Special Design Task

Simulation of SMR Plant for Hydrogen Production in Aspen HYSYS®

University of Bradford

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ABSTRACT

Hydrogen production has seen a steady increase in demand over the last decades. With this increase, there exists a need to analyse H_2 plants through means such as process simulation. In the present work a Steam Reforming Hydrogen plant was modelled in Aspen HYSYS© using Natural Gas as feedstock, producing a final H_2 purity of 99.9% at 400+ t/day. Reaction kinetics were considered within the Steam Reformer. The Shift section consists of High Temperature Shift operating at 500^{o}C, and Low Temperature Shift operating at 200^{o}C, modelled as equilibrium reactors. Validation shows generally accurate model results for Reforming and Shift sections.

CONTENTS

"Hydrogen has been the fuel of the future for decades, always promising to deliver huge benefits in about five years' time." – Forbes, 2020

1 INTRODUCTION

Steam Methane Reforming (SMR) has been in use for several decades and is considered a "benchmark process" for the production of Hydrogen (Speight, 2020).

Though Hydrogen production through hydrolysis has been a well-understood process for well over a century and its efficiency is generally higher compared to SMR, the high capital investment needed for a plant of the same capacity as SMR is still a substantial barrier to entry (CarbonCommentary.com, 2017). Furthermore, the energy used for Hydrolysis is mostly sourced from the commercial electricity grid, which in the UK consists mostly (over 40%) of electricity produced using natural gas as a fuel source (Department for Business, Energy & Industrial Strategy, 2019), essentially ending up with the same fuel source as SMR.

While Hydrogen might be considered the green fuel of the future by some, SMR can in no way be considered a "green" technology. That being said, Carbon Capture and Storage (CCS) development has also seen a significant interest due to policies such as the UK's 2050 Net-Zero Carbon goal: Currently studied CCS systems generally show a potential CO_2 emission decrease of around 85-90% (Leung, et al., 2014).

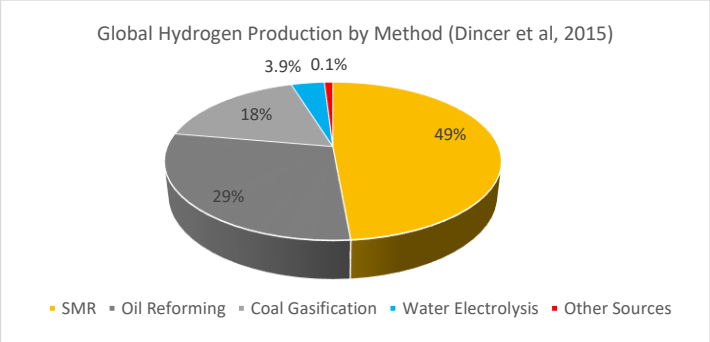

Figure 1: Global Hydrogen Production by Method (Dincer & Acar, 2015)

Whether or not SMR has a place within a green hydrogen economy is debateable, but the statistics (Dincer & Acar, 2015) clearly show that the primary global source of Hydrogen is SMR – therefore the need to examine the process through methods such as process simulation is proven.

2 SELECTION OF SOFTWARE

Aspen HYSYS offers a strong emphasis on Petrochemical and Petroleum Refining. The models that are available include a variety of reactors such as conversion, equilibrium, and PFR models. Also available within the software are separation units such as condensate drums. The software allows for dynamic simulation, with an "active" mode updating the flowsheet results in real-time. Crucially, its main area of application lies in the oil, gas, and energy sector. Natural gas being the feedstock for this plant, it follows that HYSYS is a suitable option for simulation of this process. Further proof supporting that HYSYS is very much capable of simulating Hydrogen plants is the many examples of successful steam reforming simulations such as those by Aspen Tech, or Durán et al (2020).

The full name of software and version is listed in *Table 1*.

Table 1

Software Name	Version
Aspen HYSYS®	V11 (37.0.0.395)

3 METHODOLOGY

The Pre-Reforming reactions were considered to follow the general equation (Speight, 2020):

$$C_nH_m + nH_2O \rightleftharpoons nCO + \left(\frac{m}{2} + n\right) H_2$$

Additionally, the SR, DSR, and WGSR reactions are considered within the SR (Rashid, et al., 2017).

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

$$CH_4 + 2H_2O \rightleftharpoons CO_2 + 4H_2$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

The only reaction considered within the shift reactors is the name-giving Water-Gas-Shift-Reaction, as seen above (equation X).

The entire list of equations – alongside their specified type and reaction set within HYSYS – is listed below in *Table 2*.

Table 2: Reaction Sets With Their Corresponding Equations

Reaction Set	Reaction	Reaction Type	Equation	Reaction No.
Set-1	PR-1	Conversion	$C_2H_6 + 2H_2O \rightarrow 2CO + 5H_2$	(1)
	PR-2		$C_3H_8 + 3H_2O \rightarrow 3CO + 7H_2$	(2)
	PR-3		$C_4H_{10} + 4H_2O \rightarrow 4CO + 9H_2$	(3)
	PR-4		$C_5H_{10} + 5H_2O \rightarrow 5CO + 11H_2$	(4)
	PR-5		$C_6H_{14} + 6H_2O \rightarrow 6CO + 13H_2$	(5)
	SR		$CH_4 + H_2O \rightarrow CO + 3H_2$	(6)
Set-2	SR	Kinetic	$CH_4 + H_2O \rightarrow CO + 3H_2$	
	DSR		$CH_4 + 2H_2O \rightarrow CO_2 + 4H_2$	(7)
	WGSR	Equilibrium	$CO + H_2O \leftrightarrow CO_2 + H_2$	(8)
Set-3	WGSR	Equilibrium	$CO + H_2O \leftrightarrow CO_2 + H_2$	

3.1 Assumptions Made

[1] Steady state and isothermal process.
[2] Ideal gas behaviour.
[3] No heat losses were considered.
[4] Reverse reactions were not considered, except for WGSR (equilibrium based).
[5] Pressure drops only considered within Heaters, Coolers, and Shift Reactors (200kPa for all).
[6] Outlet pressure of mixing streams set to be equal to lowest of inlet streams.
[7] Feed stream considered to be completely de-sulphurised.
[8] All streams with names “0”,”00”,”000” have no molar flow.
[9] Streams “H2O-1”, “H2O-2” are pure steam, with “H2O-3” being pure liquid water.
[10] 5% of Hydrogen Product gets adsorbed within PSA (95% H_2 recovery).
[11] PSA can achieve purity of 99.9+% (Fahim, et al., 2010)

3.2 Feed

Natural Gas compositions vary widely, therefore the feed composition must be clearly defined. The feed NG composition was chosen to be representative of raw natural gas from Norway, as this is the primary source of Natural Gas for the United Kingdom. The composition of the feed stream is listed in *Table 3*.

Table 3

Component	Formula	Mole Fraction
Methane	CH_4	0.9381
Ethane	C_2H_6	0.0452
Propane	C_3H_8	0.0038
n-Butane	C_4H_{10}	0.0004
n-Pentane	C_5H_{12}	0.0002
n-Hexane	C_6H_{14}	0.0003
Water	H_2O	0
Carbon Monoxide	CO	0
Carbon Dioxide	CO_2	0.0047
Hydrogen	H_2	0
Nitrogen	N_2	0.0073

Inlet conditions of the NG stream as well as steam streams are listed in **Table 4**.

