances within the system. The concentration of KOH in the electrolyte solution increases the ionic strength, improving the conductivity of the solution as shown in fig. 4a. The entropy of the product increased due to increased molar number of KOH . Potassium hydroxide works to enhance the electrolysis efficiency, enabling faster production of hydrogen. With more KOH , the electrolysis reaction can proceed more efficiently, possibly increasing the molar flow rate of hydrogen gas as shown in fig. 4b.



(a)

(b)

FIG. 3: Reactor efficiency with changes in mass entropy (a) and molar flow (b)

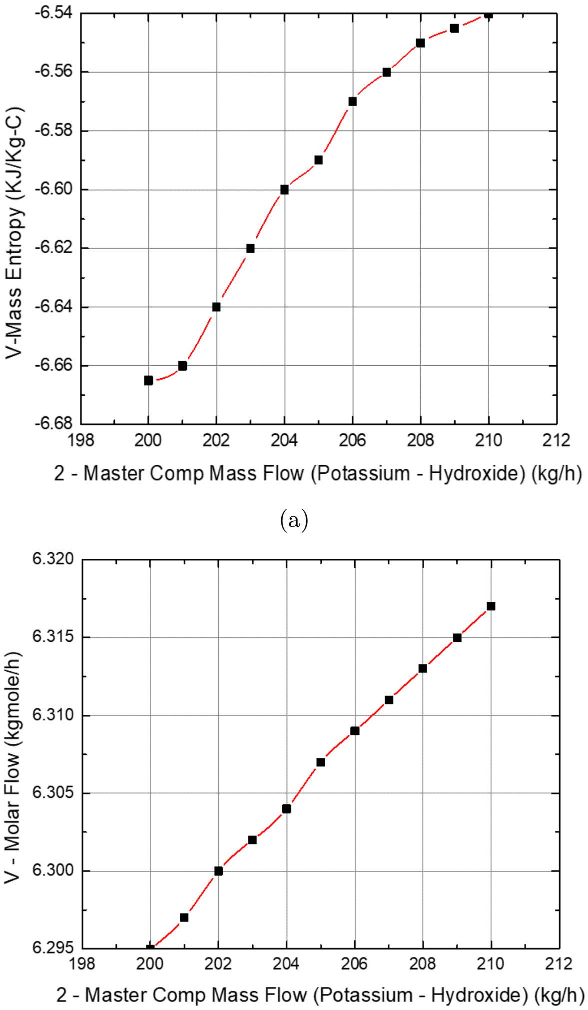
IV. CONCLUSION

The simulation results from the production of green hydrogen using Aspen HYSYS provide valuable insights into the mass and energy balance, entropy changes, and the effects of key process parameters on efficiency:

- The process is sensitive to the energy inputs, with the molar flow rate of hydrogen being influenced by temperature and reactor conditions.
- As temperature increases, the entropy of the system rises due to increased molecular disorder, which can impact the overall energy efficiency.

TABLE IV: Energy balance in hydrogen production simulation.

Inlet	**Energy Flow**	**Outlet**	**Energy Flow**
Stream 1	1.587×10^7 kJ/h	Stream 4	-1.739×10^6 kJ/h
P	8.280×10^5 kJ/h	H_2 Pure	-1.319×10^4 kJ/h
Q4	3967 kJ/h	O_2 Pure	-108.1 kJ/h
QH	8.988×10^4 kJ/h	REC-2	-1.571×10^7 kJ/h
Qqq	6529 kJ/h		
Stream 2	-3.237×10^6 kJ/h		
Total Inlet	-1.747×10^7 kJ/h	**Total Outlet**	-1.747×10^7 kJ/h



(a)

(b)

FIG. 4: The effect of KOH concentration on Mass entropy (a), and molar flow (b)

- The reactor's efficiency is strongly affected by changes in molar flow and entropy. Increasing the molar flow of reactants can improve hydrogen production but also raises entropy, reducing energy efficiency.
- The molar number of potassium hydroxide (KOH) plays a significant role in the electrolysis process. Higher KOH concentrations improve electrolyte conductivity, enhancing hydrogen production and reactor efficiency.
- The study's results provide a solid foundation for further research in production of green hydrogen.

DECLARATION OF COMPETING INTEREST

The authors declare no conflicts of interest regarding the publication of this paper.

REFERENCES

[1] A. Mio et al. Sustainability analysis of hydrogen production processes. *International Journal of Hydrogen Energy*, 54:540–553, 2024.

[2] Q. Hassan et al. Green hydrogen: A pathway to a sustainable energy future. *International Journal of Hydrogen Energy*, 50:310–333, 2024.

[3] D. Cao, Y. Sun, and G. Wang. Direct carbon fuel cell: fundamentals and recent developments. *Journal of Power Sources*, 167(2):250–257, 2007.

[4] S. Sikiru et al. Hydrogen-powered horizons: Transformative technologies in clean energy generation, distribution, and storage for sustainable innovation. *International Journal of Hydrogen Energy*, 56:1152–1182, 2024.

[5] T. Hai et al. Assessing and optimizing a cutting-edge renewable-driven system for green hydrogen production/utilization, highlighting techno-economic and sustainability aspects. *International Journal of Hydrogen Energy*, 61:934–948, 2024.

[6] Q. Hassan et al. Renewable energy-to-green hydrogen: A review of main resources routes, processes and evaluation. *International Journal of Hydrogen Energy*, 48(96):37862–37889, 2023.

[7] S. E. Hosseini and M. A. Wahid. Hydrogen from solar energy, a clean energy carrier from a sustainable source of energy. *International Journal of Energy Research*, 44(6):4110–4131, 2020.

[8] B. I. Elzaki et al. Analysis of aviation fuel performance. *Journal of Karary University for Engineering and Science*, 3(1), 2024.

[9] H. K. Mohajan. Greenhouse gas emissions, global warming and climate change. In *Proceedings of the 15th Chittagong Conference on Mathematical Physics*, 2017.

[10] S. E. Hosseini and M. A. Wahid. Hydrogen production from renewable and sustainable energy resources: Promising green energy carrier for clean development. *Renewable and Sustainable Energy Reviews*, 57:850–866, 2016.

[11] A. T. Zamorano et al. Green hydrogen production by photovoltaic-assisted alkaline water electrolysis: A review on the conceptualization and advancements. *International Journal of Hydrogen Energy*, 70:753–777, 2024.

[12] S. S. Kumar and H. Lim. An overview of water electrolysis technologies for green hydrogen production. *Energy Reports*, 8:13793–13813, 2022.

[13] C. Li and J.-B. Baek. The promise of hydrogen production from alkaline anion exchange membrane electrolyzers. *Nano Energy*, 87:106162, 2021.

[14] K. Górecki, M. Górecka, and P. Górecki. Modelling properties of an alkaline electrolyser. *Energies*, 13(12):3073, 2020.