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(Research Article)

Simulation and Optimization Blue Hydrogen Production by Steam Reforming Natural Gas

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Abstract

One of the most significant industrial processes for producing hydrogen is steam methane reforming. It is now essential to integrate carbon capture technology in order to convert to blue hydrogen due to the growing environmental challenges. This study integrates a CO_2 collection unit as a component splitter and PSA hydrogen purification as a component splitter separator to simulate the production of blue hydrogen using Unisim software R390.1. The simulation was run with a steam-to-carbon ratio of 3:1, a reformer outlet temperature of 830°C, and a pressure of 14 bar and water gas shift high temperature 300°C and low temperature 200 °C. The goal of this study is to optimize the process to produce more hydrogen while lowering emissions.

Keywords: Blue Hydrogen; Optimization; Unisim; Steam Reforming; Carbon Capture

1. Introduction

Hydrogen is expected to contribute towards the decarbonrization of the global economy. The high energy content, flexibility, and abundance of this chemical element are reasons why many sectors can benefit from it in the so-called hydrogen economy. However, almost all hydrogen produced today comes from fossil fuels (mostly from natural gas via steam methane reforming) and has a high associated carbon footprint this is known as gray but when emerged with carbon capture knows as blue. Hydrogen production from more environmentally friendly sources has been an area of intensive research for the last years. It began by assigning green and gray “colors” to hydrogen to distinguish between a “nonpolluting” hydrogen production and one with associated carbon dioxide emissions. The definition of green hydrogen is now widely understood as hydrogen produced from water electrolysis powered by renewable energy sources. However, other energy sources could power electrolysis and produce hydrogen with no carbon dioxide emissions, e.g., nuclear energy (1).

Blue hydrogen production via steam methane reforming (SMR) presents a promising pathway for low-carbon energy, yet it faces challenges related to efficiency, environmental impact, and economic viability. The levelized cost of hydrogen (LCOH) for blue hydrogen ranges from 1.62 *to* 2.00/kg, with lifecycle emissions between 3.85 and 5.74 kg CO2-eq/kg H2, significantly influenced by carbon capture technologies like piperazine and advanced flash strippers, which can reduce energy penalties by over 36% compared to traditional methods [2] [3] [4]. Additionally, innovative processes such as sorption-enhanced steam reforming can lower LCOH to approximately £2.85/kg, outperforming other methods like autothermal reforming with carbon capture [5]. The integration of policy incentives, such as the 45Q tax credit, further enhances economic feasibility, while the potential for job creation in hydrogen clusters underscores the socio-economic benefits of scaling up blue hydrogen production [2] [6]. Overall, blue hydrogen's market potential is bolstered

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by its alignment with net-zero goals, though ongoing advancements in technology and supportive policies are crucial for its widespread adoption.

While blue hydrogen offers a transitional solution towards a low-carbon economy, challenges remain. The high energy consumption and costs associated with carbon capture technologies can hinder commercialization. Additionally, the environmental benefits depend heavily on the efficiency of carbon capture and the carbon intensity of the electricity used in the process. As green hydrogen technologies advance and become more cost-competitive, the role of blue hydrogen may diminish unless further innovations and policy support are implemented.

The Unisim software design model simulation steam reforming natural gas to produce hydrogen with optimization factors operation temperature and pressure and steam carbon ratio and that result to increase hydrogen production and improvement process.

2. Methodology

2.1. Process Description

The present study investigates the production of blue hydrogen from natural gas via the steam methane reforming integrated with carbon capture using MDEA absorption and purification via PSA (Pressure Swing Adsorption). The process simulation was implemented using UniSim Design R390.1, steady-state process simulator widely adopted in industrial gas processing applications.

The process flow diagram (PFD) is structured into five main units

- Feed Conditioning Unit: where natural gas is desulfurized and preheated.
- Primary Reforming Reactor: where methane reacts with steam at high temperature and moderate pressure to form syngas.
- Water Gas Shift (WGS) Reactor: to convert CO to CO_2 and increase H_2 production.
- Carbon Capture Unit: using a 30 wt.% MDEA aqueous solvent to selectively absorb CO_2 from the syngas.
- Hydrogen Purification Unit: employing PSA to recover high-purity hydrogen (≥99.9%).

2.2. Thermodynamic and Reaction Modeling

The Peng Robinson equation of state was selected as the global thermodynamic model for vapor–liquid equilibrium (VLE) calculations. The main chemical reactions in the SMR process were incorporated via conversion reactors and equilibrium reactors depending on the simulation phase

The key reactions modeled are

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2 \qquad \Delta H = +206\, kJ/mol$$

Water-Gas Shift Reaction

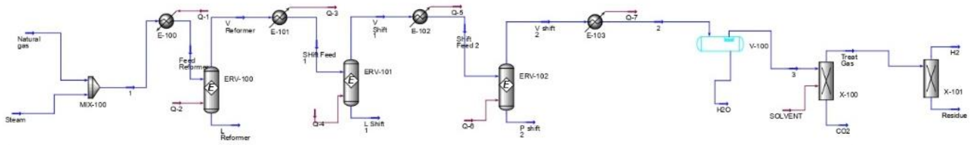
$$CO + H_2O \rightleftharpoons CO_2 + H_2 \qquad \Delta H = -41\, kJ/mol$$

The reforming reaction is highly endothermic and was modeled in a conversion reactor with a base conversion assumption of 80_90 % of methane at reformer temperatures between 800–900 °C, while the water gas shift (WGS) reaction was simulated in an equilibrium reactor operating at 200_300 °C.

