MASTER'S THESIS ASSIGNMENT

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Study program:	**Master of Automotive Engineering**		
Branch of study:	**Advanced Powertrains**		

II. Master's thesis details

Master's thesis title in English:

Hydrogen production, storage and distribution for a powertrain test laboratory

Master's thesis title in Czech:

Výroba, skladování a rozvod vodíku na zkušebně pohonů

Guidelines:

Carry out a literature and a market search of available means for hydrogen supply for powertrain test laboratory.
Carry out a comparison of various concepts for on-site hydrogen production.
Propose and size the hydrogen storage and distribution system.
Consider various laboratory testing scenarious with different power demands.
Take into account the possibility of testing the hydrogen internal combustion engines for heavy duty application.

Bibliography / sources:

SAE Digital Library
Elsevier
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Date of master's thesis assignment: **30.10.2020** Deadline for master's thesis submission: **06.01.2021**

Assignment valid until: ____________

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Supervisor's signature	Head of department's signature	Dean's signature

III. Assignment receipt

The student acknowledges that the master's thesis is an individual work. The student must produce his thesis without the assistance of others, with the exception of provided consultations. Within the master's thesis, the author must state the names of consultants and include a list of references.

Date of assignment receipt	Student's signature

Czech Technical University In Prague

Faculty Of Mechanical Engineering

Master Of Automotive Engineering

Thesis Report

Hydrogen production, storage and distribution for a powertrain test laboratory

Supervisor: Ing. Vávra Jiří Ph.D., Faculty of Mechanical Engineering

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Date: 04-01-2021

Czech Technical University in Prague

Declaration

I, Abhishek Vijay Senghani declare that this report is completely written by me as a result of my own research and work. All the external sources used directly or indirectly are clearly marked and quoted. The sources are all acknowledged in the right manner.

This work has neither been submitted in part or full to any institute or authority for other qualification, nor it has been published elsewhere.

Prague January 4, 2021

Abhishek Vijay Senghani

Abstract

The main objective of the report was to carry out a literature search of available means for hydrogen supply for powertrain test laboratory. Carry out a comparison of various concepts of on-site hydrogen production. Propose and size hydrogen storage and distribution system.

In this study, a brief explanation of currently used hydrogen production and hydrogen storage systems are discussed. A detailed study on hydrogen requirement for a single cylinder dual fuel engine was calculated based on certain operating conditions.

Based on these hydrogen requirements the cylinder requirement was calculated by three different gas models. Market survey was done and suppliers were selected and compared based on their product specification.

A survey of hydrogen onsite production suppliers was also done based on flow rate required for low hydrogen demand and high hydrogen demand of the powertrain laboratory.

Models of the most widely used hydrogen production technologies was also developed and validated in this thesis. Based on the results from these models the fuel requirements and cost of producing hydrogen for these most widely used technologies was calculated.

Keywords: Hydrogen Storage, Hydrogen Production, Distribution of Hydrogen, Powertrain Test Laboratory.

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I would especially like to thank Dr. Ing. Gabriela Achtenová who guided me all through my master's study in Prague. Last but not the least, I am grateful to my parents for all the love and support given throughout my stay abroad.

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Abbreviations

SMR – steam methane reforming

WGS – Water gas Shift Reaction

SRK – Soave Redlich Kwong

BTE – Brake Thermal Efficiency

PEM –Proton Exchange Membrane

LHV –Lower Heating Value

PSA –Pressure Swing Absorption

1. Introduction

1.1. Motivation

In upcoming years, decrease in supply of fossil fuels will change. World of automotive will change drastically and new vehicles will have become an essential part of day-to-day commute for humans and goods transport. When it comes to the fuel for future hydrogen is a promising candidate. When this new change will come there will be a need to update the current testing facilities to accommodate this new change.

1.2. Objective

The foremost purpose of this research work is to study the available technology for hydrogen production, hydrogen storage and to calculate the required amount of hydrogen. To achieve these goals, the following objectives are defined:

- To build a model to calculate amount of required hydrogen of a dual fuel engine operating on hydrogen and diesel.
- To calculate the number of cylinders that will be required to store this hydrogen.
- To model hydrogen production of best commercially available technology.
- To perform a market survey of available suppliers and compare them.
- To estimate fuel costs for these available technologies.

2. Literature review

2.1. Background of hydrogen production

Hydrogen is the simplest and most abundant element on earth. Hydrogen has a heating value of 120MJ/kg [1], this energy is extracted during the combustion in dual fuel engine. Since hydrogen is abundant and as fossil fuel continues to decline hydrogen being a clean fuel with less emissions can be used in fuel cells for powering automobiles by generating electricity. Hydrogen has a very high energy yield of 122KJ/kg and is 2.75 times more than hydrocarbon fuels [2].

2.2. Hydrogen production methods

Hydrogen global production has so far been mostly done by a conversion from fossil fuels, with the many different technologies. There are many methods described in figure 2.1, But only the two most commonly used being the steam reforming of hydrocarbons such as methane, other being electrolysis of water [3] are discussed in this study.

