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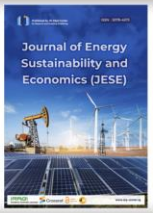

Sensitivity Analysis-Based Simulation and Optimization of Steam Methane Reforming in Aspen Plus for Improved Hydrogen Production

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Abstract

Rising demand for clean energy has increased interest in hydrogen as a sustainable energy carrier due to its high energy content and low emissions. Steam methane reforming (SMR) remains the dominant industrial production method because of its efficiency and economic viability. This study simulates hydrogen production via SMR using Aspen Plus to evaluate reactor performance and operating parameters. The process includes steam generation, reforming reactions, separation, and recycle streams under steady-state conditions. The reformer is modeled using an equilibrium (RGibbs) reactor with the PRSK equation of state. Sensitivity analysis shows that increasing temperature enhances hydrogen yield due to the endothermic reaction, while higher pressure reduces hydrogen production because of equilibrium constraints. Increasing the steam-to-carbon ratio improves methane conversion, though gains diminish at high steam levels. Optimal conditions involve high temperature, low pressure, and moderate steam ratio, producing a hydrogen-rich stream with minimal unreacted methane.

Introduction

The increasing global demand for energy, coupled with the current reliance on fossil fuels and their associated environmental damage and emissions, has spurred the search for alternative energy sources

that are readily available and have minimal environmental impact [1]. Hydrogen is the simplest and most abundant element in the universe, which makes it a promising candidate for widespread use as an energy carrier, despite the challenges in isolating it in pure form on Earth [2]. However, due to its high chemical reactivity, it's never found in its pure form on Earth, always combined with compounds like water, hydrocarbons, alcohols, and biomass[3]. Energy is required to split hydrogen from these molecules, Hydrogen has emerged as a potential solution to global energy problems due to its promising properties Hydrogen is a critical component of the global energy transition and a key to achieving carbon neutrality. Hydrogen higher heating value (HHV) which about 141.8 MJ/kg at 298 K, and its lower heating value (LHV) is approximately 120 MJ/kg, which is significant greater than that of conventional fuels such as gasoline (44 MJ/kg). Hydrogen can be used to store energy for a longer period and facilitate the integration of renewable energy sources into the energy mix [4]. Hydrogen can also be used as a viable alternative to fossil fuels for the decarbonization of sectors such as heavy industry, chemicals, steel production, and long-distance transportation while supporting energy security, creating jobs, and driving economic growth Hydrogen is produced using several methods, the most common steam methane reforming (SMR) of natural gas, and over 80% of them depend on the steam conversion of fossil fuels[5].

. Green hydrogen is also produced through the electrolysis of water using renewable energy sources as the power source for the electrolysis process [6]. Therefore, hydrogen produced using these methods are considered clean hydrogen with no associated emissions [7]. Around 55 million tonnes of hydrogen are produced annually globally, increasing at a rate of around 6% annually[8]. A variety of feedstock's, such as natural gas, oil, coal, water, biomass, and industrial by-products, can be used to produce hydrogen. Nowadays, natural gas SMR accounts for almost half of the world's produced hydrogen, following with 30% from oil and naphtha reforming in chemical and refinery sectors, 18% from coal gasification, around 3.9% from water electrolysis[9]. These results in greenhouse gas emissions, making hydrogen produced in its current form not an ideal solution to emissions problems [10]. This study aims to simulate the hydrogen production process using Steam Methane Reforming with Aspen Plus software and to conduct sensitivity analyses of changes in reactor pressure and temperature on the conversion ratio and hydrogen produced.

Steam methane reforming:

Steam methane reforming (SMR) is currently the most widely used and cost-effective method for producing hydrogen on an industrial scale. Its widespread adoption is mainly due to its high efficiency and relatively low operating and production costs [11]. Natural gas is the primary feedstock used in this process, although lighter hydrocarbons, methanol, and other oxygenated compounds can also serve as raw materials.

The SMR process generally consists of two main stages. In the first stage, the hydrocarbon feed is mixed with steam and introduced into a tubular catalytic reactor [12]. Under high temperatures, the reaction produces synthesis gas (syngas), which is mainly composed of hydrogen and carbon monoxide, with a relatively small amount of carbon dioxide. Heat required for the reaction is typically supplied by partially combusting a portion of the feed using air or oxygen. In the second stage, the produced gas mixture passes through a water–gas shift reactor, where carbon monoxide reacts with steam to form additional hydrogen and carbon dioxide. To prevent catalyst deactivation, the feedstock must be free from sulfur-containing compounds [13]. Operating conditions vary depending on the feedstock; temperatures may be as low as about 180 °C for methanol reforming but usually exceed 500 °C for conventional hydrocarbons. Catalysts used in SMR are mainly classified into two categories: precious metal catalysts (such as platinum and rhodium) and non-precious metal catalysts, particularly nickel-based systems [14].