Table 4: Feed Conditions

Stream Name	Pressure (kPa)	Temperature (^oC)
NG	2800	35
H2O-1	2300	550
H2O-2	2000	950

Calculation of Steam feeds is done simply by performing a brief Carbon (C) balance on the NG stream and multiplying by the desired ratio. As some water leaves the PR, the water already present in Stream 4 (4199 kmol/h) is subtracted to achieve the correct ratio in the SR feed. *Table 5* lists ratio alongside the calculated feed flowrate for steam.

Table 5: Calculation of Required Steam via S/C Ratio

Block	Carbon Balance (kmol/h)	Desired S/C Ratio	Required Steam Feed (kmol/h)	Stream
PR	2255	2.5	2255*2.5 = 5638	H2O-1
SR	2255	4	(2255*4)-4199 = 4822	H2O-2

3.3 Reactions

Aspen HYSYS offers a variety of reactor models, including conversion, equilibrium, and Gibbs reactors. Crucially, HYSYS also offers a detailed model for Plug-Flow reactors, which is the type SRs generally use, therefore it was chosen as the model for the main SR. *Table 6* lists all blocks and their type, alongside their reactions.

Table 6: Blocks Used For HYSYS Simulation Including Description

Block	Type	Reactions	Description
PR	Conversion Reactor	PR-1 through PR-5, SR	Reforms heavier hydrocarbons with 100% conversion. Exception: SR (Methane) at 60% conversion.
SR	PFR	SR, DSR, WGSR	Kinetic reactions for SR and DSR. WGSR is equilibrium-based.
HTS	Equilibrium Reactor	WGSR	Equilibrium-based modelling of WGSR reaction at operating temp of 550^{o}C.
LTS	Equilibrium Reactor	WGSR	Equilibrium-based modelling of WGSR reaction at operating temp of 350^{o}C.
D-1	Drum	Separation only	Separation of Water and Syngas. 0.3mol% water still present in outlet.
PSA	Splitter	Separation only	Hydrogen and Nitrogen in outlet only.

The kinetic factors for SR and DSR reactions occurring within the PFR (*SR*) as shown by Rashid et al are listed in *Table 7*. It is worth noting that the basis for both reactions is defined as "Partial Pressure", the base units are "kPa", and the rate unit is kmol/m^{3}s, as defined by the source literature.

Table 7: Pre-Exponential Factors and Kinetic Factors for SR and DSR Reactions (Rashid, et al., 2017)

Reaction	k_{ji} (kmol kg^{-1}h^{-1})	E_i (kJ mol^{-1})
SR	4.225×10^{15} bar$^{0.5}$	240.100
DSR	1.955 × 106 bar^{-1}	67.130

4 MAIN PROCESS FLOWSHEET

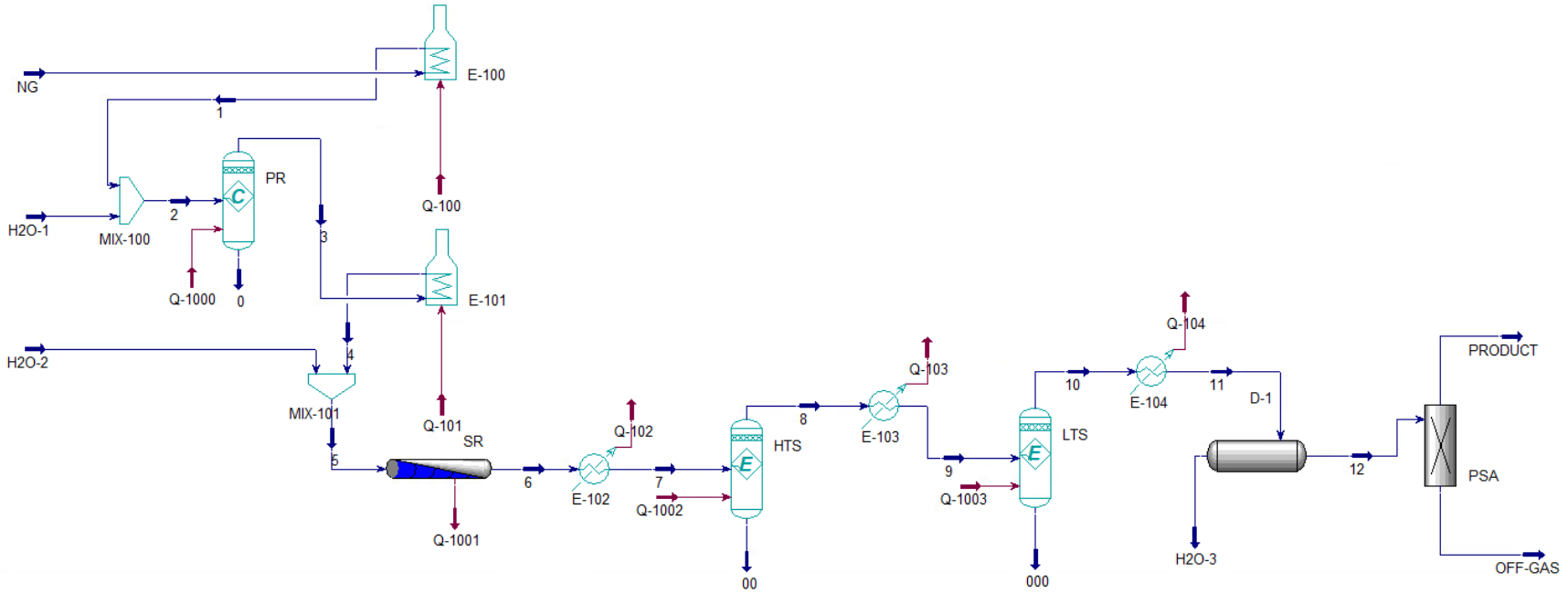

Figure 2: Main Process Flowsheet

5 RESULTS & DISCUSSION

5.1 Heaters and Coolers

The primary source of heat for the incoming NG streams is through the convective zone of the SR furnace. Although more complex models for heating are available in Aspen HYSYS (such as the "Fired Heater" or "Heat Exchanger" models), the choice was made to use the more simplified "Heater" model. Paralleling the setup of the heaters, the heat exchangers downstream of the SR were assigned the "Cooler" model. Pressure drops for all heaters and coolers were defined as 200kPa. Results are listed in *Table 8*.

Table 8: Heat Exchanger Energy Stream Results (Output)

Unit Name	T_{in} (^oC)	T_{out} (^oC)	ΔT (^oC)	Energy Stream	Heat Flow ([kJ/h]*10^8)
E-100	39.58	550	510.4	Q-100	6.424
E-101	550	950	400	Q-101	2.61
E-102	949.5	500	-449.5	Q-102	-4.348
E-103	500	200	-300	Q-103	-2.692
E-104	200	35	-165	Q-104	-6.51

5.2 Reforming Section

The aim of a pre-reformer is to reform the larger hydrocarbons. This process requires multiple reactions occurring simultaneously, so the initial reaction set was chosen to be based on conversion. A critical assumption made was that hydrocarbons with 2 or more C atoms were converted 100% within the pre-reformer. The amount of steam required for the desired S/C ratio of 2.5 is added beforehand, as seen in *Table 5*. The steam-rich natural gas feed (*Stream 5*) enters the reactor at a temperature of 550^{o}C with a flowrate of 15490kmol/h. Reactions 1-5 are set at a conversion of 100%, reforming all heavier hydrocarbons completely. Results from previous work (Reeves, et al., 2021) show the conversion of Methane would lie at around 60%, which was chosen as the conversion for the SR reaction.