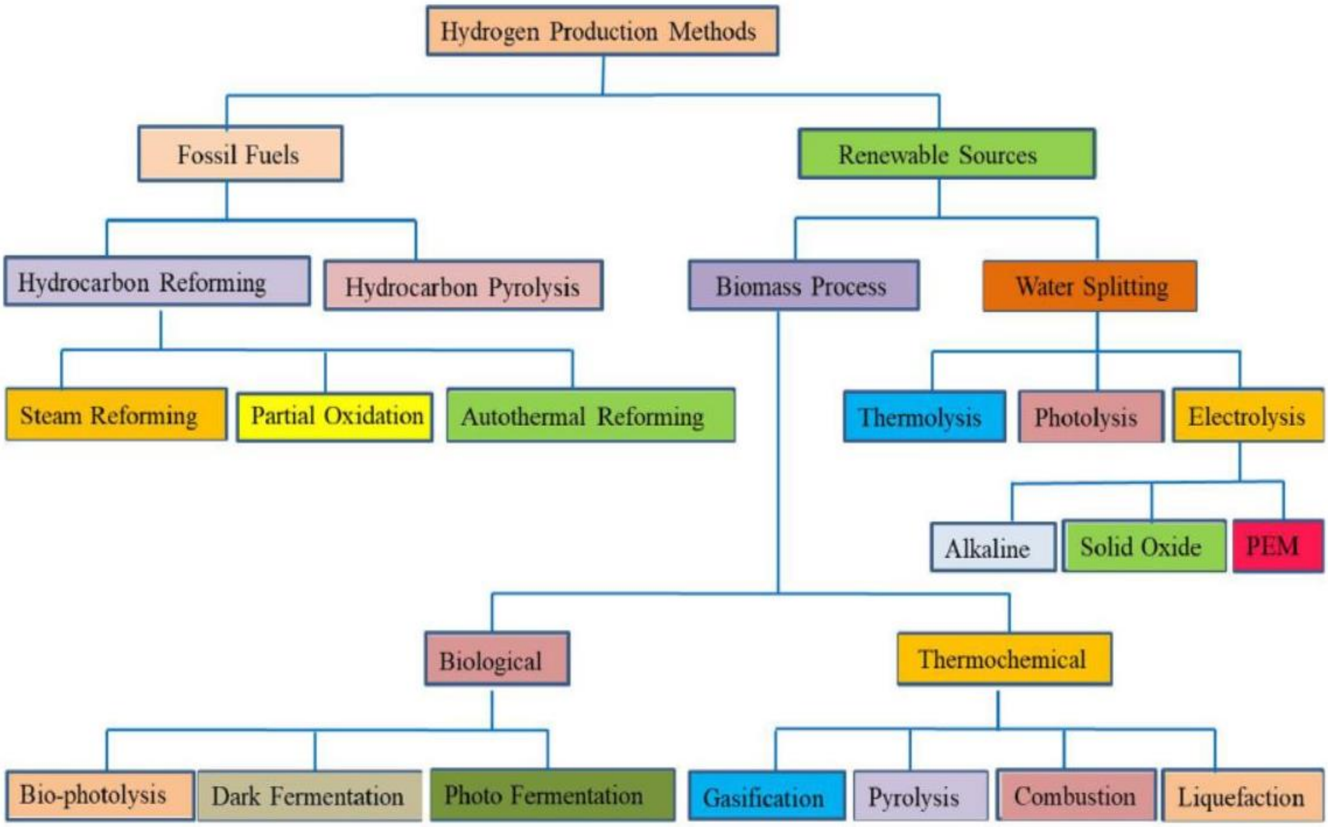


Figure 2.1 Hydrogen production methods [4]

2.3. Steam reforming

Steam methane reforming (SMR) is the technology used to produce hydrogen. Fuel used to produce hydrogen is Natural gas as it is very common and is easily available as a fuel. Infrastructure already exists for extracting, transporting, and storing of natural gas. Furthermore, SMR can be operated using other hydrocarbons such as gasoline and methanol in its process. Mostly 75% of the world’s hydrogen production is produced by using methane and natural gas.

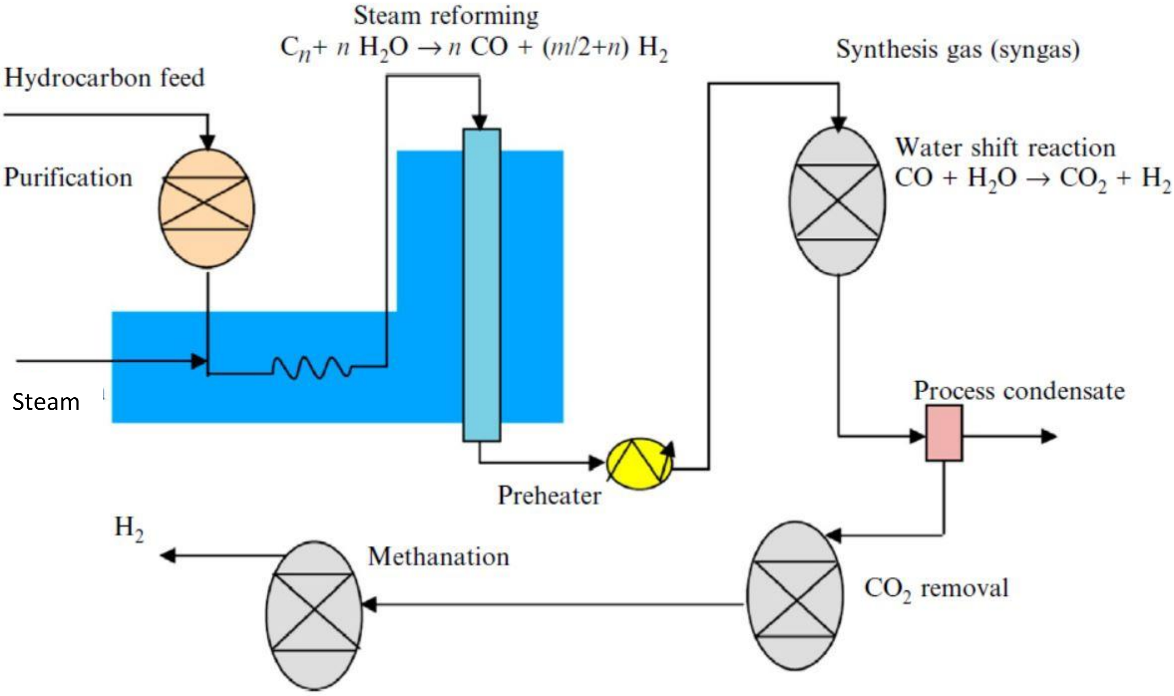


Figure 2.2 Steam methane reforming process [5]

2.3.1. SMR working process

- Hydrocarbon feed consisting of natural gas is purified and fed into reformer. purification mainly involves desulphurization process, in which all Sulphur content present in hydrocarbon feed must be removed because Sulphur is very poisonous for steam reforming catalyst after purification all Sulphur will be converted to hydrogen sulphide [6].