Although noble metals show excellent catalytic performance, their high cost limits industrial use, making nickel catalysts the most practical and commonly used option. In conventional reformers, heat and mass transfer limitations often control reactor performance rather than reaction kinetics, further supporting the use of economical nickel catalysts [15].

The main reaction involved in methane steam reforming is an endothermic process:

$$CH_4 + H_2O \leftrightarrow CO + 3H_2$$

This reaction produces up to three moles of hydrogen per mole of methane. Additional hydrogen can be generated through the water–gas shift reaction:

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

Because methane molecules contain strong C–H bonds, high temperatures (typically 700–1100 °C) and pressures between 3 and 35 bar are required to achieve efficient conversion. Increasing the steam-to-methane ratio improves hydrogen production but also raises energy consumption. At lower temperatures, carbon deposition becomes more significant, leading to catalyst deactivation [16].

Catalyst design plays a critical role in improving SMR performance. Supports such as alumina, silica, spinel structures, zirconia, and ceria enhance catalyst stability, reduce coke formation, and improve resistance to sintering [17]. Bimetallic catalysts and promoter additives are also used to increase activity, selectivity, and durability. Despite these improvements, sulfur poisoning, carbon deposition, and particle sintering remain major operational challenges [18].

Recent research has focused on process intensification techniques to improve hydrogen yield and energy efficiency. Membrane reactors, for example, allow selective removal of hydrogen or carbon dioxide, shifting the reaction equilibrium toward greater hydrogen production, with yields exceeding 90% in some cases [19]. Carbon dioxide capture methods using chemical absorbents or membrane technologies also show promising potential for reducing emissions.

Industrial SMR processes typically achieve thermal efficiencies of around 70–85%; however, a key disadvantage is the significant production of carbon dioxide, approximately 7 kg of CO_2 per kg of hydrogen produced [20]. To address this issue, new approaches such as electrically assisted catalysis, structured catalysts with improved heat transfer, microwave heating, and the use of renewable biomethane or biomass-derived feedstocks are being explored [21]. These developments aim to make SMR more sustainable while maintaining its economic advantages as the leading hydrogen production technology [21].

METHODOLOGY:

Process Description:

The steam methane reforming (SMR) process was simulated using Aspen Plus to evaluate hydrogen production performance under different operating conditions. The developed process flow diagram consists of steam generation, reforming reaction, gas–liquid separation, and recycle streams designed to represent a simplified industrial hydrogen production system.

Water was first introduced into a steam generator (STGEN), where it was converted into superheated steam. The steam stream was then combined with methane prior to entering the reforming reactor. The methane feed flow rate was fixed at 200 mol/h, while the steam flow rate was maintained at 840 mol/h, corresponding to a steam-to-carbon (S/C) ratio of approximately 4.2, which is commonly employed to suppress carbon deposition and enhance methane conversion.

The mixed feed entered the reforming reactor operating at elevated temperature and pressure conditions. Inside the reactor, methane reacted with steam to produce synthesis gas primarily composed of hydrogen, carbon monoxide, carbon dioxide, and small amounts of unreacted methane.

The reactor outlet stream was directed to a first flash separator (FLASH1) to achieve vapor–liquid phase separation. The vapor phase was further processed in a second flash unit (FLASH2) to obtain a hydrogen-rich gas stream as the main product. Liquid streams from the separation units were combined, partially recycled to improve water utilization, and the remaining fraction was discharged as wastewater. Unreacted methane was recycled to the reactor inlet to improve overall process efficiency and hydrogen yield [fig1].

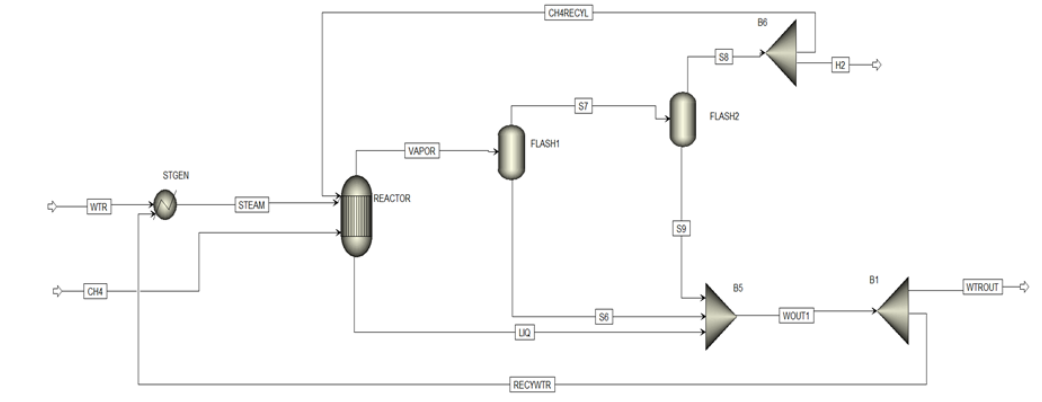

Figure1: steam methane reforming process pfd.