Table 9: Reformer Section Results

Component	NG	1	H2O-1	2	3	4	H2O-2	5	6
CH_4	0.9381	0.9381	0	0.259	0.0756	0.0756	0	0.0521	0
C_2H_6	0.0452	0.0452	0	0.0125	0	0	0	0	0
C_3H_8	0.0038	0.0038	0	0.001	0	0	0	0	0
C_4H_{10}	0.0004	0.0004	0	0.0001	0	0	0	0	0
C_5H_{12}	0.0002	0.0002	0	0.0001	0	0	0	0	0
C_6H_{14}	0.0003	0.0003	0	0.0001	0	0	0	0	0
CO	0	0	0	0	0.1349	0.1349	0	0.0929	0.0585
CO_2	0.0047	0.0047	0	0.0013	0.0009	0.0009	0	0.0007	0.0734
N_2	0.0073	0.0073	0	0.002	0.0015	0.0015	0	0.001	0.0009
H_2O	0	0	1	0.7239	0.3938	0.3938	1	0.5825	0.4075
H_2	0	0	0	0	0.3933	0.3933	0	0.2708	0.4597
Mole Flow	2150	2150	5638	7788	10660	10660	4822	15490	17100
Temperature	40	550	550	547.7	550	950	950	949.6	730.2
Pressure	3400	3200	3200	3200	3200	3000	3000	3000	3000

Leaving the PR is a stream which no longer contains any hydrocarbons other than Methane the composition (stream 3) is displayed in *Table 9*. This stream is combined with the right amount of steam to achieve a S/C ratio of 4 (*Table 5*). Then it enters the main steam reformer, in which the SR reaction as well as DSR reaction will be defined as kinetic. Kinetic factors were defined from available literature (Rashid, et al., 2017) and are displayed in *Table 7*. The governing equations as defined by Aspen HYSYS are:

$$r = k * f(Basis) \qquad k = k_{ji} * \exp\left(-\frac{E_i}{RT}\right)$$

The Water-Gas shift reaction (WGSR) is also introduced into this reaction set, modelled as an equilibrium-based reaction. K_{eq} is based on Gibbs Free Energy, according to the equation:

$$\ln(K_{eq}) = -\frac{\Delta G(reaction)}{RT}$$

Basis is set as "Activity" and phase is selected as "VapourPhase". To achieve the desired S/C ratio for the SR, the required additional steam (see *Table 5*) is added via MIX-101. The resulting stream 5 enters the SR at 950^{o}C and 3000kPa (30 Bar), which is considered suitable operating conditions for Steam Reformers (Shagdar, et al., 2020). Tube dimensions were specified as 12m long with an internal diameter of 5cm, and the NT was manually specified to be 30, as lower values failed to produce a sufficient conversion of Methane. The final product leaving the SR can be considered Syngas, its composition (Stream 6) is displayed in *Table 9*.

5.3 Shift Section

The aim of the WGS reactions is to convert the remaining CO to CO_2 in presence of Water, thereby releasing Hydrogen. A two-stage shift section was selected, as a single HTS was found to produce a low CO conversion (67%, see Appendix B).

The third reaction set has the WGSR defined as an equilibrium reaction, with the same parameters as within the SR reaction set. It will be applied to both the HTS and LTS, the main difference between the two being the operating temperature, which lies at 500^{o}C and 200^{o}C, respectively.

Table 10: Shift Section Results

Component	6	7	8	9	10
CO	0.0585	0.0585	0.0263	0.0263	0.0008
CO_2	0.0734	0.0734	0.1056	0.1056	0.1311
N_2	0.0009	0.0009	0.0009	0.0009	0.0009
H_2O	0.4075	0.4075	0.3754	0.3754	0.3499
H_2	0.4597	0.4597	0.4918	0.4918	0.5173
Mole Flow	17100	17100	17100	17100	17100
Temperature	730.2	500	500	200	200
Pressure	3000	2800	2600	2400	2200

The CO conversion across the entire shift section (Stream 6 to Stream 10) is calculated as:

$$X_{CO} = 1 - \left(\frac{n_{CO,out}}{n_{CO,in}}\right) = 1 - \left(\frac{13.68\frac{kmol}{h}}{1000.35\frac{kmol}{h}}\right) = 98.62\%$$

5.4 Purification Section

The initial purification step is the condensate drum (*D-1*). The results show that a small amount (0.3mol%) of water still leaves the condensate drum, due to incomplete condensation within cooler *E-104*.

Table 11: Purification Section Results

Component	Stream 10	H2O-3	Stream 11	Stream 12
CO	0.0008	0.0008	0	0.0013
CO_2	0.1311	0.1311	0.0015	0.2003
N_2	0.0009	0.0009	0	0.0014
H_2O	0.3499	0.3499	0.9985	0.0032
H_2	0.5173	0.5173	0	0.7938
Mole Flow	17100	17100	5957	11140
Temperature	200	35	35	35
Pressure	2200	2000	2000	2000

The final unit operation within the purification phase is Pressure-Swing Adsorption (*PSA*) unit. HYSYS offers a variety of gas-liquid adsorption models but modelling of a solid-gas adsorption such as PSA is not an intended use case for the program. Therefore, the "Splitter" model was selected to simulate this operation, as has been done in other simulations of this operation (Rusten, 2010). The available literature (Fahim, et al., 2010) supports the assumption, that all impurities such as CO, CO_2, and even N_2 can effectively be removed through the PSA process, achieving a purity of 99.9% or higher. Using an adsorption medium such as Zeolite 5A, with Assumption [10] adding the requirement for 5% of Hydrogen product being desorbed into the *OFF-GAS* stream (95% H_2 recovery). Thus, the Splitter was configured to allow 95% of H_2 and 50% of N_2 in the exit stream.

5.5 Product

The product feed is obtained with a flowrate of 8412 kmol/h, equivalent to 411.84t/day. The final product has a purity of 99.81%. The only impurity present is Nitrogen.

Table 12: Product Composition and Conditions

Component	Mole Fract.
N_2	0.0009
H_2	0.9991
Mole Flow	8412
Mass Flow (kg/h)	17160
Mass Flow (t/day)	411.84
Temperature	40
Pressure	2000

5.6 Energy

The total energy consumption of the plant lies at $5.38*10^8$ kJ/h (= $1.29*10^7$ MJ/day, see Appendix A).

6 MODEL VALIDATION

As Hydrogen plant configurations vary widely, it is hard to find a single comparative source. Therefore, the main unit operation (Steam Reformer) was validated against results obtained by Shagdar et al. (2020).

Identical feed conditions as the model proposed by Shagdar et al. (2020) were fed into the SR. The flowsheet for this experiment is displayed in Figure 8.