- Hydrocarbon feed must include certain content of hydrogen for hydrodesulphurization process in order to protect the catalyst in downstream in the reformer [6].It is typically required for Sulphur based species to be reduced to 0.01ppm [7].

- Steam is fed in reformer based on a certain steam to carbon ratio (S/C) with amount of carbon present in hydrocarbon feed. This ratio is very important and has a value of 3 or above [3] to avoid carbon formation.
- Steam and natural gas enter the reformer which is generally operated in range of 800˚C-1000˚C temperature and 1.4-2.5Mpa pressure [7].
- The reactions in reformer occurs over a Ni based metal catalyst because they have a high tolerance for Sulphur and are less costly compared to other metal-based catalyst [7].

Reforming reaction

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2 \quad (\Delta H_{298} = +206 kJ/mol)$$

Watergas shift reaction (WGS)

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \quad (\Delta H_{298} = -41.2 kJ/mol)$$

- Steam reforming reaction is strongly endothermic and water gas shift reaction is weakly exothermic, therefore it is required to occur at different temperatures.
- After WGS reaction the condensate which is mainly water is extracted from syngas, also carbon dioxide is separated, most commercial used method to purify hydrogen is Pressure Swing Absorption Technology (PSA) after passing through PSA absorber the output gas contains maximum amount of pure hydrogen.

2.3.2. Steam methane reforming advantages

- SMR is most efficient, economical and most widely used technology for producing hydrogen.
- The efficiency of SMR is around 70% to 85% which is very high compared to many other currently available technologies to produce hydrogen [8].
- The cost of hydrogen produced is currently tied to price of natural gas and due to this SMR is the least expensive way to produce hydrogen in bulk.

2.3.3. Steam methane reforming limitations

- Operating SMR at higher temperature can lead to higher methane conversion but currently this temperature is limited by tube material limitations.
- Higher temperature with low S/C ratio can lead to coke formation which may block the tubes inside reformer and can lead to hot spots and can cause catalyst deactivation.
- If we try to decrease the coke formation by increasing the S/C ratio we will require more energy, thereby decreasing the efficiency of system
- SMR also causes formation of CO_2 and CO as a by-product which leads to greenhouse effect and causes environmental damage.

2.3.4. Typical operating conditions of SMR

Parameter	Unit	Value
Outlet temperature from furnace	˚C	880
Outlet pressure from furnace	bar	24
H_2O/C molar ratio	-	4.0

Table 2.1 Typical operating parameters of SMR [7]

2.4. Electrolysis

The electrolysis is the process of separating water molecules by supplying electrical energy, this method is normally used in production of hydrogen by renewable energy resources such as wind, solar and geothermal.

2.4.1. Electrolyser working process

- Water is fed into the anode side of electrolyser where it gets split into oxygen (O2), and (H+) and (e-).
- These (H+) protons then travel via conducting medium this maybe Proton Exchange Membrane (PEM), Alkaline electrolyte or solid oxide. To cathode side.
- The electrons travel through external circuit and combine with (H+) protons to form H_2 at cathode side. The Illustration of this process is shown in Fig.2.3

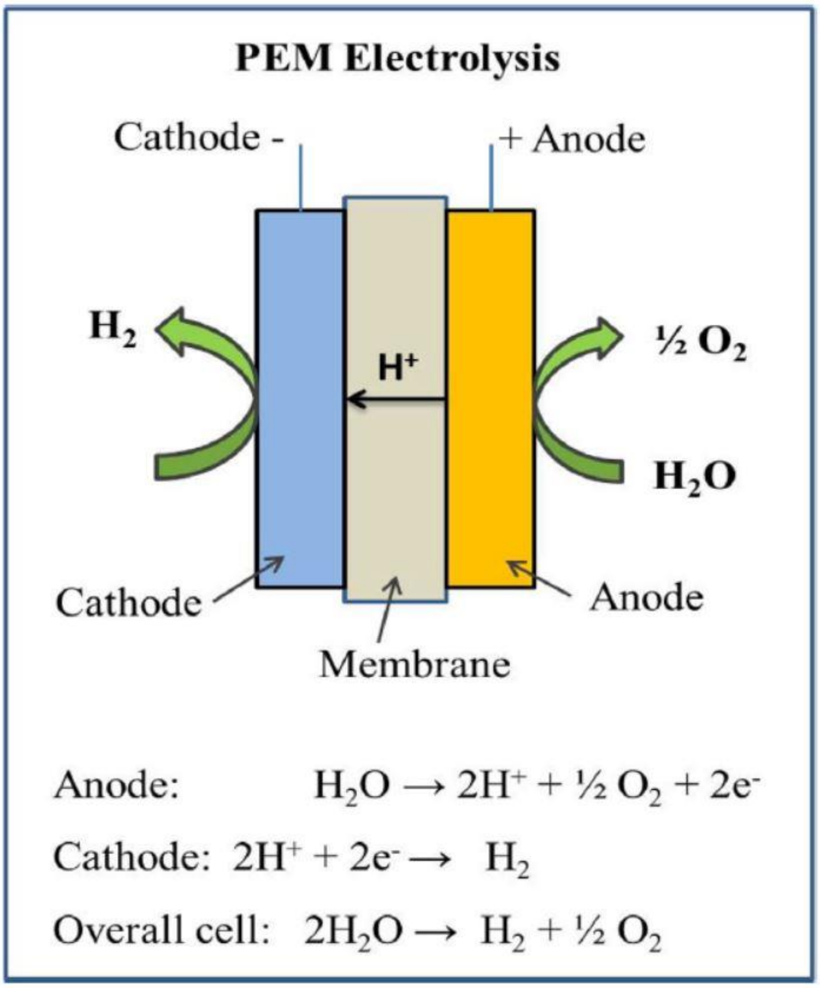


Figure 2.3 Schematic illustration of PEM water electrolysis [8]