Table 1. Process Units and Their Functions in the Aspen Plus SMR Simulation.

Unit ID	Unit Name	Unit Type (Aspen Plus)	Function in Process
STGEN	Steam Generator	Heater	Converts feed water into steam before entering the reactor
REACTOR	Reforming Reactor	RGibbs (Equilibrium Reactor)	Performs steam methane reforming and water–gas shift reactions to produce syngas
FLASH1	First Separator	Flash Drum	Separates reactor outlet into vapor and liquid phases
FLASH2	Second Separator	Flash Drum	Produces hydrogen-rich gas stream through additional phase separation
B5	Mixer	Mixer	Combines liquid outlet streams from separation units
B1	Splitter	Splitter	Divides water stream into recycle and purge streams
B6	Splitter/Compressor	Gas Handling Unit	Directs hydrogen product and methane recycle stream
Recycle Loop	Recycle Stream	Recycle Block	Returns unreacted methane and water to improve conversion efficiency

Table 2. Process Streams Description and Composition.

Stream Name	Phase	Main Components	Description
WTR	Liquid	H_2O	Fresh water feed entering steam generator
STEAM	Vapor	H_2O	Generated steam supplied to reactor
CH4	Vapor	CH_4	Methane feedstock entering reformer
VAPOR	Vapor	H_2, CO, CO_2, CH_4, H_2O	Reactor outlet vapor stream

LIQ	Liquid	H_2O	Condensed liquid leaving reactor/separator
S7	Vapor	H_2-rich gas mixture	Vapor stream from FLASH1 to FLASH2
S8	Vapor	H_2 (major)	Hydrogen product stream
S9	Liquid	Water + dissolved gases	Liquid stream from FLASH2
WOUT1	Liquid	H_2O	Combined liquid stream before splitting
WTROUT	Liquid	H_2O	Wastewater purge stream
RECYWTR	Liquid	H_2O	Recycled water stream
CH4RECYL	Vapor	CH_4	Recycled unreacted methane back to reactor
H2	Vapor	H_2	Final hydrogen product stream

Simulation Setup:

The SMR process was modeled using Aspen Plus steady-state simulation software. The PRSK (Predictive Redlich–Kwong–Soave) thermodynamic property method was selected to accurately represent vapor–phase behavior and phase equilibria under high-temperature and high-pressure reforming conditions.

The following components were included in the simulation:

- Methane (CH_4)
- Water (H_2O)
- Hydrogen (H_2)
- Carbon monoxide (CO)
- Carbon dioxide (CO_2)

Methane and steam were introduced at flow rates of 200 mol/h and 840 mol/h, respectively. All simulations were performed under steady-state conditions.

Reactor Model and Reaction System:

The reforming reactor was modeled using an equilibrium reactor (RGibbs), which determines product composition by minimizing the Gibbs free energy of the system. This approach assumes that chemical equilibrium is achieved within the reactor and is widely applied for high-temperature reforming processes.

The principal reactions considered in the reactor include:

Steam Methane Reforming (SMR):

$$CH4+H2O \rightleftharpoons CO+3H2$$

The reactor was operated at a base condition of 920 °C and 32 bar, with vapor–liquid phases enabled in the simulation environment [fig 2] [fig 3].

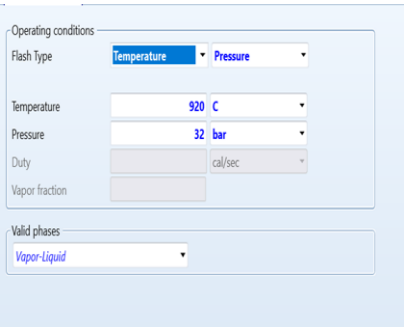

Fig 2. Reactor pressure and temperature conditions.

	Units	STEAM	CH4	
− MIXED Substream				
Phase		Vapor Phase	Vapor Phase	
Temperature	C	237.548	75	
Pressure	bar	32	32	
Molar Vapor Fraction		1	1	
Molar Liquid Fraction		0	0	
Molar Solid Fraction		0	0	
Mass Vapor Fraction		1	1	
Mass Liquid Fraction		0	0	
Mass Solid Fraction		0	0	
Molar Enthalpy	cal/mol	-56385	-17454.8	
Mass Enthalpy	cal/gm	-3129.84	-1088.02	
Molar Entropy	cal/mol-K	-13.5652	-24.9808	
Mass Entropy	cal/gm-K	-0.752984	-1.55714	
Molar Density	mol/cc	0.000855984	0.00112583	
Mass Density	gm/cc	0.0154208	0.0180614	
Enthalpy Flow	cal/sec	-1.31565e+07	-969709	
Average MW		18.0153	16.0428	
+ Mole Flows	kmol/hr	840	200	

Figure 3: Inlet streams to reactor

Sensitivity Analysis

A sensitivity analysis was performed using Aspen Plus to evaluate the influence of reactor operating conditions on hydrogen production in the steam methane reforming (SMR) process. Reactor temperature and pressure were selected as key independent variables due to their strong impact on reaction equilibrium and methane conversion. In addition, the effect of steam feed flowrate was investigated because the steam-to-carbon ratio plays a critical role in hydrogen generation, reaction equilibrium, and catalyst stability.

