

Special Design Task

# Simulation of SMR Plant for Hydrogen Production in Aspen HYSYS®

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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<sub>2</sub> 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<sub>2</sub> 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°C, and Low Temperature Shift operating at 200°C, modelled as equilibrium reactors. Validation shows generally accurate model results for Reforming and Shift sections.

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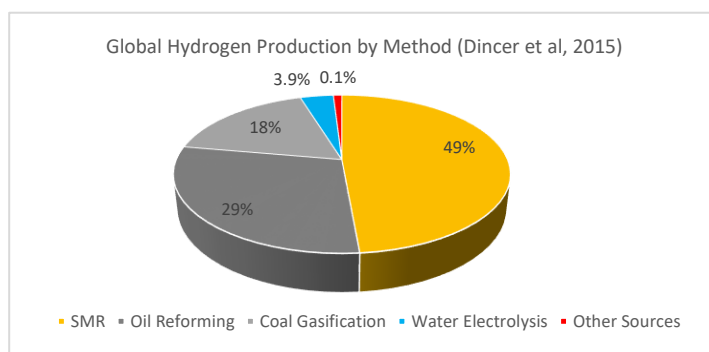
*“Hydrogen has been the fuel of the future for decades, always promising to deliver huge benefits in about five years’ time.” – Forbes, 2020*

## 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<sub>2</sub> 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).

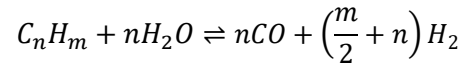
The full name of software and version is listed in *Table 1*.

**Table 1**

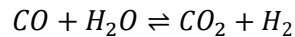
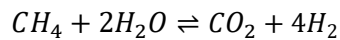
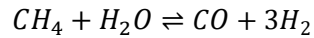
Software Name	Version
Aspen HYSYS®	V11 (37.0.0.395)

### 3 METHODOLOGY

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



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



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	$CH_4 + H_2O \rightarrow CO + 3H_2$	(7)
	DSR		$CH_4 + 2H_2O \rightarrow CO_2 + 4H_2$	
	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<sub>2</sub> 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 <sub>4</sub>	0.9381
Ethane	C <sub>2</sub> H <sub>6</sub>	0.0452
Propane	C <sub>3</sub> H <sub>8</sub>	0.0038
n-Butane	C <sub>4</sub> H <sub>10</sub>	0.0004
n-Pentane	C <sub>5</sub> H <sub>12</sub>	0.0002
n-Hexane	C <sub>6</sub> H <sub>14</sub>	0.0003
Water	H <sub>2</sub> O	0
Carbon Monoxide	CO	0
Carbon Dioxide	CO <sub>2</sub>	0.0047
Hydrogen	H <sub>2</sub>	0
Nitrogen	N <sub>2</sub>	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 (°C)
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°C.
LTS	Equilibrium Reactor	WGSR	Equilibrium-based modelling of WGSR reaction at operating temp of 350°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<sup>3</sup>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 <sup>-1</sup> h <sup>-1</sup> )	$E_i$ (kJ mol <sup>-1</sup> )
SR	$4.225 \times 10^{15} \text{ bar}^{0.5}$	240.100
DSR	$1.955 \times 10^6 \text{ bar}^{-1}$	67.130