2.4.2. Types of electrolyser cell configuration

- Unipolar configuration

  This type of arrangement of cells is also called mono polar configuration or arrangement of cells in parallel. This type of configuration has a cell voltage of about 2.2V. This type of configuration is simple and easy to maintain, but has high ohmic losses at low voltages [9].

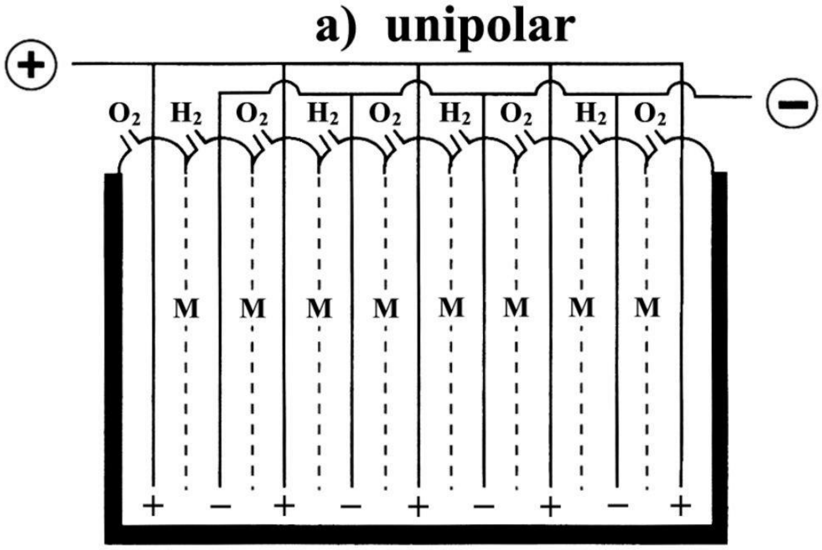


Figure 2.4 Unipolar cell configuration [9]

- Bipolar Configuration

  This type of arrangement of cells is also called series arrangement. The typical cell voltage of a bipolar configuration is 2.2 x (n-1) V, where n is no of electrodes. This type of arrangement has low ohmic losses but requires high precision in design and manufacturing to avoid gas leakages between cells [9].This type of electrolyser configuration are most commonly manufactured nowadays [10].

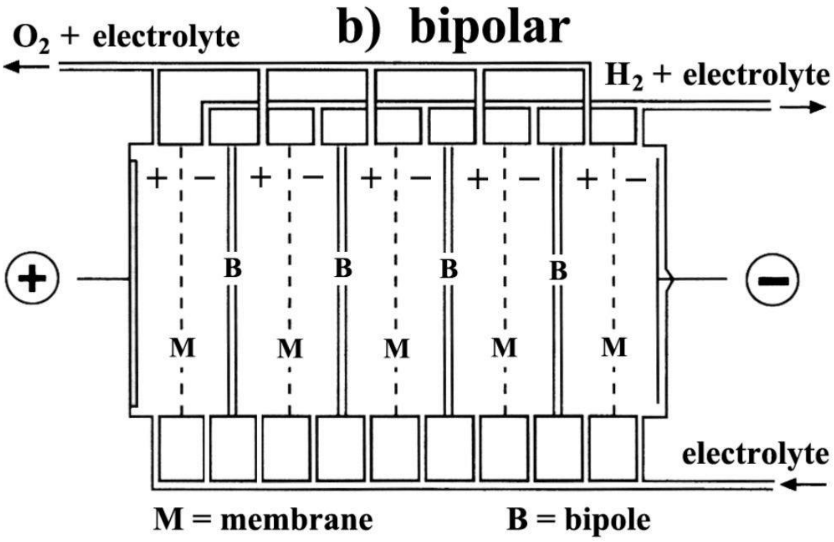


Figure 2.5 Bipolar cell configuration [9]

Parameter	Unit	Value
Power	MW	10^{-6}-10
Active area	cm^2	1-1500
Power density	$W*cm^{-2}$	1.8-3.6
Current density	$A*cm^{-2}$	1-2.5
Nominal cell voltage	V	1.8 at 1 $A*cm^{-2}$
Nominal temperature	˚C	50-70
Maximal temperature	˚C	80
Nominal O_2 pressure	bar	1-25
Nominal H_2 pressure	bar	1-70
Nominal ΔP	bar	10

Table 2.2 Typical operating parameters of conventional PEM cell [11]

2.4.3. Comparison between SMR and electrolysis

Steam Methane Reforming	Electrolysis
Efficiency around 70-85% **[8]**	Efficiency around 50-70% [8]
Releases greenhouse gases as a byproduct	By product of electrolysis is oxygen
It is mostly used technology for high scale hydrogen production	This technology is used in small to medium scale production of hydrogen
Cost of production of hydrogen is low but as it is a complex process more components are required increasing initial cost	Cost of production is high since electrical energy required for splitting water molecules is high, but it is fairly simple process and less components are required compared to SMR lowering initial cost
Uses hydrocarbon fuel as feed to generate hydrogen	Uses water as feed to generate hydrogen
Cost of maintaining is high	Low cost of maintaining

Table 2.3 SMR and electrolysis comparison

2.5. Hydrogen storage

Hydrogen has a very low density by volume which results in large storage vessels required to store hydrogen. There are many ways to navigate this problem such as pressurizing hydrogen gas, lowering temperature of gas and liquefying hydrogen, or storing hydrogen in metal hydride. The most common used method used to store hydrogen is by compressing it at high pressures this is because it is a very simple method with less cost of storing compared with other methods [12]. For this reason, only hydrogen storage in compressed form is discussed in this thesis.