The investigated operating ranges were:

- Temperature: 900–1200 °C
- Pressure: 26–40 bar
- Steam flowrate: 500–1500 mol/h

During the sensitivity analysis, hydrogen mole fraction and hydrogen production rate were monitored as primary performance indicators. Temperature variation was used to evaluate the thermodynamic limitations of the endothermic reforming reactions, while pressure effects were examined to assess equilibrium shifts and process feasibility under industrial conditions. The steam flowrate analysis was conducted to determine the influence of steam availability on methane conversion and hydrogen formation, as well as to identify the optimal steam-to-carbon ratio that maximizes hydrogen production while avoiding unnecessary energy consumption.

Results and Discussions:

The steam methane reforming reactor was supplied with methane and steam at flow rates of 200 mol/h and 840 mol/h, respectively, corresponding to a steam-to-carbon ratio of 4.2. The reactor outlet stream was entirely in the vapor phase with a total molar flow rate of 1415.12 mol/h, indicating significant generation of gaseous products during the reforming reactions. A substantial change in stream composition was observed between inlet and outlet conditions. While the feed streams consisted of pure methane and steam, the reactor products contained hydrogen, carbon monoxide, residual steam, and a small amount of unreacted methane. The outlet mole fractions were 0.3976 for H_2, 0.1325 for CO, 0.461 for H_2O, and only 0.00879 for CH_4, confirming extensive methane consumption inside the reactor [fig4].

Methane conversion was evaluated based on inlet and outlet molar flow rates. Using the outlet methane mole fraction and total molar flow rate, the remaining methane flow was calculated as approximately 12.43 mol/h, corresponding to a methane conversion of about 93.8%. This high conversion demonstrates efficient reactor performance under the selected operating conditions. The significant hydrogen mole fraction indicates successful progression of the endothermic steam methane reforming reaction, where methane reacts with steam to produce synthesis gas rich in hydrogen. The increase in total molar flow rate from 1040 mol/h at the inlet to 1415.12 mol/h at the outlet further confirms hydrogen formation, as reforming reactions generate additional gas moles.

Carbon monoxide formation with a mole fraction of 0.1325 suggests partial completion of the water–gas shift reaction, which is typical for high-temperature reformers operating near thermodynamic equilibrium. Meanwhile, the relatively high remaining steam fraction indicates operation with excess steam, which helps suppress carbon deposition and enhances catalyst stability but also dilutes the hydrogen concentration in the product gas. Mass and volumetric flow rates increased significantly across the reactor, with outlet volumetric flow reaching 72,852 L/min, reflecting gas expansion caused by hydrogen production. Additionally, the enthalpy flow values confirm the strongly endothermic nature of the reforming process, emphasizing the requirement for continuous external heat supply.

	Units	CH4	STEAM	LIQ	VAPOR	
Molar Enthalpy	cal/mol	-17454.8	-56385		-23014.9	
Mass Enthalpy	cal/gm	-1088.02	-3129.84		-1775.7	
Molar Entropy	cal/mol-K	-24.9808	-13.5652		4.006	
Mass Entropy	cal/gm-K	-1.55714	-0.752984		0.309081	
Molar Density	mol/cc	0.00112583	0.000855984		0.000323743	
Mass Density	gm/cc	0.0180614	0.0154208		0.00419603	
Enthalpy Flow	cal/sec	-969709	-1.31565e+07		-9.0469e+06	
Average MW		16.0428	18.0153		12.961	
+ Mole Flows	**kmol/hr**	**200**	**840**	**0**	**1415.12**	
− Mole Fractions						
H2O		0	1		0.461049	
H2		0	0		0.39762	
CH4		1	0		0.0087906	
CO		0	0		0.13254	
+ Mass Flows	**kg/hr**	**3208.55**	**15132.8**		**18341.4**	
+ Mass Fractions						
Volume Flow	l/min	2960.78	16355.4		72852.1	
+ Vapor Phase						
<add properties>						

Figure 4: Summary of Reactor Stream Results Showing Inlet Streams (CH_4 and Steam) and Outlet Vapor and Liquid Phases

Sensitivity Analysis of reactor temperature:

A sensitivity analysis was performed to evaluate the effect of reactor temperature on hydrogen production performance. The reactor temperature was varied from 900°C to 1200°C, and the response variable (M), representing the hydrogen mole fraction in the product stream, was monitored [fig5 a].