2.3. Operating Conditions and Design Basis

The design was based on literature review included the following:

- Reformer temperature: 800–900 °C
- Reformer pressure: 15–30 bar
- Steam-to-carbon ratio (S/C): 2.5–3.1 mol/mol WGS reactor temperature: 200_350°C



Streams											
		Natural gas	Steam	1	Feed Reformer	V Reformer	L Reformer	SHift Feed 1	V Shift 1	L Shift 1	Shift Feed 2
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000	0.0000	1.0000	1.0000	0.0000	1.0000
Temperature	C	500.0	500.0	497.6	820.0	830.0	830.0	300.0	300.0	300.0	220.0
Pressure	kPa	3000	3000	3000	1400	1400	1400	1400	1400	1400	1400
Molar Flow	kgmole/h	100.0	300.0	400.0	400.0	571.5	0.0000	571.5	571.5	0.0000	571.5
Mass Flow	kg/h	1604	5405	7009	7009	7009	0.0000	7009	7009	0.0000	7009
Std Ideal Liq Vol Flow	m3/h	5.358	5.415	10.77	10.77	15.06	0.0000	15.06	17.41	0.0000	17.41
Heat Flow	kJ/h	-5.187e+006	-6.764e+007	-7.282e+007	-6.655e+007	-4.692e+007	0.0000	-5.748e+007	-6.065e+007	0.0000	-6.219e+007
Molar Enthalpy	kJ/kgmole	-5.187e+004	-2.255e+005	-1.821e+005	-1.664e+005	-8.211e+004	-8.211e+004	-1.006e+005	-1.061e+005	-2.535e+005	-1.088e+005
		V shift 2	P shift 2	2	H2O	3	CO2	Treat Gas	H2	Residue	
Vapour Fraction		1.0000	0.0000	0.7734	0.0000	1.0000	1.0000	1.0000	1.0000	0.0000	
Temperature	C	200.0	200.0	5.000	5.000	5.000	5.000	5.000	35.00	-240.3	
Pressure	kPa	1400	1400	1500	1500	1500	300.0	300.0	3500	3.500	
Molar Flow	kgmole/h	571.5	0.0000	571.5	129.5	442.0	84.52	357.5	342.0	15.48	
Mass Flow	kg/h	7009	0.0000	7009	2340	4669	3720	949.3	689.4	259.9	
Std Ideal Liq Vol Flow	m3/h	17.53	0.0000	17.53	2.347	15.18	4.507	10.67	9.869	0.8022	
Heat Flow	kJ/h	-6.273e+007	-0.0000	-7.211e+007	-3.729e+007	-3.482e+007	-3.336e+007	-1.445e+006	9.756e+004	-1.543e+006	
Molar Enthalpy	kJ/kgmole	-1.098e+005	-2.718e+005	-1.262e+005	-2.880e+005	-7.878e+004	-3.947e+005	-4044	285.3	-9.969e+004	

Monday Jun 30 2025, 9:23:19 Case: C:\Users\HP\Documents\UniSim Design R390\Cases\Eq optimization Paper.usc Flowsheet: Case (Main)

Figure 1 Process flow diagram of steam reforming

3. Results and Discussion

High temperatures above the optimal level cause methane cracking and carbon buildup, which slows down the reaction rate. Lowering the temperature below the optimal range also reduces the reaction rate because the process requires heat.

- The observed low pressure increases the reaction rate, but from an operational perspective, it has a minor effect on the reactor and raises costs, so a moderate pressure is used.
- The ideal steam-to-carbon ratio is crucial. If it goes above the recommended value, it leads to higher energy use and costs. If it drops below the necessary level, it causes carbon to deposit on the catalyst, which then decreases the reaction rate.
- The optimal temperature and pressure for the reformer reactor are 830 °C and 14 bar, achieving a methane conversion efficiency of 94%.
- In the water gas shift reactor, the best conditions are 300 °C and 200 °C for high and low temperatures. The final hydrogen production rate reached 344.99 kg-mol/h.

4. Conclusion

The study simulated production of hydrogen by Unisim software and found optimum operation temperature reforming natural gas 830 C and 14 bar pressure. Water gas shift reaction high temperature 300 C and low temperature 200 C final hydrogen from process 344 99kg-mol then carbon capture unit as component splitter and hydrogen purification as a component splitter also. The important is the study came from improvement process economically and environmentally.

The study recommended carry simulation model for heat distribution in reactor.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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