## 4 MAIN PROCESS FLOWSHEET

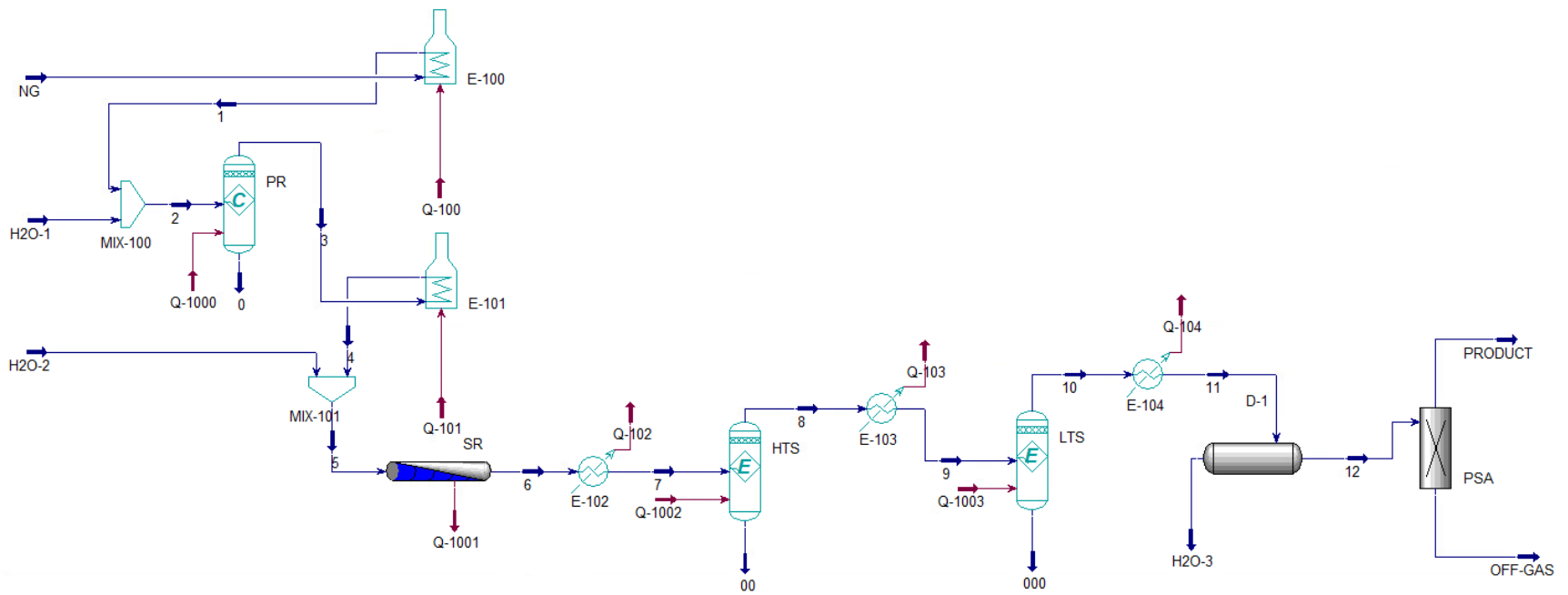


Figure 2: Main Process Flowsheet

## 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 <sub>in</sub> (°C)	T <sub>out</sub> (°C)	ΔT (°C)	Energy Stream	Heat Flow ([kJ/h]*10 <sup>8</sup> )
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°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 <sub>4</sub>	0.9381	0.9381	0	0.259	0.0756	0.0756	0	0.0521	0
C <sub>2</sub> H <sub>6</sub>	0.0452	0.0452	0	0.0125	0	0	0	0	0
C <sub>3</sub> H <sub>8</sub>	0.0038	0.0038	0	0.001	0	0	0	0	0
C <sub>4</sub> H <sub>10</sub>	0.0004	0.0004	0	0.0001	0	0	0	0	0
C <sub>5</sub> H <sub>12</sub>	0.0002	0.0002	0	0.0001	0	0	0	0	0
C <sub>6</sub> H <sub>14</sub>	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 <sub>2</sub>	0.0047	0.0047	0	0.0013	0.0009	0.0009	0	0.0007	0.0734
N <sub>2</sub>	0.0073	0.0073	0	0.002	0.0015	0.0015	0	0.001	0.0009
H <sub>2</sub> O	0	0	1	0.7239	0.3938	0.3938	1	0.5825	0.4075
H <sub>2</sub>	0	0	0	0	0.3933	0.3933	0	0.2708	0.4597
<b>Mole Flow</b>	2150	2150	5638	7788	10660	10660	4822	15490	17100
<b>Temperature</b>	40	550	550	547.7	550	950	950	949.6	730.2
<b>Pressure</b>	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:

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

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°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<sub>2</sub> 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°C and 200°C, respectively.

**Table 10: Shift Section Results**

<b>Component</b>	<b>6</b>	<b>7</b>	<b>8</b>	<b>9</b>	<b>10</b>
CO	0.0585	0.0585	0.0263	0.0263	0.0008
CO <sub>2</sub>	0.0734	0.0734	0.1056	0.1056	0.1311
N <sub>2</sub>	0.0009	0.0009	0.0009	0.0009	0.0009
H <sub>2</sub> O	0.4075	0.4075	0.3754	0.3754	0.3499
H <sub>2</sub>	0.4597	0.4597	0.4918	0.4918	0.5173
<b>Mole Flow</b>	17100	17100	17100	17100	17100
<b>Temperature</b>	730.2	500	500	200	200
<b>Pressure</b>	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 <sub>2</sub>	0.1311	0.1311	0.0015	0.2003
N <sub>2</sub>	0.0009	0.0009	0	0.0014
H <sub>2</sub> O	0.3499	0.3499	0.9985	0.0032
H <sub>2</sub>	0.5173	0.5173	0	0.7938
<b>Mole Flow</b>	17100	17100	5957	11140
<b>Temperature</b>	200	35	35	35
<b>Pressure</b>	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<sub>2</sub>, and even N<sub>2</sub> 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<sub>2</sub> recovery). Thus, the Splitter was configured to allow 95% of H<sub>2</sub> and 50% of N<sub>2</sub> 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 <sub>2</sub>	0.0009
H <sub>2</sub>	0.9991
<b>Mole Flow</b>	8412
<b>Mass Flow (kg/h)</b>	17160
<b>Mass Flow (t/day)</b>	411.84
<b>Temperature</b>	40
<b>Pressure</b>	2000

## 5.6 Energy

The total energy consumption of the plant lies at  $5.38 \cdot 10^8$  kJ/h (=  $1.29 \cdot 10^7$  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.