To estimate our hydrogen storage required, we cannot use Ideal gas model for estimating volume occupied by hydrogen at different temperature and pressure because of following reasons.

- Real gases have small attraction and repulsion forces between gas particles and ideal gases do not have such forces.
- Real gas particles occupy a volume and ideal gas particles are assumed to occupy no volume.
- Real gas particles have collisions which are inelastic (Energy is lost in collisions) and ideal gas particles collide elastically.

Hence, real gas models such as Van Der Waals Gas Model and Soave Redlich Kwong (SRK) Model will be used to predict hydrogen storage requirements.

2.5.1. Van Der Waals Gas Model

The equation of state by Van Der Waal is given by

$$P = \frac{RT}{V - b} - \frac{a}{V^2}$$

Where, P = Pressure, V = Volume, R = Universal gas constant,

T = Temperature, “a” and “b” are physical parameters specific to fluid.

The results given by van der waals are generally qualitatively in agreement with experimental data, but the results are not accurate enough to be used in engineering calculations. The equation by van der waal uses only two physical parameters “a” and “b” which are not enough to predict the compressibility factor [13].

2.5.2. Soave Redlich Kwong (SRK) Model

The equation of state by SRK is given by

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)}$$

The parameters are same as in Van Der Waals equation, but the physical parameters i.e. “a” and “b” in SRK model accounts for acentric factor which is conceptual number given by Kenneth Pitzer in year 1955 which takes into account the non-sphericity of molecules thereby increasing the accuracy of results very close experimental values.

Van Der Waal equation gives largest error in liquid region and SRK equation gives much better results in vapor region [13].

A convenient approach to adjust the behavior for real gas from Ideal gas is to use compressibility factor denoted by Z. The deviation of Z from 1 is deviation of real gas from Ideal gas. It is found that at ambient temperature and at a 300 bar pressure value of Z is found to be 1.2, this means that hydrogen in vessel at ambient temperature and 300 bar pressure will occupy 20% more volume than what is predicted by Ideal gas equation of state [14].

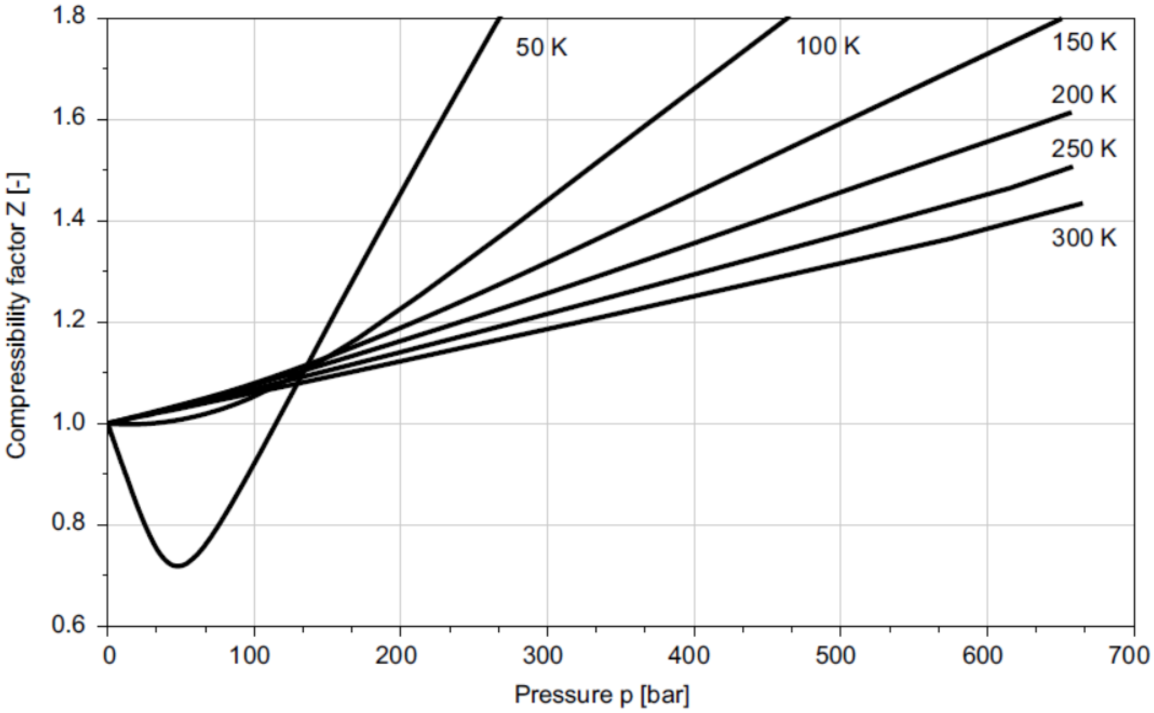
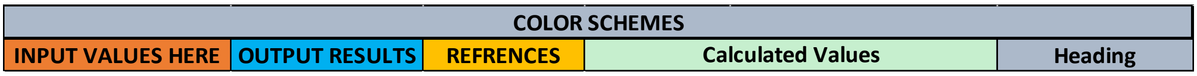


Figure 2.6 Compressibility factor Z for hydrogen [14]