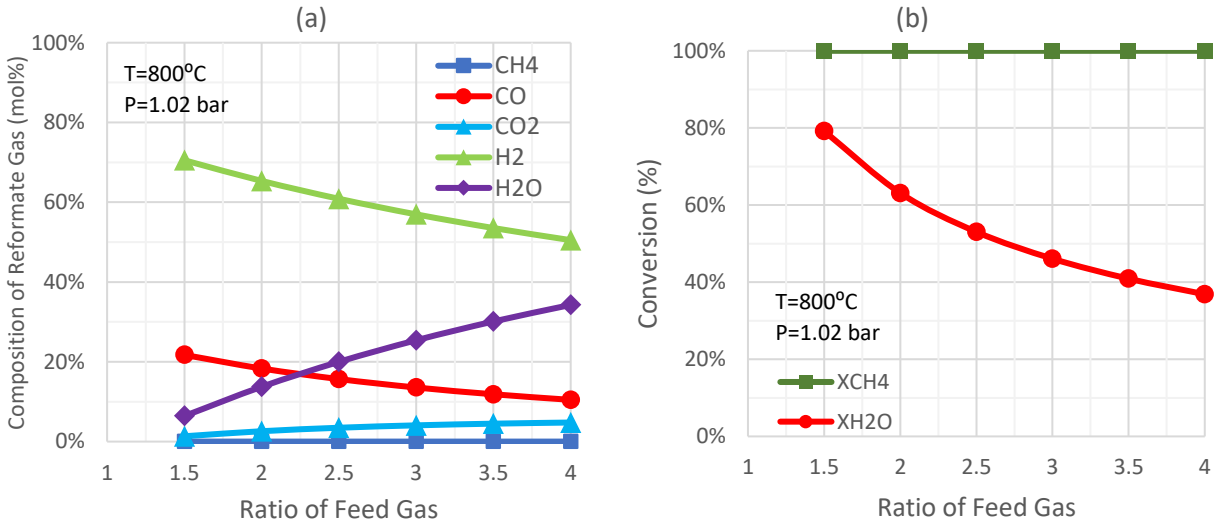

Figure 3: Effect of the mass flow ratio of feed gas on the SMR process (present work): (a) composition of reformate gas; (b) conversion rates of methane and steam

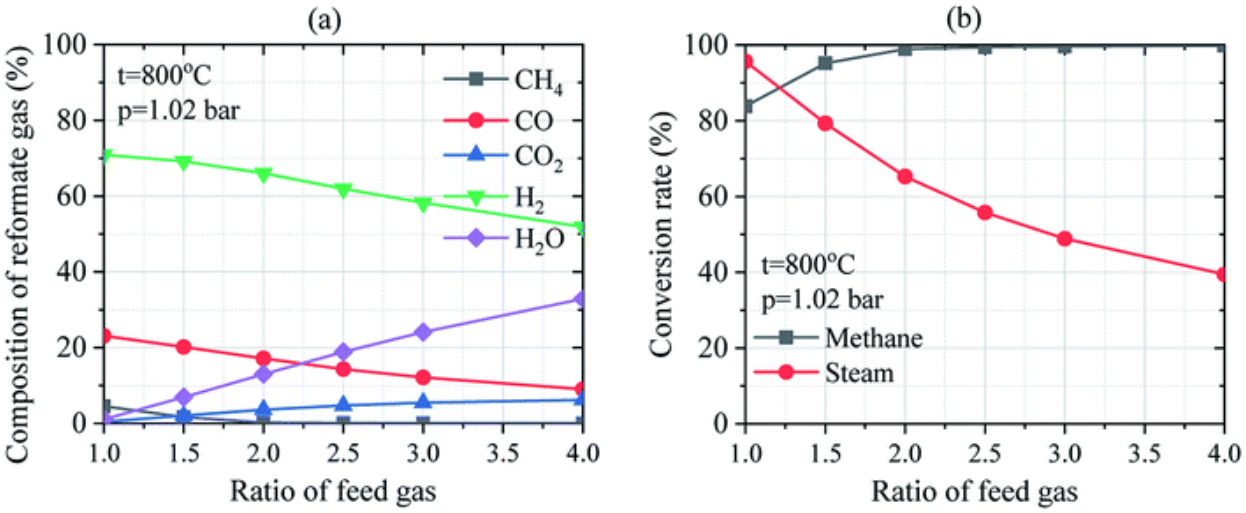

Figure 4: Effect of the mass flow ratio of feed gas on the SMR process (Shagdar, et al., 2020): (a) composition of reformate gas; (b) conversion rates of methane and steam

From the results in Figure 4, it can be observed that the proposed HYSYS model shows a high similarity to the results obtained by Shagdar et al. (2020). The main difference is observed in the Conversion of CH_4, which stems from the fact that no reverse SR and DSR reactions were considered (see Assumption [4]), therefore the conversion of Methane lies at a constant 100%.

For further validation, a temperature sensitivity analysis was performed. The same effect as observed in Figure 3 is present, with 100% conversion of Methane.

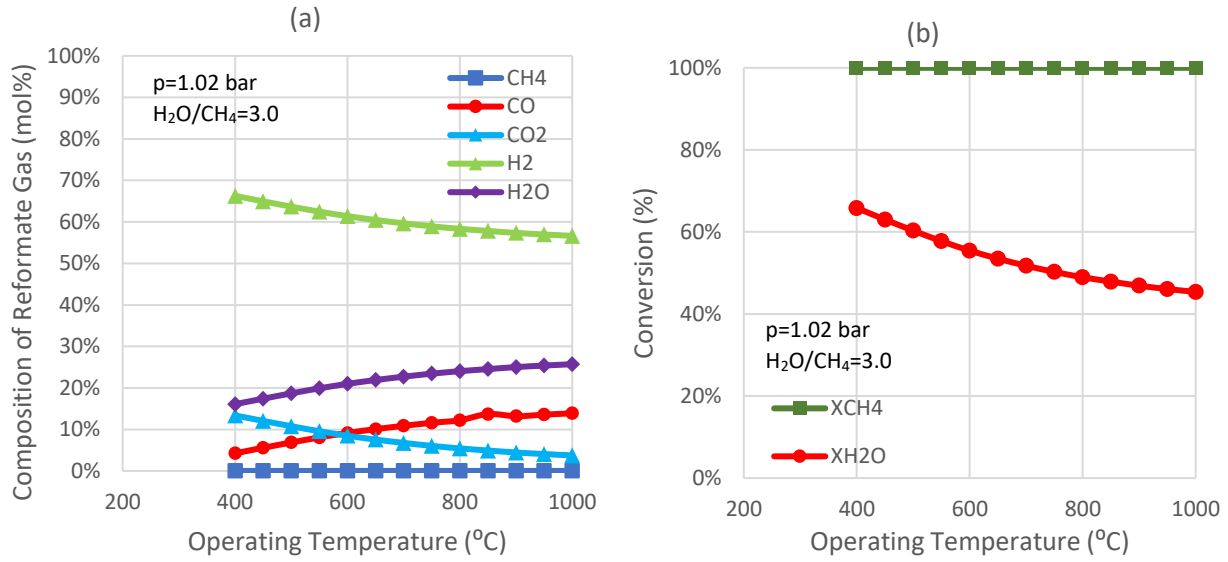

Figure 5: Effect of operating temperature on the SMR process (present work): (a) composition of reformate gas; (b) conversion rates of methane and steam