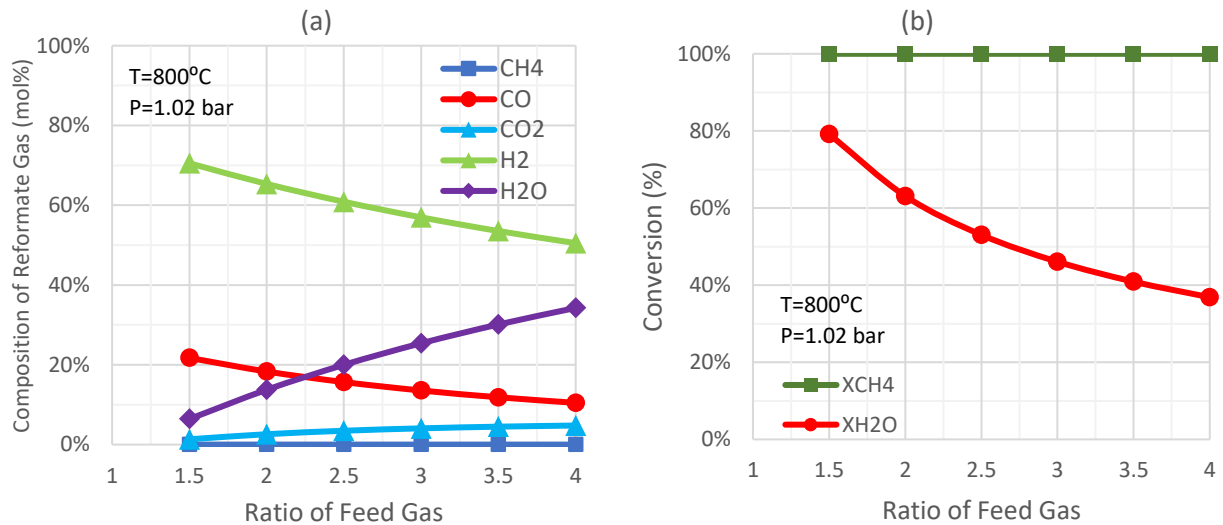


Figure 3: Effect of the mass flow ratio of feed gas on the SMR process (present work): (a) composition of reformate gas; (b) conversion rates of methane and steam

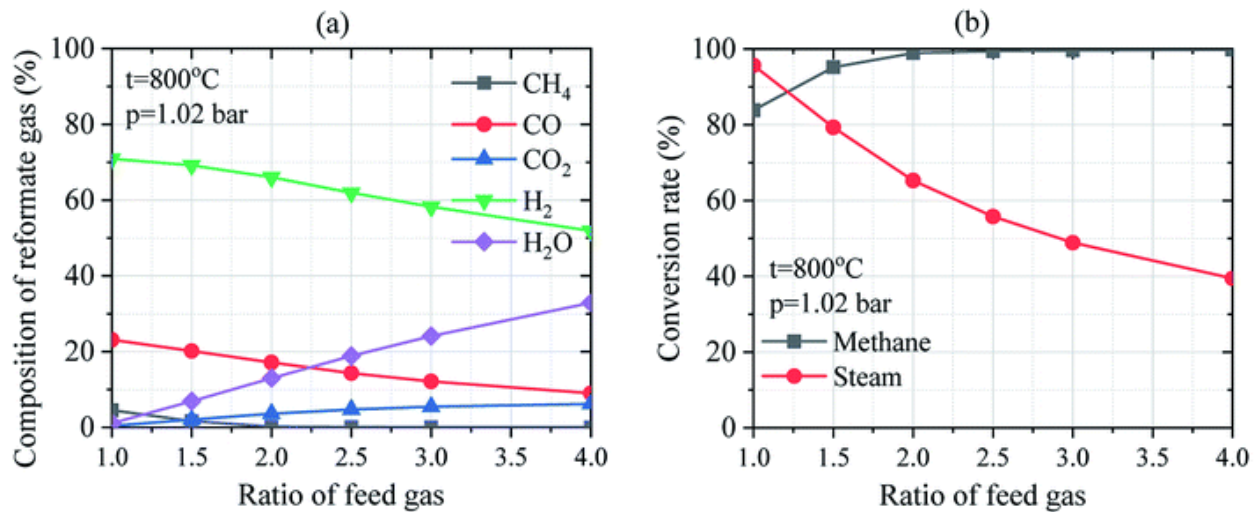


Figure 4: Effect of the mass flow ratio of feed gas on the SMR process (Shagdar, et al., 2020): (a) composition of reformate gas; (b) conversion rates of methane and steam

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<sub>4</sub>, 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.

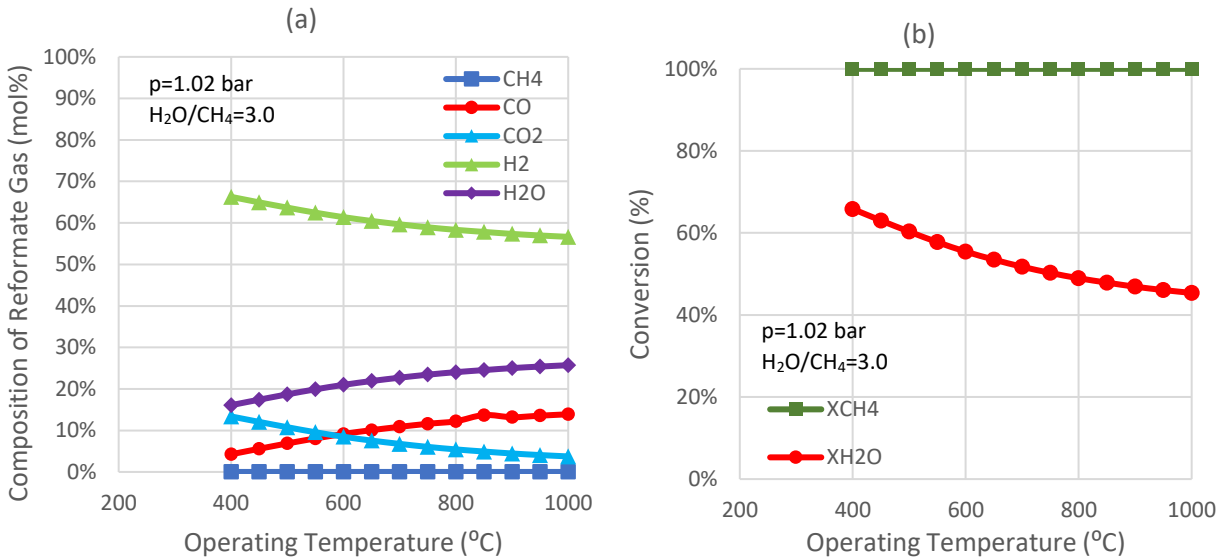


Figure 5: Effect of operating temperature on the SMR process (present work): (a) composition of reformate gas; (b) conversion rates of methane and steam