3. Hydrogen requirement calculation model for laboratory

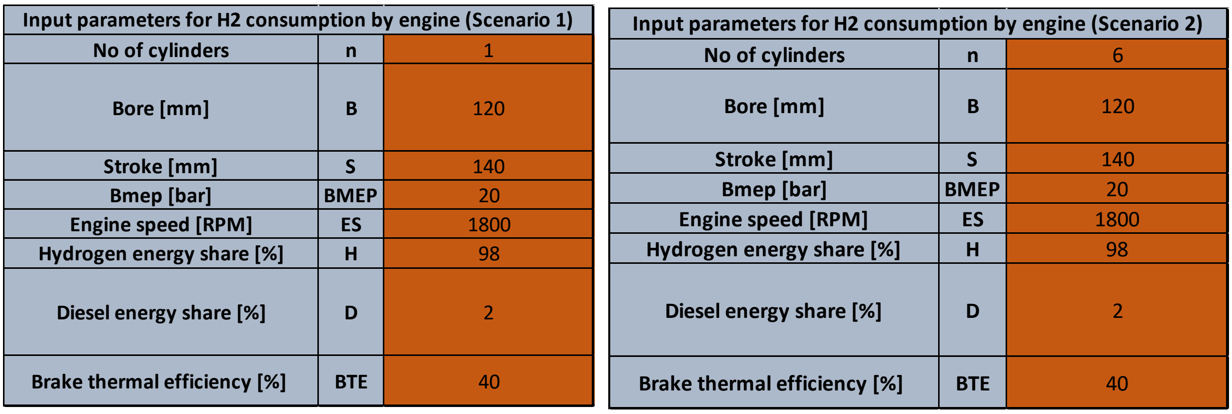
The Model is developed with the objective to calculate hydrogen requirement for multiple cylinder engines operating at different loads with variable hydrogen to diesel fuel ratio and other parameters such as break thermal efficiency, bore, stroke, Engine speed parameters which can be changed according to the requirements. It is important to describe the color scheme that will be used to describe various model in this thesis with image given in figure 3.1.



COLOR SCHEMES				
INPUT VALUES HERE	OUTPUT RESULTS	REFRENCES	Calculated Values	Heading

Figure 3.1 Color scheme

There are two Scenarios that are considered depending on Engine Size with all parameters being same but with the difference being in no of cylinders of engine. The images for input parameters for Scenario 1 and Scenario 2 are given from model made in excel in below figure 3.2.



Input parameters for H2 consumption by engine (Scenario 1)		
No of cylinders	n	1
Bore [mm]	B	120
Stroke [mm]	S	140
Bmep [bar]	BMEP	20
Engine speed [RPM]	ES	1800
Hydrogen energy share [%]	H	98
Diesel energy share [%]	D	2
Brake thermal efficiency [%]	BTE	40

Input parameters for H2 consumption by engine (Scenario 2)		
No of cylinders	n	6
Bore [mm]	B	120
Stroke [mm]	S	140
Bmep [bar]	BMEP	20
Engine speed [RPM]	ES	1800
Hydrogen energy share [%]	H	98
Diesel energy share [%]	D	2
Brake thermal efficiency [%]	BTE	40

Figure 3.2 Input parameters for H_2 requirement calculation

3.1. Basic relations used in model

Piston Area (m^2) [1] $A=\frac{\pi}{4}*\left(B*10^{-3}\right)^2$

Displacement Volume (dm^3) [1] $V_d=n*\frac{\pi}{4}*\left(B*10^{-3}\right)^2*S$

Brake Torque (Nm) [1] $T_b=\frac{V_d\ [dm^3]*BMEP\ [kPa]}{6.28*n_R}$

Brake Power (kW) [1] $P_b=\frac{BMEP\ [kPa]*V_d\ [dm^3]*ES\ [RPM]}{n_R*10^3*60}$

Mass flow rate diesel (kg/h) [15] $M_D = \frac{P_b\,[kW]*3.6}{Q_{LHV(D)}\ [\text{MJ/kg}]*BTE[\%]*0.01} * \left(\frac{\text{D}\ [\%]}{100}\right)$

Mass flow rate H₂ (kg/h) [15] $M_H = \frac{P_b\,[kW]*3.6}{Q_{LHV(H_2)}\ [\text{MJ/kg}]*BTE[\%]*0.01} * \left(\frac{H\ [\%]}{100}\right)$

Brake specific fuel consumption (g/kWh) [15] $BSFC = \frac{M_D[kg/h]+M_H[kg/h]}{P_b[kW]} * 10^3$

Brake specific energy consumption (MJ/kWh)

$$BSEC = \frac{M_D[kg/h]*Q_{LHV(d)}[MJ/kg]+M_{H_2}[kg/h]*Q_{LHV(H_2)}[MJ/kg]}{P_b\ [kW]} = \frac{1}{BTE\ [\%]*0.01} * 3.6$$