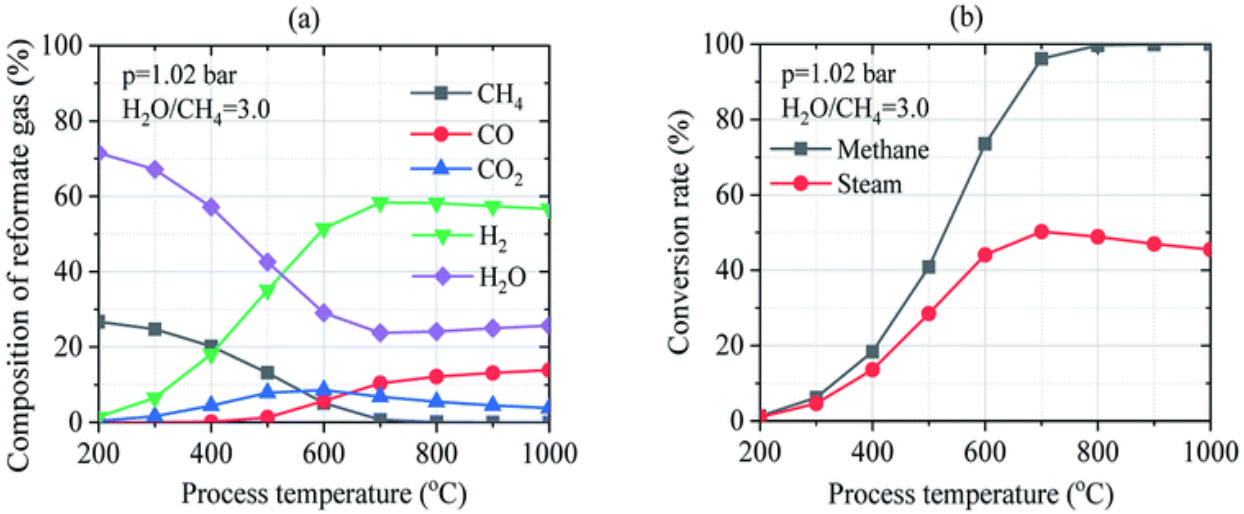

Figure 6: Effect of operating temperature on the SMR process (Shagdar, et al., 2020): (a) composition of reformate gas; (b) conversion rates of methane and steam

Initially the results may show a strong discrepancy between the models. Yet, upon further analysis the presented model shows a low error at operating temperatures above 700°C (average of 1% absolute error where CH_4 values are omitted). This is confirmed by an error analysis which is displayed in Figure 7.

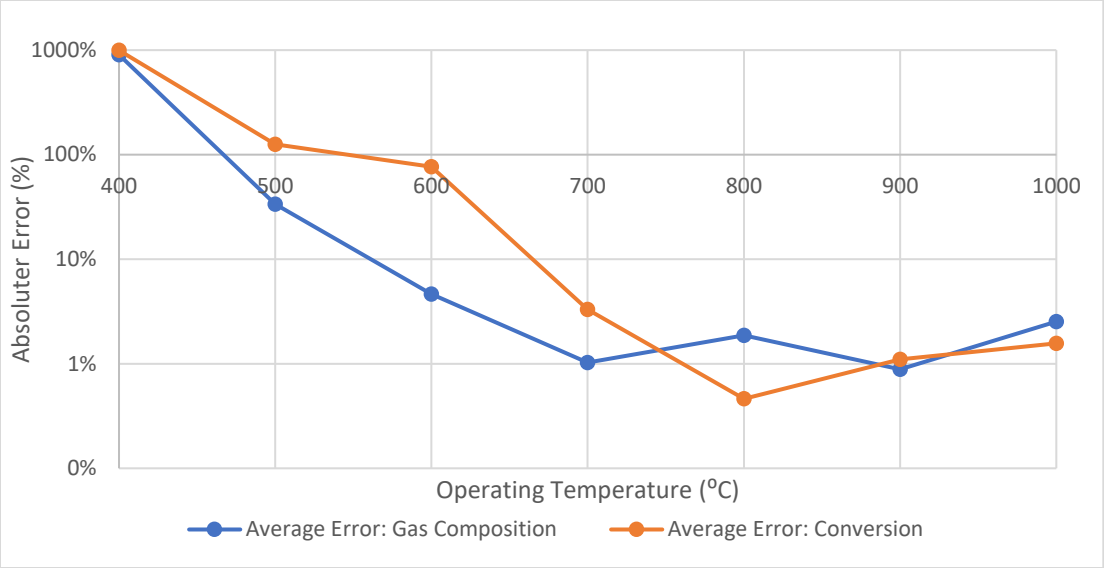

Figure 7: Average Absolute Error of the Present Model against Shagdar et al. (2020) [CH_4 omitted, Logarithmic scale]

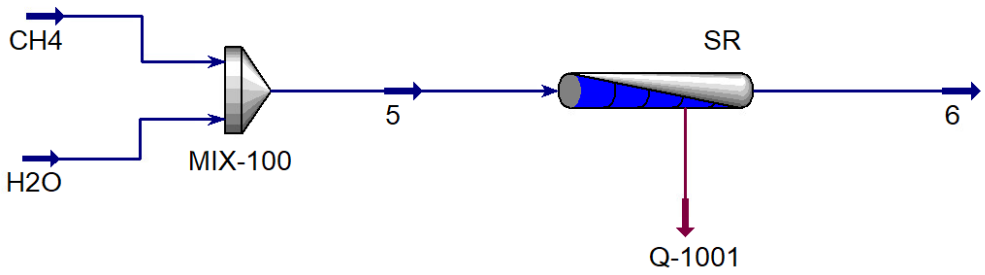

Figure 8: Flowsheet for Model Validation (Identical Settings to Main Model)

7 CONCLUSION

The initial task was to create a simulation of a Hydrogen plant that produces 400t/day at a purity of 99.9%. Results show this has been achieved with a NG feed of 2150 kmol/h and a total energy consumption of $6.16*10^8$ kJ/h. The total water (steam) consumption is 10460 kmol/h (= 188.28 t/h). CH_4 conversion is 100% within the SR, and CO conversion within the Shift section is 98.62%. The model validation shows the proposed model is generally accurate, with error at the chosen operating temperature (950°C) being around 1% (Figure 7). The off-gas leaves the PSA at a flowrate of 2733 kmol/h, with a CO_2 purity of 80%. This means CO_2 emissions lie at around 98.3t/h, or 2358.19 t/day. With appropriate CCS integration, the environmental impact can be greatly reduced.

Overall, the goal was achieved successfully, providing a robust representation of a steam reforming plant.