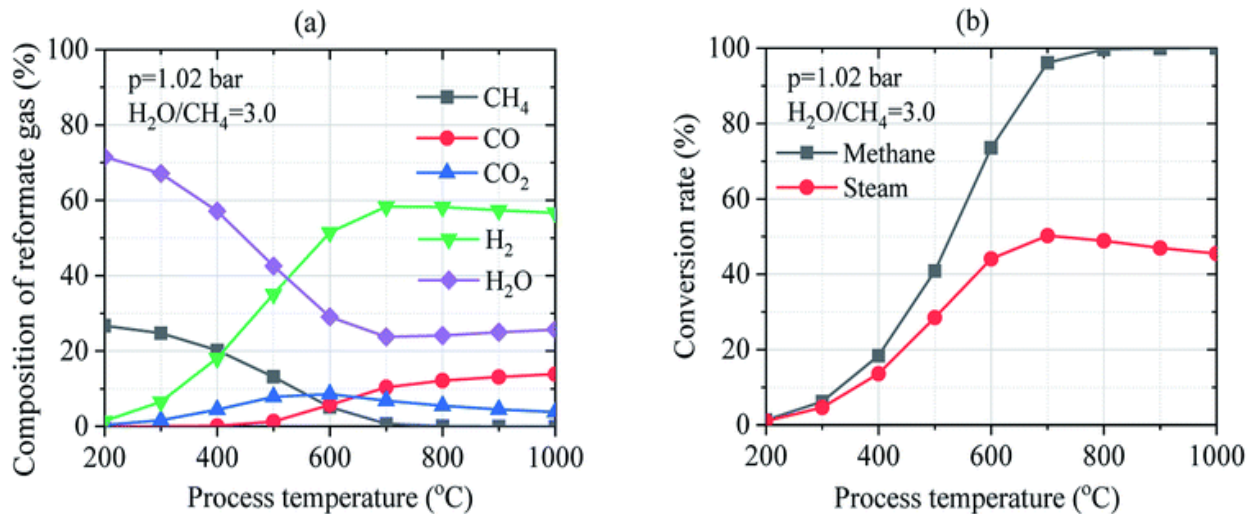


Figure 6: Effect of operating temperature on the SMR process (Shagdar, et al., 2020): (a) composition of reformate gas; (b) conversion rates of methane and steam

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<sub>4</sub> values are omitted). This is confirmed by an error analysis which is displayed in Figure 7.

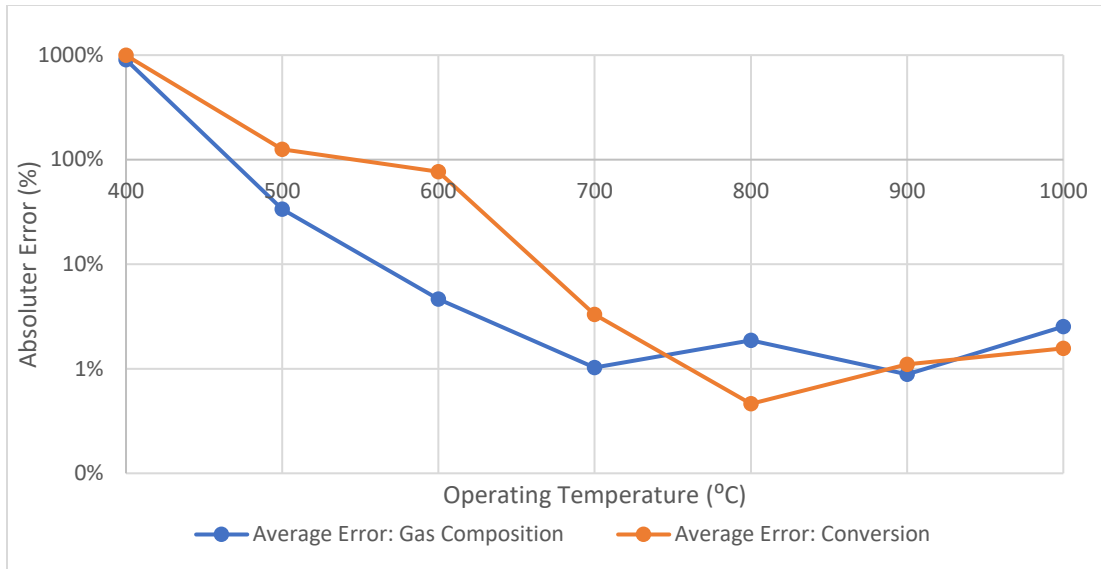


Figure 7: Average Absolute Error of the Present Model against Shagdar et al. (2020) [CH<sub>4</sub> omitted, Logarithmic scale]

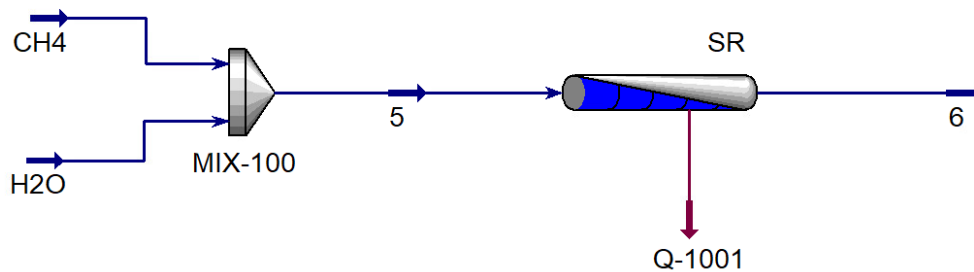


Figure 8: Flowsheet for Model Validation (Identical Settings to Main Model)

## 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  $6.16 \times 10^8$  kJ/h. The total water (steam) consumption is 10460 kmol/h (= 188.28 t/h). CH<sub>4</sub> 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<sub>2</sub> purity of 80%. This means CO<sub>2</sub> 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 <sub>2</sub>	Carbon Dioxide	PR	Pre-Reformer
CH <sub>4</sub>	Methane	SR	Steam-Reformer
DR	Direct Reforming Reaction	SMR	Steam Methane Reforming
H <sub>2</sub> O	Water	S/C	Steam-to-Carbon ratio
H <sub>2</sub>	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 °C.
4. All Pressures in kPa.