The simulation results indicate a clear positive relationship between reactor temperature and hydrogen production. As shown in Table and Figure (S-1 Results Summary), increasing the reactor temperature leads to a continuous increase in the hydrogen mole fraction. At 900°C, the hydrogen mole fraction was 0.3908. When the temperature increased to 933°C, the value rose to approximately 0.401, indicating a significant improvement in hydrogen formation at relatively small temperature increments. Further temperature increases continued to enhance hydrogen production, reaching 0.4113 at 1000°C [fig 5].

Beyond 1000°C, the rate of increase becomes smaller. The hydrogen mole fraction gradually increases from 0.4135 at 1033°C to 0.4164 at 1200°C. This behavior suggests that the system approaches a thermodynamic limitation where additional temperature increases provide only marginal improvements [22].

The observed trend can be explained by the endothermic nature of the steam methane reforming reaction, where higher temperatures shift the equilibrium toward hydrogen and carbon monoxide formation, thereby enhancing methane conversion and hydrogen yield. Similar behavior was reported by Mozdzierz et al. (2016), who demonstrated that increasing reaction temperature significantly enhances methane conversion, resulting in an increase in hydrogen mole fraction accompanied by a decrease in methane and steam concentrations along the reformer length. This agreement between the present simulation results and previous studies confirms that reactor temperature is a dominant parameter governing reforming equilibrium and hydrogen production efficiency [23].

a

Row/Case	Status	VARY 1 REACTOR PARAM TEMP C	M
1	OK	900	0.390789
2	OK	920	0.39762
3	OK	933.333	0.401216
4	OK	966.667	0.407586
5	OK	1000	0.411328
6	OK	1033.33	0.413494
7	OK	1066.67	0.41475
8	OK	1100	0.415486
9	OK	1133.33	0.415924
10	OK	1166.67	0.41619
11	OK	1200	0.416355

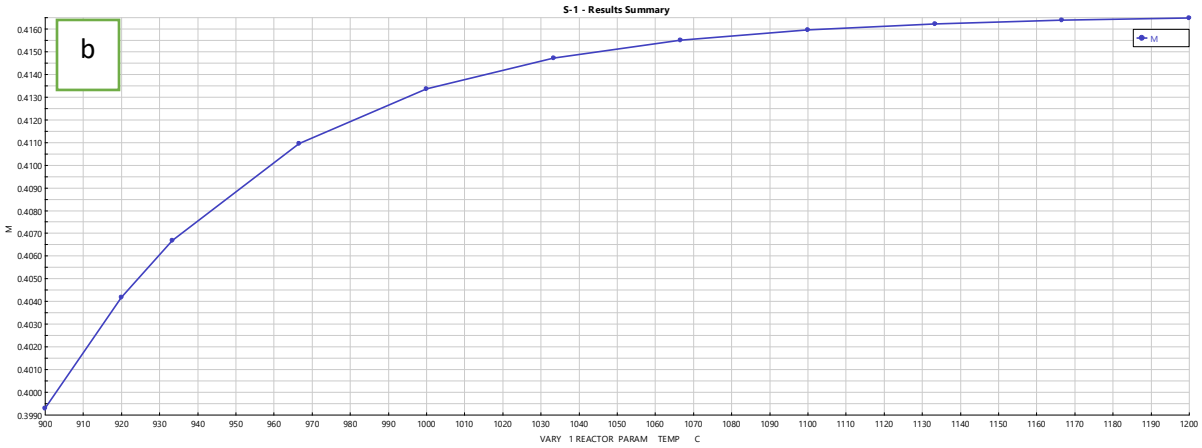

Figure 5. Sensitivity analysis of hydrogen mole fraction in the vapor outlet stream as a function of reactor temperature.

(a) Tabulated results obtained from Aspen Plus sensitivity analysis showing the variation in hydrogen mole fraction using the parameter VARY 1 – REACTOR parameter: temperature.

(b) Graphical representation illustrating the effect of reactor temperature (x-axis) on the hydrogen mole fraction response (y-axis) in the reactor product stream.

Sensitivity Analysis of reactor pressure:

A sensitivity analysis was performed to investigate the effect of reactor pressure on hydrogen production in the steam reforming of methane (SMR). The pressure was varied within the range of 26–40 bar, while other operating conditions remained constant. The hydrogen mole fraction was used as a performance indicator, as an increase in the mole fraction corresponds to an increase in hydrogen production.

The results shown in Figure 6 demonstrate that the hydrogen mole fraction decreases gradually with increasing pressure. At 26 bar, the mole fraction is approximately 0.4033, while at 40 bar, it decreases to approximately 0.3895. This continuous decrease indicates an inverse relationship between reactor pressure and hydrogen production.

This behavior can be explained based on the principles of chemical equilibrium and Le Chatelier's Principle. The steam reforming of methane:

Increases the number of moles of gas from 2 moles in the reactants to 4 moles in the products. As the pressure increases, the equilibrium shifts towards the side with fewer moles, i.e., the reactants, thus reducing hydrogen formation and lowering its molar fraction in the reactor product.[24]

Increasing the pressure also affects the water-gas shift reaction, which relatively limits the formation of additional hydrogen. Therefore, operating at relatively low pressures is more suitable for achieving higher hydrogen production from a thermodynamic perspective [25].