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Nomenclature

CCS	Carbon Capture & Storage	NT	Number of Tubes
CO	Carbon Monoxide	PFR	Plug-Flow Reactor
CO_2	Carbon Dioxide	PR	Pre-Reformer
CH_4	Methane	SR	Steam-Reformer
DR	Direct Reforming Reaction	SMR	Steam Methane Reforming
H_2O	Water	S/C	Steam-to-Carbon ratio
H_2	Hydrogen	WGSR	Water-Gas-Shift Reaction
NG	Natural Gas		

APPENDIX A: SIMULATION RESULTS

Note:

1. **All fractions are in mol%.**
2. **All flows are in kmol/h.**
3. **All temperatures in ^oC.**
4. **All Pressures in kPa.**

Unless stated otherwise

Kinetic Factors (Rashid, et al., 2017)

Reaction	**k_{ji} (kmol $kg^{-1}h^{-1}$)**	**E_i (kJ mol^{-1})**
SR	4.225×10^{15} $bar^{0.5}$	240.100
DSR	1.955×106 bar^{-1}	67.130

Feed

Component	**Formula**	**Mole Fract.**
Methane	CH_4	0.9381
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Propane	C_3H_8	0.0038
n-Butane	C_4H_{10}	0.0004
n-Pentane	C_5H_{12}	0.0002
n-Hexane	C_6H_{14}	0.0003
Water	H_2O	0
Carbon Monoxide	CO	0
Carbon Dioxide	CO_2	0.0047
Hydrogen	H_2	0
Nitrogen	N_2	0.0073
Mole Flow	2150 kmol/h	

S/C Ratio Results

Block	Carbon Balance (kmol/h)	Desired S/C Ratio	Required Steam Feed (kmol/h)	Stream
PR	2255	2.5	2255*2.5 = 5638	H2O-1
SR	2255	4	(2255*4)-4199 = 4822	H2O-2

Reforming Section Results

Component	NG	1	H2O-1	2	3	4	H2O-2	5	6
CH_4	0.9381	0.9381	0	0.259	0.0756	0.0756	0	0.0521	0
C_2H_6	0.0452	0.0452	0	0.0125	0	0	0	0	0
C_3H_8	0.0038	0.0038	0	0.001	0	0	0	0	0
C_4H_{10}	0.0004	0.0004	0	0.0001	0	0	0	0	0
C_5H_{12}	0.0002	0.0002	0	0.0001	0	0	0	0	0
C_6H_{14}	0.0003	0.0003	0	0.0001	0	0	0	0	0
CO	0	0	0	0	0.1349	0.1349	0	0.0929	0.0585
CO_2	0.0047	0.0047	0	0.0013	0.0009	0.0009	0	0.0007	0.0734
N_2	0.0073	0.0073	0	0.002	0.0015	0.0015	0	0.001	0.0009
H_2O	0	0	1	0.7239	0.3938	0.3938	1	0.5825	0.4075
H_2	0	0	0	0	0.3933	0.3933	0	0.2708	0.4597
Mole Flow	2150	2150	5638	7788	10660	10660	4822	15490	17100
Temperature	40	550	550	547.7	550	950	950	949.6	730.2
Pressure	3400	3200	3200	3200	3200	3000	3000	3000	3000

Shift Section Results

Component	6	7	8	9	10
CO	0.0585	0.0585	0.0263	0.0263	0.0008
CO_2	0.0734	0.0734	0.1056	0.1056	0.1311
N_2	0.0009	0.0009	0.0009	0.0009	0.0009
H_2O	0.4075	0.4075	0.3754	0.3754	0.3499
H_2	0.4597	0.4597	0.4918	0.4918	0.5173
Mole Flow	17100	17100	17100	17100	17100
Temperature	730.2	500	500	200	200
Pressure	3000	2800	2600	2400	2200

Purification Section Results

Component	Stream 10	H2O-3	Stream 11	Stream 12

CO	0.0008	0.0008	0	0.0013
CO_2	0.1311	0.1311	0.0015	0.2003
N_2	0.0009	0.0009	0	0.0014
H_2O	0.3499	0.3499	0.9985	0.0032
H_2	0.5173	0.5173	0	0.7938
Mole Flow	17100	17100	5957	11140
Temperature	200	35	35	35
Pressure	2200	2000	2000	2000

Product

Component	**Mole Fract.**
N_2	0.0009
H_2	0.9991
Mole Flow	8412
Mass Flow (kg/h)	17160
Mass Flow (t/day)	411.84
Temperature	40
Pressure	2000

Off-Gas

Component	**Mole Fract.**
CO	0.0051
CO_2	0.8171
H_2O	0.0130
H_2	0.1619
Mole Flow	2733
Temperature	41.07
Pressure	2000

Energy Streams (Energy OUT, Temperatures in ^oC)

Stream Name	**Unit Name**	**T_{in}**	**T_{out}**	**ΔT**	**Value (kJ/h)**
Heaters					
Q-100	E-100	40	550	510	4.062*10^008
Q-101	E-101	550	950	400	1.65*10^008
Coolers					
Q-102	E-102	950	500	-450	-1.424*10^008
Q-103	E-103	500	200	-300	-1.776*10^008
Q-104	E-104	200	35	-165	-3.607*10^008

Reactors					
Q-1000	PR	550	550	0	-3.133*10^008
Q-1001	SR	950	950	0	-1.544*10^008
Q-1002	HTS	500	500	0	3.377*10^007
Q-1003	LTS	200	200	0	4.956*10^006
Total Energy					-5.38*10^008

Note:
The negative values mean energy is required for operation, positive values describe energy output. Arrows on flowsheet might not correspond to this notation.

APPENDIX B: SINGLE SHIFT RESULTS

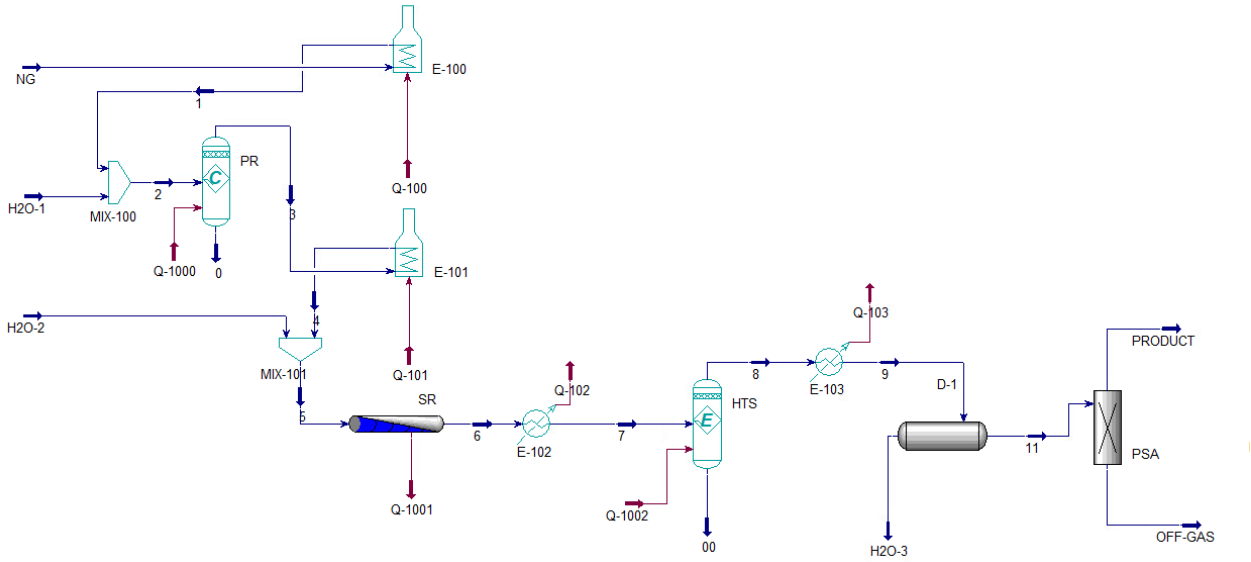

Figure 9: Flowsheet for Single HTS Reactor

Shift Section Results (Single HTS)