Unless stated otherwise

*Kinetic Factors (Rashid, et al., 2017)*

Reaction	$k_{ji}$ (kmol kg <sup>-1</sup> h <sup>-1</sup> )	$E_i$ (kJ mol <sup>-1</sup> )
SR	$4.225 \times 10^{15} \text{ bar}^{0.5}$	240.100
DSR	$1.955 \times 106 \text{ bar}^{-1}$	67.130

*Feed*

Component	Formula	Mole Fract.
Methane	CH <sub>4</sub>	0.9381
Ethane	C <sub>2</sub> H <sub>6</sub>	0.0452
Propane	C <sub>3</sub> H <sub>8</sub>	0.0038
n-Butane	C <sub>4</sub> H <sub>10</sub>	0.0004
n-Pentane	C <sub>5</sub> H <sub>12</sub>	0.0002
n-Hexane	C <sub>6</sub> H <sub>14</sub>	0.0003
Water	H <sub>2</sub> O	0
Carbon Monoxide	CO	0
Carbon Dioxide	CO <sub>2</sub>	0.0047
Hydrogen	H <sub>2</sub>	0
Nitrogen	N <sub>2</sub>	0.0073
<b>Mole Flow</b>	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 <sub>4</sub>	0.9381	0.9381	0	0.259	0.0756	0.0756	0	0.0521	0
C <sub>2</sub> H <sub>6</sub>	0.0452	0.0452	0	0.0125	0	0	0	0	0
C <sub>3</sub> H <sub>8</sub>	0.0038	0.0038	0	0.001	0	0	0	0	0
C <sub>4</sub> H <sub>10</sub>	0.0004	0.0004	0	0.0001	0	0	0	0	0
C <sub>5</sub> H <sub>12</sub>	0.0002	0.0002	0	0.0001	0	0	0	0	0
C <sub>6</sub> H <sub>14</sub>	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 <sub>2</sub>	0.0047	0.0047	0	0.0013	0.0009	0.0009	0	0.0007	0.0734
N <sub>2</sub>	0.0073	0.0073	0	0.002	0.0015	0.0015	0	0.001	0.0009
H <sub>2</sub> O	0	0	1	0.7239	0.3938	0.3938	1	0.5825	0.4075
H <sub>2</sub>	0	0	0	0	0.3933	0.3933	0	0.2708	0.4597
<b>Mole Flow</b>	2150	2150	5638	7788	10660	10660	4822	15490	17100
<b>Temperature</b>	40	550	550	547.7	550	950	950	949.6	730.2
<b>Pressure</b>	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 <sub>2</sub>	0.0734	0.0734	0.1056	0.1056	0.1311
N <sub>2</sub>	0.0009	0.0009	0.0009	0.0009	0.0009
H <sub>2</sub> O	0.4075	0.4075	0.3754	0.3754	0.3499
H <sub>2</sub>	0.4597	0.4597	0.4918	0.4918	0.5173
<b>Mole Flow</b>	17100	17100	17100	17100	17100
<b>Temperature</b>	730.2	500	500	200	200
<b>Pressure</b>	3000	2800	2600	2400	2200

*Purification Section Results*

Component	Stream 10	H2O-3	Stream 11	Stream 12
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CO	0.0008	0.0008	0	0.0013
CO <sub>2</sub>	0.1311	0.1311	0.0015	0.2003
N <sub>2</sub>	0.0009	0.0009	0	0.0014
H <sub>2</sub> O	0.3499	0.3499	0.9985	0.0032
H <sub>2</sub>	0.5173	0.5173	0	0.7938
<b>Mole Flow</b>	17100	17100	5957	11140
<b>Temperature</b>	200	35	35	35
<b>Pressure</b>	2200	2000	2000	2000

*Product*

<b>Component</b>	<b>Mole Fract.</b>
N <sub>2</sub>	0.0009
H <sub>2</sub>	0.9991
<b>Mole Flow</b>	8412
<b>Mass Flow (kg/h)</b>	17160
<b>Mass Flow (t/day)</b>	411.84
<b>Temperature</b>	40
<b>Pressure</b>	2000

*Off-Gas*

<b>Component</b>	<b>Mole Fract.</b>
CO	0.0051
CO <sub>2</sub>	0.8171
H <sub>2</sub> O	0.0130
H <sub>2</sub>	0.1619
<b>Mole Flow</b>	2733
<b>Temperature</b>	41.07
<b>Pressure</b>	2000

*Energy Streams (Energy OUT, Temperatures in °C)*

<b>Stream Name</b>	<b>Unit Name</b>	<b>T<sub>in</sub></b>	<b>T<sub>out</sub></b>	<b>ΔT</b>	<b>Value (kJ/h)</b>
<i>Heaters</i>					
Q-100	E-100	40	550	510	4.062*10 <sup>008</sup>
Q-101	E-101	550	950	400	1.65*10 <sup>008</sup>
<i>Coolers</i>					
Q-102	E-102	950	500	-450	-1.424*10 <sup>008</sup>
Q-103	E-103	500	200	-300	-1.776*10 <sup>008</sup>
Q-104	E-104	200	35	-165	-3.607*10 <sup>008</sup>