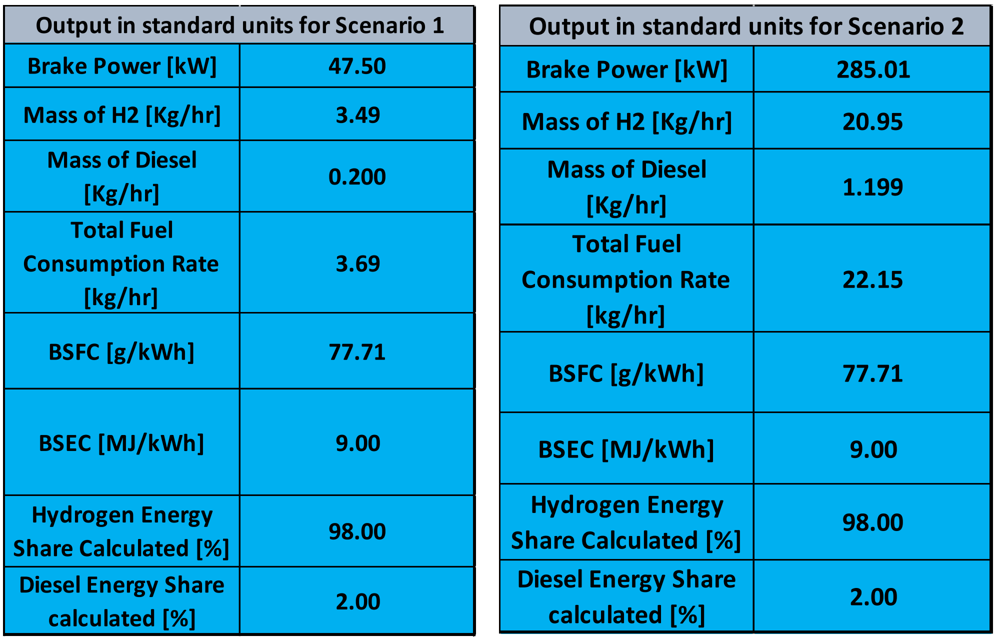
Hydrogen energy share (%) [16] $H = \frac{\dot{m}_{H_2} * Q_{LHV(H_2)}}{\dot{m}_d * Q_{LHV(d)} + \dot{m}_{H_2} * Q_{LHV(H_2)}}$

Diesel energy share (%) $D = \frac{\dot{m}_d * Q_{LHV(d)}}{\dot{m}_d * Q_{LHV(d)} + \dot{m}_{H_2} * Q_{LHV(H_2)}}$

- The values if $Q_{LHV(H2)}$ is 120 MJ/kg and $Q_{LHV(D)}$ is 42.8 MJ/kg [1].

3.2. Mapping engine at full load

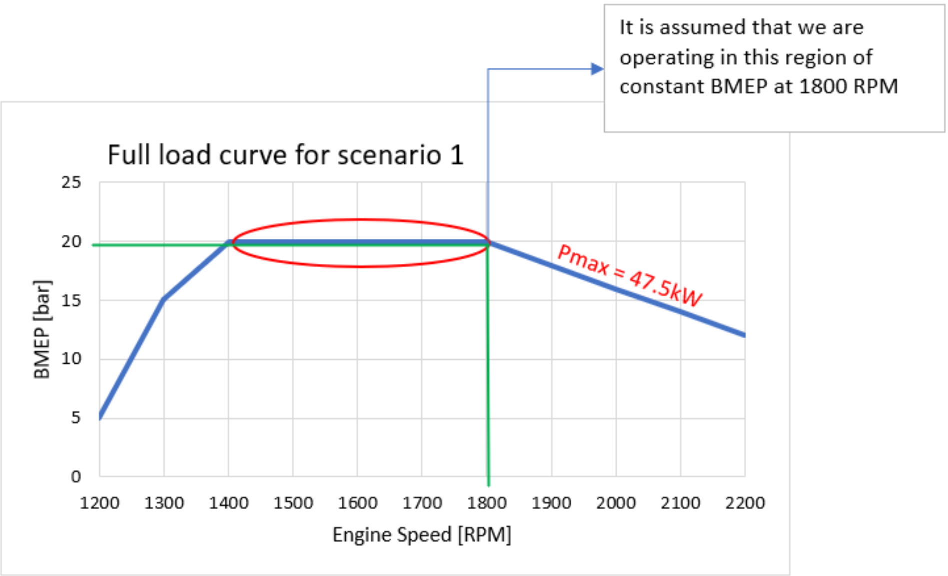
For the engine with Scenario 1 and Scenario 2 at its maximum brake power we get our requirement of hydrogen for a single test for running engine for 1 hour we get the following results described in figure 3.3.



Output in standard units for Scenario 1	
Brake Power [kW]	47.50
Mass of H2 [Kg/hr]	3.49
Mass of Diesel [Kg/hr]	0.200
Total Fuel Consumption Rate [kg/hr]	3.69
BSFC [g/kWh]	77.71
BSEC [MJ/kWh]	9.00
Hydrogen Energy Share Calculated [%]	98.00
Diesel Energy Share calculated [%]	2.00

Output in standard units for Scenario 2	
Brake Power [kW]	285.01
Mass of H2 [Kg/hr]	20.95
Mass of Diesel [Kg/hr]	1.199
Total Fuel Consumption Rate [kg/hr]	22.15
BSFC [g/kWh]	77.71
BSEC [MJ/kWh]	9.00
Hydrogen Energy Share Calculated [%]	98.00
Diesel Energy Share calculated [%]	2.00