Component	7	8	9
CO	0.0523	0.0263	0.0263
CO_2	0.0796	0.1056	0.1056
N_2	0.0009	0.0009	0.0009
H_2O	0.4286	0.3754	0.3754
H_2	0.4386	0.4918	0.4918
Mole Flow	17100	17100	17100
Temperature	500	500	200
Pressure	2800	2600	2400

X_{CO} = 1 - (450/1361) = 66.94%

APPENDIX C: VALIDATION RESULTS

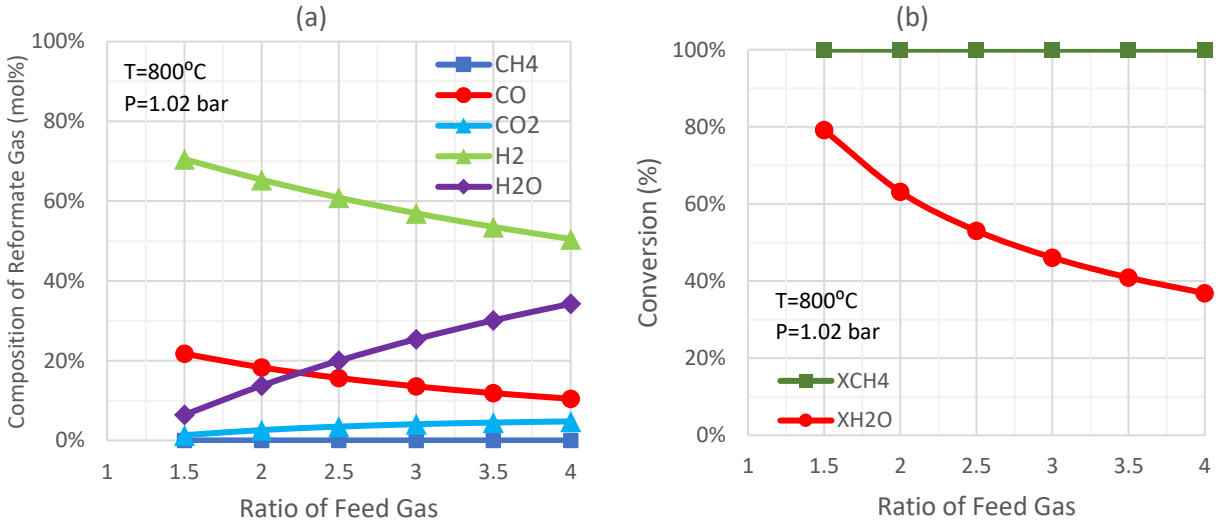

Figure 10: Effect of the mass flow ratio of feed gas on the SMR process (present work): (a) composition of reformate gas; (b) conversion rates of methane and steam

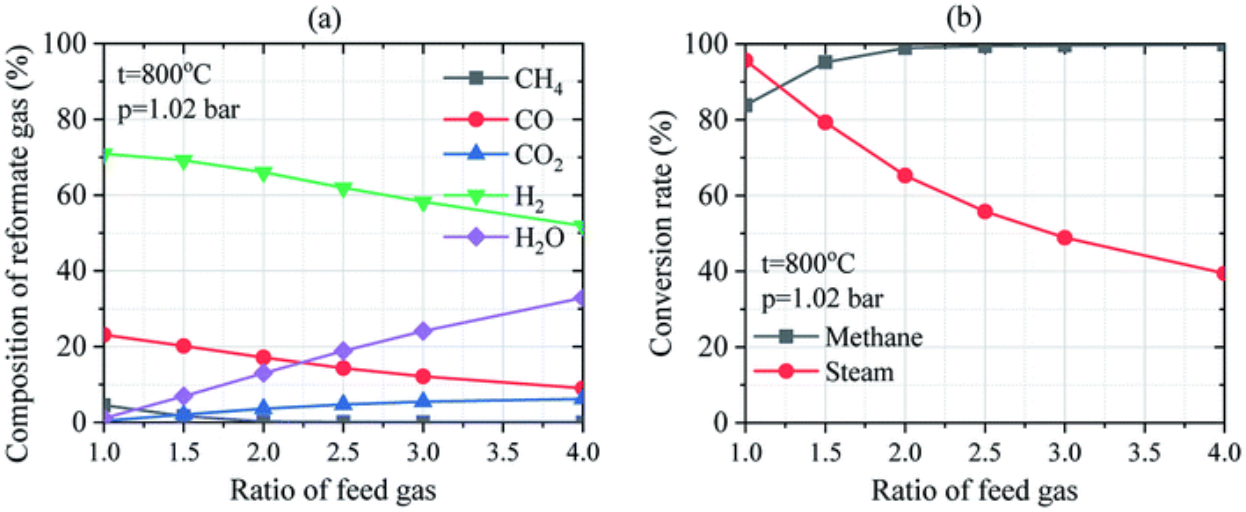

Figure 11: Effect of the mass flow ratio of feed gas on the SMR process (Shagdar, et al., 2020): (a) composition of reformate gas; (b) conversion rates of methane and steam

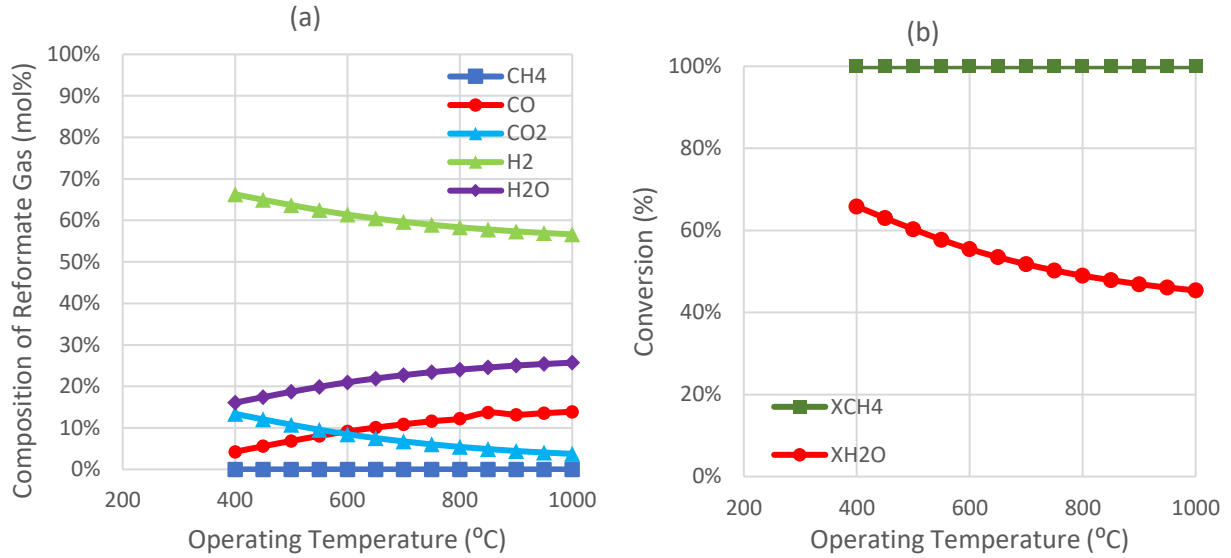

Figure 12: Effect of operating temperature on the SMR process (present work): (a) composition of reformate gas; (b) conversion rates of methane and steam