*Reactors*

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

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

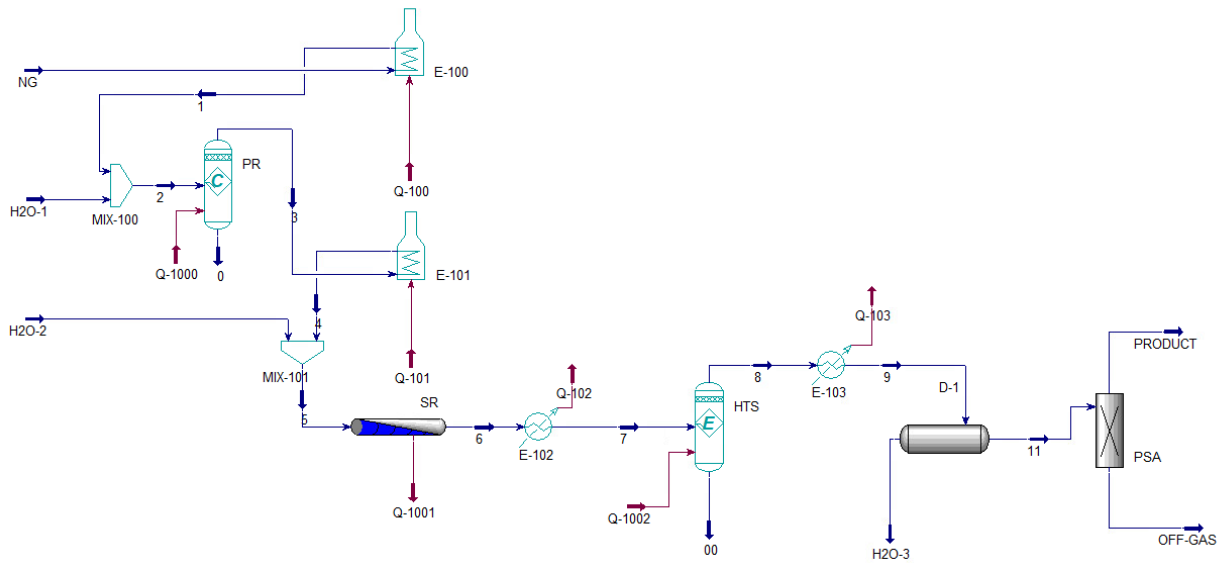


Figure 9: Flowsheet for Single HTS Reactor

### Shift Section Results (Single HTS)

Component	7	8	9
CO	0.0523	0.0263	0.0263
CO <sub>2</sub>	0.0796	0.1056	0.1056
N <sub>2</sub>	0.0009	0.0009	0.0009
H <sub>2</sub> O	0.4286	0.3754	0.3754
H <sub>2</sub>	0.4386	0.4918	0.4918
<b>Mole Flow</b>	17100	17100	17100
<b>Temperature</b>	500	500	200
<b>Pressure</b>	2800	2600	2400

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

## APPENDIX C: VALIDATION RESULTS

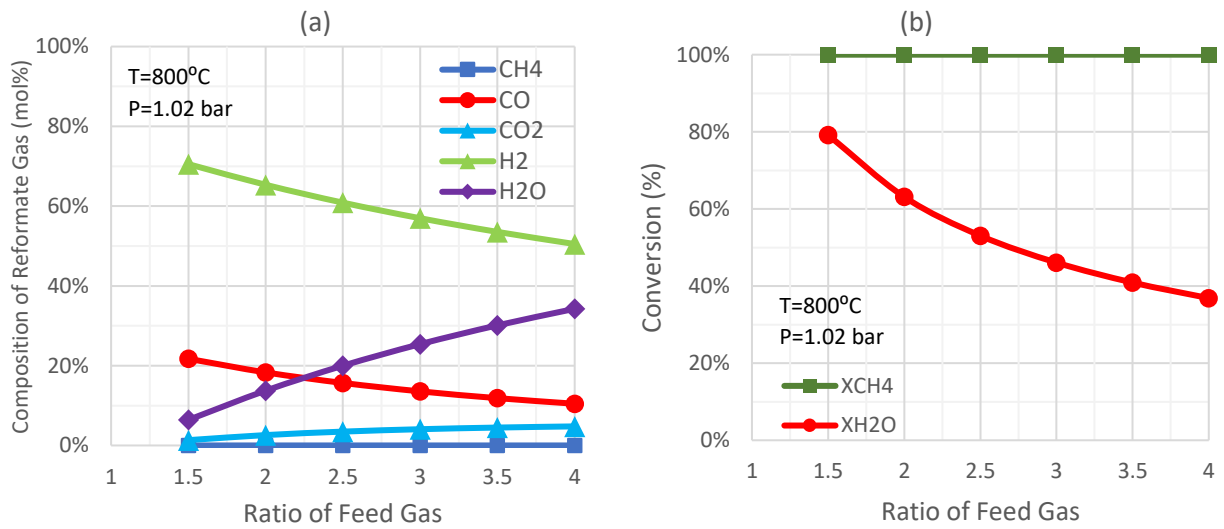


Figure 10: Effect of the mass flow ratio of feed gas on the SMR process (present work): (a) composition of reformate gas; (b) conversion rates of methane and steam