Although higher pressures may be beneficial for reducing the size of industrial equipment and improving subsequent separation processes, the current simulation results show that increasing the pressure leads to a decrease in hydrogen yield within the studied operating range. Based on the sensitivity analysis results, lower pressures within the studied range can be considered more suitable for maximizing hydrogen production in the SMR process [26].

Row/Case	Status	VARY 1 REACTOR PARAM PRES BAR	PC
1	OK	26	0.403294
2	OK	26.4828	0.402858
3	OK	26.9655	0.402417
4	OK	27.4483	0.401973
5	OK	27.931	0.401525
6	OK	28.4138	0.401074
7	OK	28.8966	0.400619
8	OK	29.3793	0.40016
9	OK	29.8621	0.399699
10	OK	30.3448	0.399234
11	OK	30.8276	0.398767
12	OK	31.3103	0.398297
13	OK	31.7931	0.397824
14	OK	32	0.39762
15	OK	32.2759	0.397348
16	OK	32.7586	0.39687

Row/Case	Status	VARY 1 REACTOR PARAM PRES BAR	PC
16	OK	32.7586	0.39687
17	OK	33.2414	0.39639
18	OK	33.7241	0.395908
19	OK	34.2069	0.395423
20	OK	34.6897	0.394937
21	OK	35.1724	0.394448
22	OK	35.6552	0.393958
23	OK	36.1379	0.393466
24	OK	36.6207	0.392973
25	OK	37.1034	0.392478
26	OK	37.5862	0.391981
27	OK	38.069	0.391484
28	OK	38.5517	0.390985
29	OK	39.0345	0.390485
30	OK	39.5172	0.389983
31	OK	40	0.389481

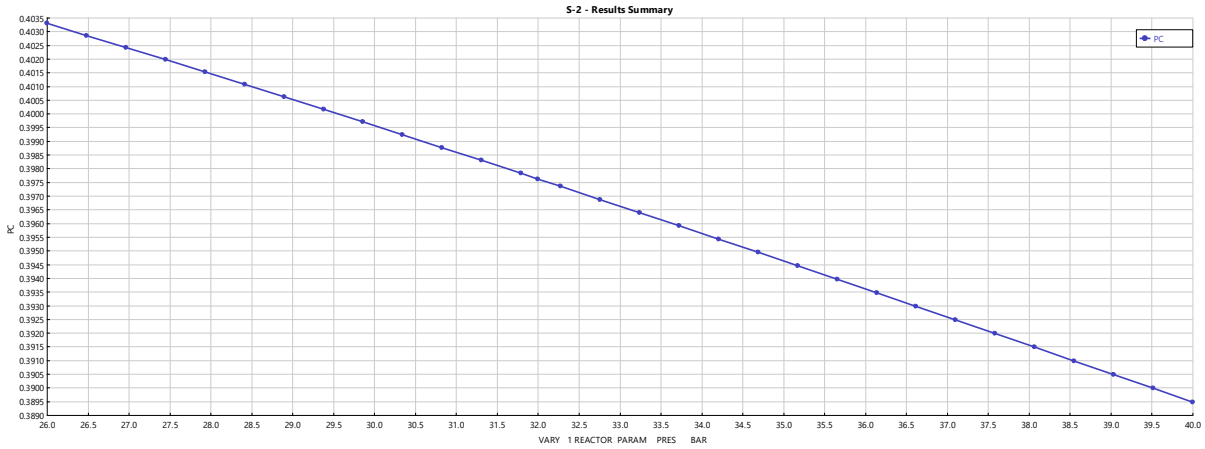

Figure 6: Sensitivity analysis of hydrogen mole fraction in the vapor outlet stream as a function of reactor pressure.

(a) Tabulated results obtained from Aspen Plus sensitivity analysis showing the variation in hydrogen mole fraction using the parameter VARY 1 – REACTOR parameter: pressure.

(b) Graphical representation illustrating the effect of reactor pressure (x-axis) on the hydrogen mole fraction response (y-axis) in the reactor product stream.

Sensitivity Analysis of Steam Flow rate:

A sensitivity analysis was conducted to investigate the influence of steam feed flowrate on hydrogen production in the steam methane reforming reactor. The steam flowrate entering the reactor was varied from 500 mol/h to 1500 mol/h, while other operating conditions were maintained constant, and the resulting hydrogen molar flowrate at the reactor outlet was monitored. The simulation results demonstrate a clear positive relationship between steam flowrate and hydrogen production. As the steam input increased from 500 mol/h to approximately 772.7 mol/h, the hydrogen production increased significantly from 508.05 mol/h to 556.05 mol/h, indicating that additional steam strongly promotes methane conversion during the initial operating range [fig 7].