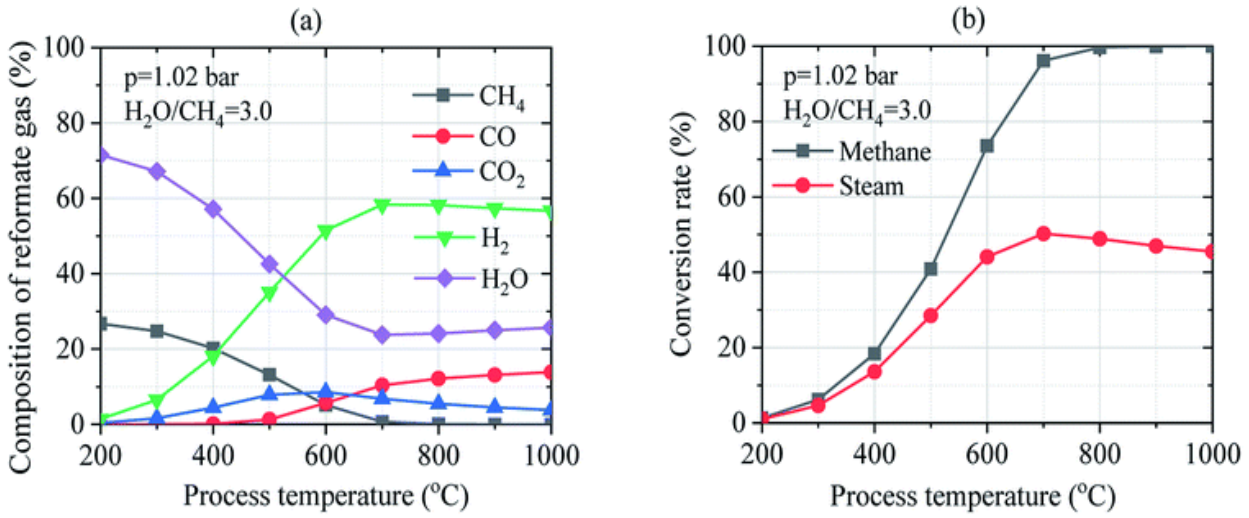

Figure 13: Effect of operating temperature on the SMR process (Shagdar, et al., 2020): (a) composition of reformate gas; (b) conversion rates of methane and steam

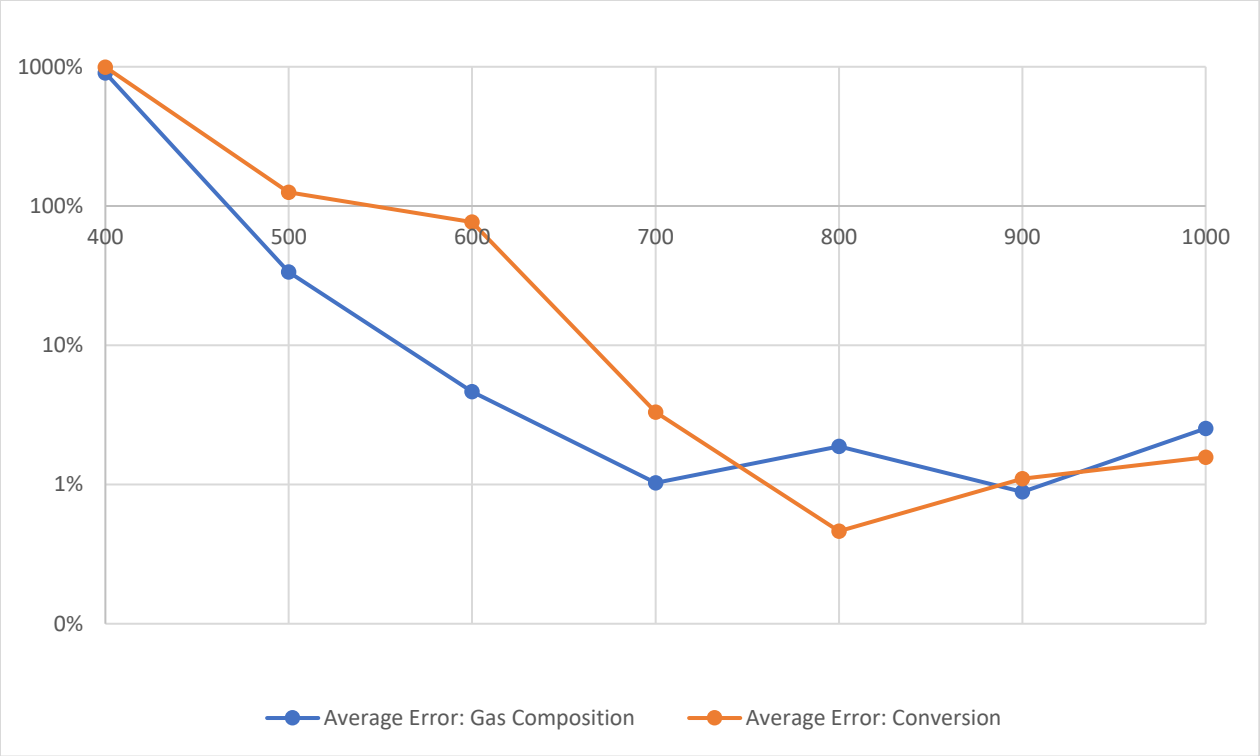

Figure 14: Average Absolute Error of the Present Model against Shagdar et al. (2020) [CH_4 omitted, Logarithmic scale]

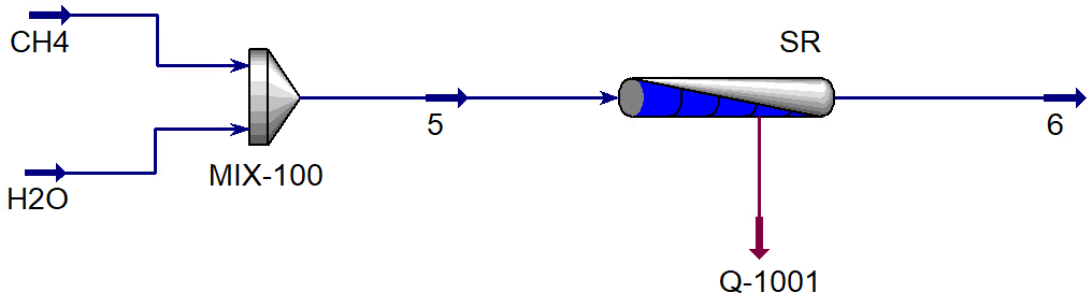

Figure 15: Flowsheet for Model Validation (Identical Conditions to Main Model)