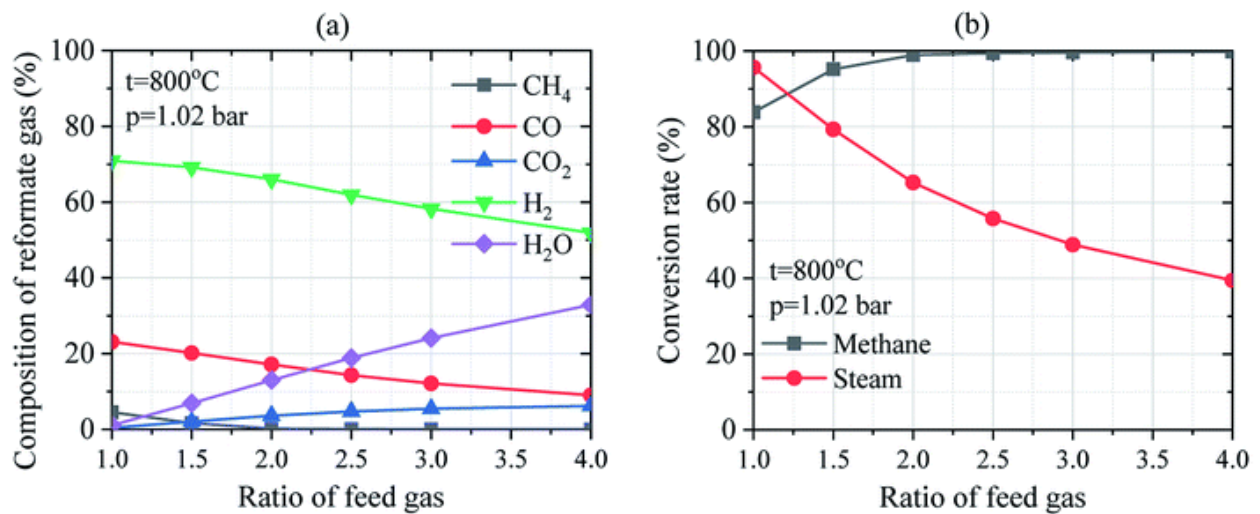


Figure 11: Effect of the mass flow ratio of feed gas on the SMR process (Shagdar, et al., 2020): (a) composition of reformate gas; (b) conversion rates of methane and steam

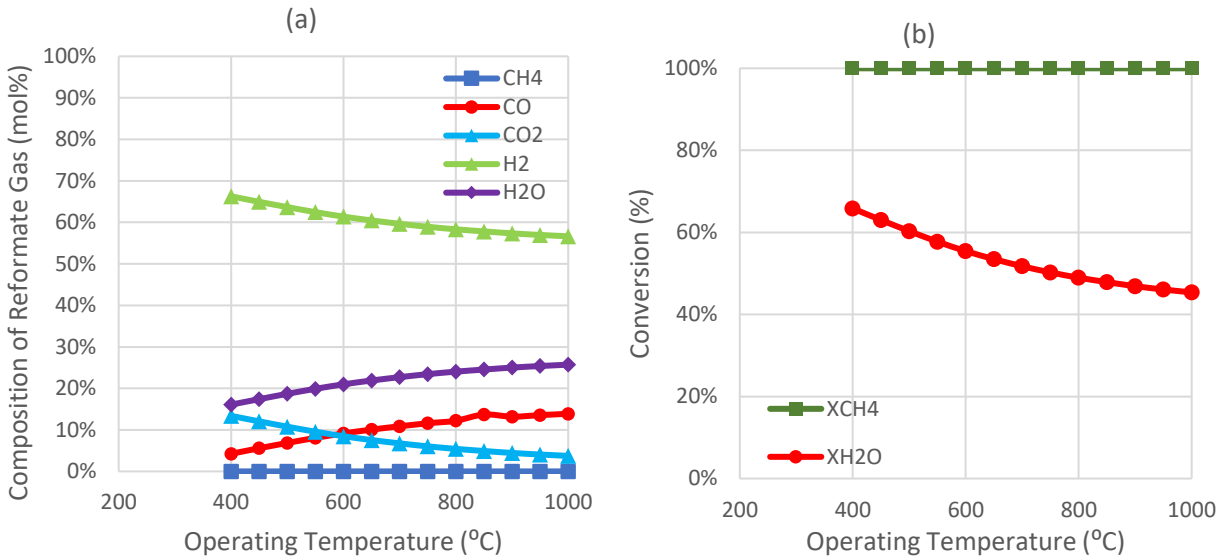


Figure 12: Effect of operating temperature on the SMR process (present work): (a) composition of reformate gas; (b) conversion rates of methane and steam