Further increases in steam flowrate continued to enhance hydrogen generation; however, the rate of improvement gradually decreased. At a steam flowrate of 1045.45 mol/h, hydrogen production reached 576.44 mol/h, while increasing steam to 1500 mol/h resulted in a hydrogen flowrate of 589.86 mol/h. This behavior indicates diminishing returns at higher steam flowrates, where additional steam produces only marginal increases in hydrogen output. The observed trend can be explained by the thermodynamic characteristics of steam methane reforming, an endothermic reaction in which excess steam shifts the equilibrium toward hydrogen formation according to Le Chatelier's principle. Higher steam concentrations also reduce carbon deposition risk and enhance catalyst stability[27][28].

However, once methane conversion approaches equilibrium limits, the system becomes less sensitive to further increases in steam. Excess steam begins to act mainly as a diluent rather than a reactive component, leading to reduced efficiency in hydrogen gain relative to the additional energy required for steam generation and heating [29]. The curve obtained from the sensitivity analysis clearly shows a rapid increase in hydrogen production at low-to-moderate steam flowrates followed by a plateau region beyond approximately 1100 mol/h, suggesting that optimal reactor operation occurs within this intermediate range.

(a)

Row/Case	Status	VARY 1 STEAM MIXED TOTAL MO LEFLOW KMOL/HR	MF KMOL/HR
1	OK	500	508.052
2	OK	590.909	529.1
3	OK	681.818	544.55
4	OK	772.727	556.045
5	OK	863.636	564.71
6	OK	954.545	571.325
7	OK	1045.45	576.44
8	OK	1136.36	580.441
9	OK	1227.27	583.607
10	OK	1318.18	586.14
11	OK	1409.09	588.186
12	OK	1500	589.855

(b)

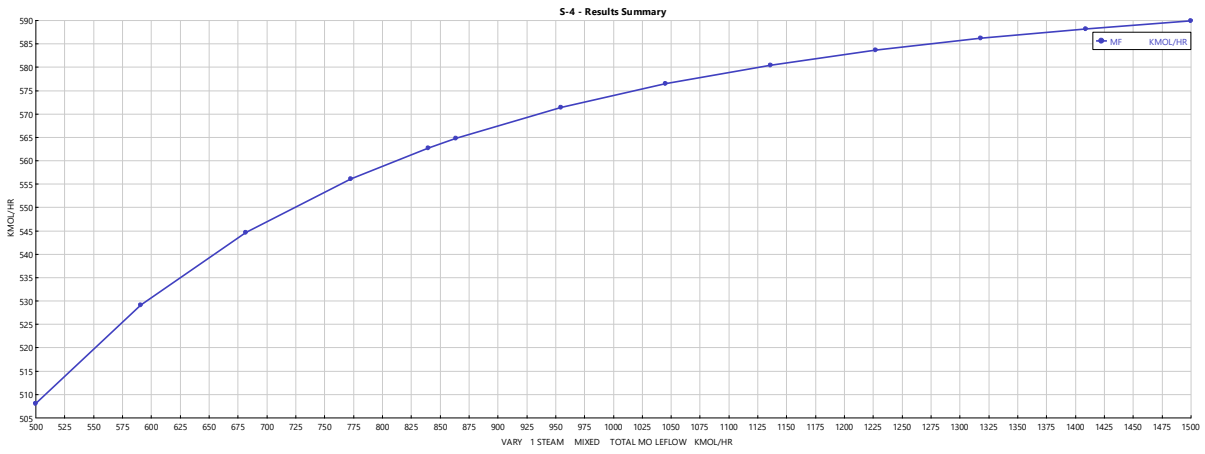

Figure 7. Sensitivity analysis of hydrogen molar flowrate in the vapor outlet stream as a function of steam feed flowrate to the reactor.
(a) Tabulated results obtained from Aspen Plus sensitivity analysis showing the variation in hydrogen molar production using the parameter VARY 1 – inlet steam stream molar flowrate.
(b) Graphical representation illustrating the effect of steam feed flowrate to the reactor (x-axis) on the hydrogen molar flowrate response (y-axis) in the reactor product stream.

Reactor Performance Analysis at Optimum Operating Conditions for Hydrogen Production:
After applying the optimum operating conditions obtained from the sensitivity analysis, the reactor performance showed a significant improvement in hydrogen production and methane conversion. Under these optimized conditions, the total outlet molar flowrate reached 2099.94 mol/h, indicating substantial gas generation as a result of the steam methane reforming reactions. The product stream consisted mainly of steam, hydrogen, and carbon monoxide, with molar flowrates of 1300.03 mol/h H_2O, 599.91 mol/h H_2, and 199.97 mol/h CO, while the remaining methane was extremely low at only 0.02896 mol/h [fig 8]. The negligible methane concentration confirms that nearly complete methane conversion was achieved,

demonstrating that the selected operating conditions successfully shifted the reaction equilibrium toward product formation.

The high hydrogen production rate reflects the strong influence of elevated temperature and optimized steam flowrate identified during the sensitivity analysis. Excess steam promotes methane reforming and enhances the water–gas shift reaction, thereby increasing hydrogen generation while suppressing carbon formation on the catalyst surface. The increase in total molar and volumetric flowrates, reaching 171,137 L/min, further verifies hydrogen formation since reforming reactions increase the number of gas moles in the system. Additionally, the large negative enthalpy flow value confirms the strongly endothermic nature of the process, meaning continuous external heat input is required to maintain reactor operation.

Although hydrogen production reached a high value under optimum conditions, a noticeable amount of carbon monoxide remains in the product stream, indicating equilibrium limitations at high reforming temperatures. This suggests that a downstream water–gas shift reactor would be beneficial to further convert CO into additional hydrogen and improve product purity. Overall, the optimized reactor conditions maximize hydrogen yield while achieving nearly complete methane conversion, confirming the effectiveness of the sensitivity analysis in determining suitable operating parameters for efficient SMR operation.

	Units	VAPOR
Molar Enthalpy	cal/mol	-28057.4
Mass Enthalpy	cal/gm	-1948.93
Molar Entropy	cal/mol-K	4.24169
Mass Entropy	cal/gm-K	0.294637
Molar Density	mol/cc	0.000204509
Mass Density	gm/cc	0.00294418
Enthalpy Flow	cal/sec	-1.63664e+07
Average MW		14.3963
− Mole Flows	**kmol/hr**	**2099.94**
H2O	kmol/hr	1300.03
H2	kmol/hr	599.913
CH4	kmol/hr	0.0289581
CO	kmol/hr	199.971
+ Mole Fractions		
+ Mass Flows	**kg/hr**	**30231.5**
+ Mass Fractions		
Volume Flow	l/min	171137
+ Vapor Phase		
<add properties>		

Figure 8: Reactor stream result after apply optimum condition from sensitive analysis.

Conclusion:

This study presented a comprehensive simulation and performance evaluation of hydrogen production via steam methane reforming (SMR) using Aspen Plus. The developed process model successfully represented the main stages of the SMR process, including feed preparation, reforming reactions, product separation, and recycle operation under steady-state conditions. The Peng–Robinson–Stryjek–Vera (PRSK/PRSK) thermodynamic model was applied to accurately predict phase behavior and reaction equilibrium for the gas-phase reforming system.

Simulation results confirmed that steam methane reforming remains an efficient and reliable method for large-scale hydrogen production. Under the base operating conditions, methane conversion reached approximately 93.8%, producing a hydrogen-rich synthesis gas stream with a significant hydrogen mole fraction. The increase in outlet molar and volumetric flowrates compared to inlet conditions verified the progression of reforming and water–gas reactions, demonstrating effective hydrogen generation within the reactor. The results also emphasized the strongly endothermic nature of the reforming reactions, highlighting the importance of continuous heat supply and thermal management for stable reactor performance.

The sensitivity analysis provided detailed insight into the influence of operating parameters on hydrogen production efficiency. Reactor temperature was identified as the most influential parameter affecting hydrogen yield. Increasing temperature enhanced methane conversion and hydrogen formation due to thermodynamic equilibrium shifting toward product formation in endothermic reactions. Conversely, increasing reactor pressure negatively affected hydrogen production, as higher pressures favor reactants according to Le Chatelier's principle. These findings agree well with industrial SMR operation, where high temperatures and moderate pressures are typically employed.

In addition, steam flowrate played a critical role in determining reactor performance. Increasing the steam-to-carbon ratio improved methane conversion and hydrogen production while reducing the likelihood of carbon formation and catalyst deactivation. However, excessive steam addition resulted in diminishing improvements in hydrogen yield and increased energy consumption associated with steam generation, indicating the existence of an optimal operational range that balances performance and energy efficiency.

Optimization of operating conditions led to nearly complete methane conversion with minimal residual methane in the product stream and hydrogen production approaching 599.9 mol/h. Despite the high hydrogen yield achieved, the presence of carbon monoxide in the reformer outlet indicates the necessity of downstream purification processes, such as the water–gas shift reaction and hydrogen separation technologies, to obtain high-purity hydrogen suitable for fuel cells or clean energy applications.

From an industrial perspective, the study demonstrates the effectiveness of process simulation as a powerful engineering tool for analyzing, optimizing, and predicting SMR reactor behavior without the need for costly experimental trials. The developed model can assist process engineers in evaluating operational trade-offs between temperature, pressure, and steam consumption, thereby improving process efficiency, reducing operational costs, and supporting safer plant operation.

Furthermore, the findings highlight the continuing importance of SMR technology during the global transition toward cleaner energy systems. While SMR is currently dependent on fossil-based feedstocks,

integration with carbon capture and storage (CCS) technologies and renewable heat sources could significantly reduce carbon emissions, enabling low-carbon or blue hydrogen production pathways.

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