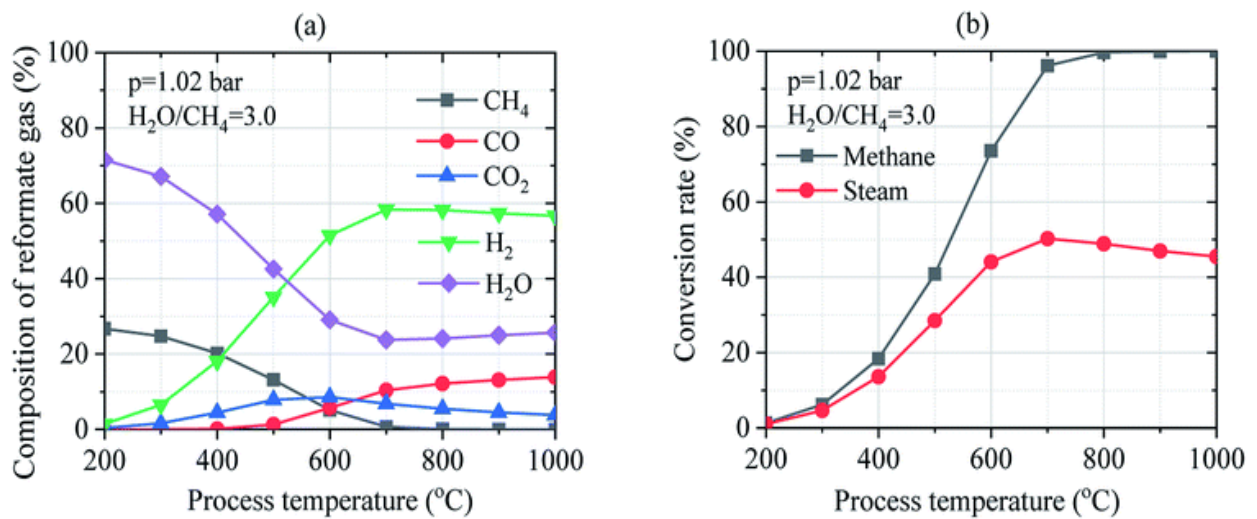


Figure 13: Effect of operating temperature on the SMR process (Shagdar, et al., 2020): (a) composition of reformate gas; (b) conversion rates of methane and steam

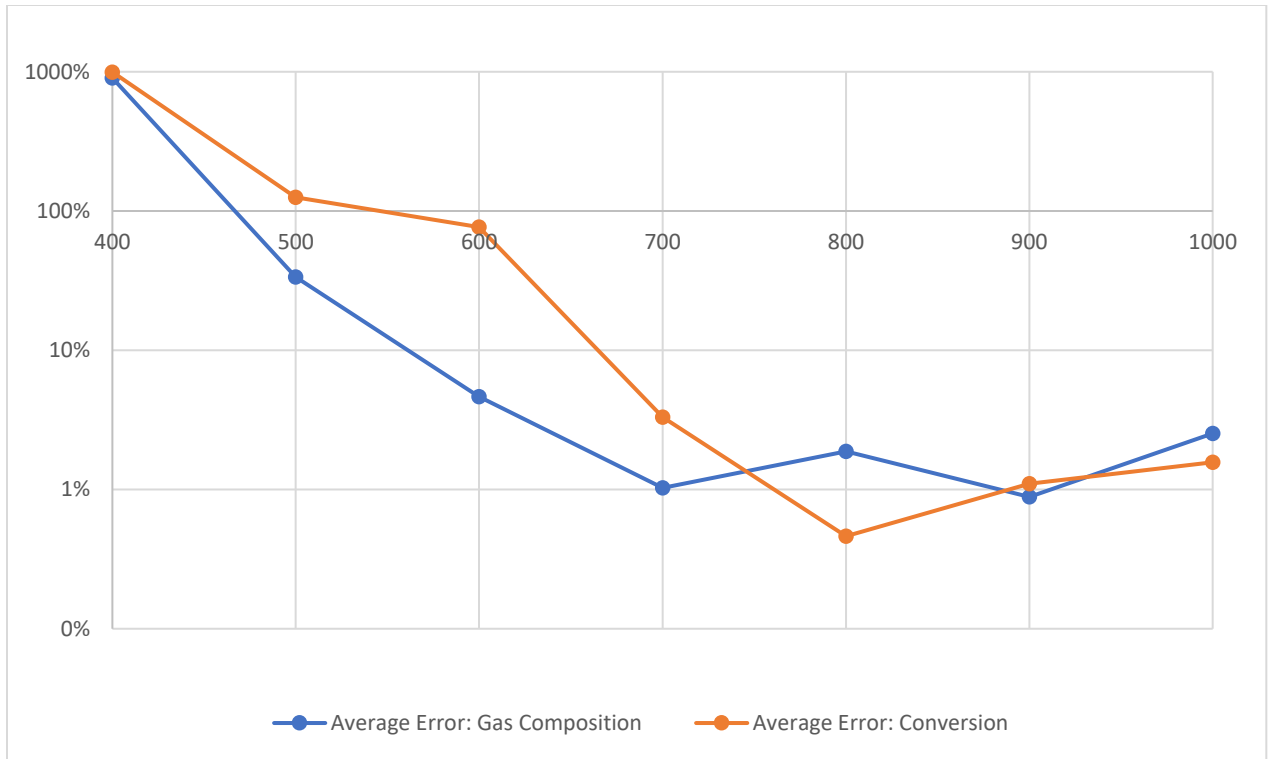


Figure 14: Average Absolute Error of the Present Model against Shagdar et al. (2020) [CH<sub>4</sub> omitted, Logarithmic scale]

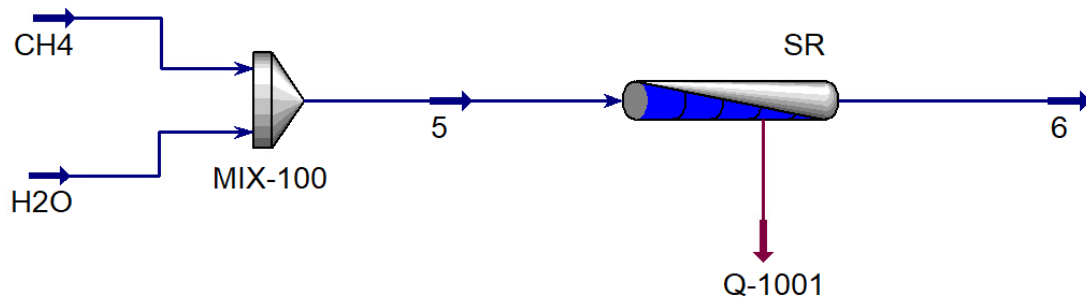


Figure 15: Flowsheet for Model Validation (Identical Conditions to Main Model)