Figure 3.3 Output for single test for running engine for 1 hour



It is assumed that we are operating in this region of constant BMEP at 1800 RPM

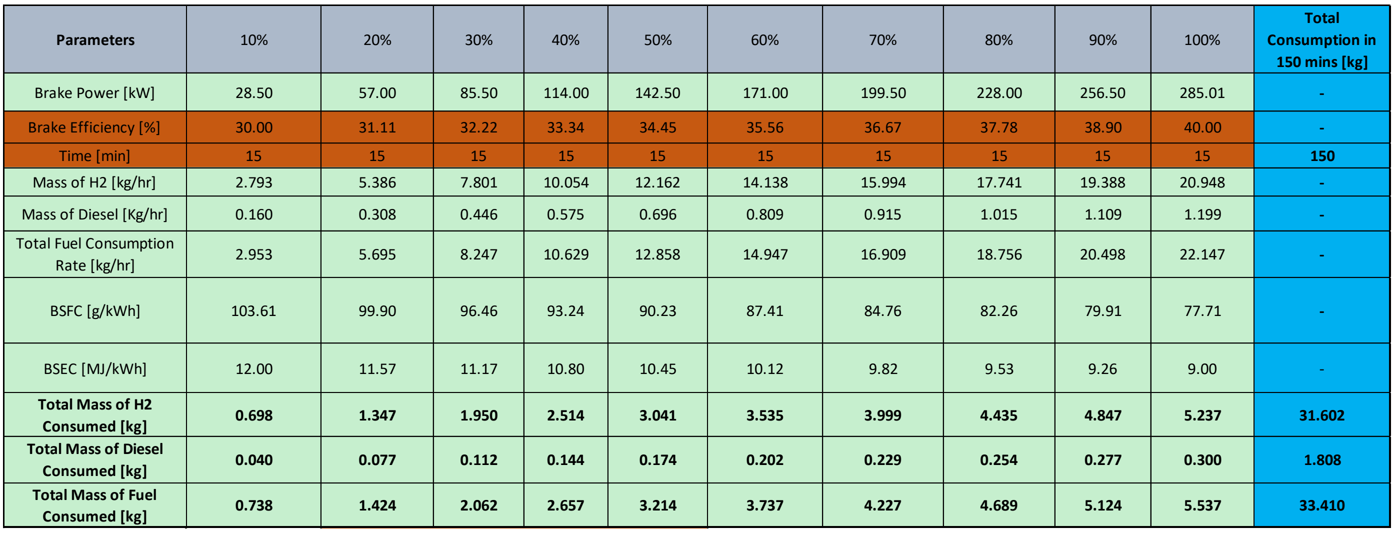
Figure 3.4 BMEP vs Engine speed graph

Assuming we will map the engine in 10 cycles, with each cycle engine operates for 15 minutes each and varying engine brake power from 10 to 100% of its value also changing the brake thermal efficiency from 30 to 40% linearly. We get our hydrogen requirement for both Scenario 1 and Scenario 2. The output for such task is described in Fig 3.5 and Fig 3.6.

Parameters	10%	20%	30%	40%	50%	60%	70%	80%	90%	100%	**Total Consumption in 150 mins [kg]**
Brake Power [kW]	4.75	9.50	14.25	19.00	23.75	28.50	33.25	38.00	42.75	47.50	-
Brake Efficiency [%]	30.00	31.11	32.22	33.34	34.45	35.56	36.67	37.78	38.90	40.00	-
Time [min]	15	15	15	15	15	15	15	15	15	15	**150**
Mass of H2 [kg/hr]	0.466	0.898	1.300	1.676	2.027	2.356	2.666	2.957	3.231	3.491	-
Mass of Diesel [Kg/hr]	0.027	0.051	0.074	0.096	0.116	0.135	0.153	0.169	0.185	0.200	-
Total Fuel Consumption Rate [kg/hr]	0.492	0.949	1.375	1.772	2.143	2.491	2.818	3.126	3.416	3.691	-
BSFC [g/kWh]	103.61	99.90	96.46	93.24	90.23	87.41	84.76	82.26	79.91	77.71	-
BSEC [MJ/kWh]	12.00	11.57	11.17	10.80	10.45	10.12	9.82	9.53	9.26	9.00	-
Total Mass of H2 Consumed [kg]	**0.116**	**0.224**	**0.325**	**0.419**	**0.507**	**0.589**	**0.666**	**0.739**	**0.808**	**0.873**	**5.267**
Total Mass of Diesel Consumed [kg]	**0.007**	**0.013**	**0.019**	**0.024**	**0.029**	**0.034**	**0.038**	**0.042**	**0.046**	**0.050**	**0.301**
Total Mass of Fuel Consumed [kg]	**0.123**	**0.237**	**0.344**	**0.443**	**0.536**	**0.623**	**0.705**	**0.782**	**0.854**	**0.923**	**5.568**

Figure 3.5 Hydrogen consumption Scenario 1

From this, we get our hydrogen consumption, but it is better to have some reserve factor therefore considering a reserve factor of 2 for both scenarios, we can conclude that we would require 11 kg of hydrogen for Scenario 1.



Parameters	10%	20%	30%	40%	50%	60%	70%	80%	90%	100%	**Total Consumption in 150 mins [kg]**
Brake Power [kW]	28.50	57.00	85.50	114.00	142.50	171.00	199.50	228.00	256.50	285.01	-
Brake Efficiency [%]	30.00	31.11	32.22	33.34	34.45	35.56	36.67	37.78	38.90	40.00	-
Time [min]	15	15	15	15	15	15	15	15	15	15	**150**
Mass of H2 [kg/hr]	2.793	5.386	7.801	10.054	12.162	14.138	15.994	17.741	19.388	20.948	-
Mass of Diesel [Kg/hr]	0.160	0.308	0.446	0.575	0.696	0.809	0.915	1.015	1.109	1.199	-
Total Fuel Consumption Rate [kg/hr]	2.953	5.695	8.247	10.629	12.858	14.947	16.909	18.756	20.498	22.147	-
BSFC [g/kWh]	103.61	99.90	96.46	93.24	90.23	87.41	84.76	82.26	79.91	77.71	-
BSEC [MJ/kWh]	12.00	11.57	11.17	10.80	10.45	10.12	9.82	9.53	9.26	9.00	-
Total Mass of H2 Consumed [kg]	**0.698**	**1.347**	**1.950**	**2.514**	**3.041**	**3.535**	**3.999**	**4.435**	**4.847**	**5.237**	**31.602**
Total Mass of Diesel Consumed [kg]	**0.040**	**0.077**	**0.112**	**0.144**	**0.174**	**0.202**	**0.229**	**0.254**	**0.277**	**0.300**	**1.808**
Total Mass of Fuel Consumed [kg]	**0.738**	**1.424**	**2.062**	**2.657**	**3.214**	**3.737**	**4.227**	**4.689**	**5.124**	**5.537**	**33.410**

Figure 3.6 Hydrogen consumption Scenario 2

We get our hydrogen requirement for scenario 2 to be approximately 64 kg.

Laboratory testing scenarios	**Hydrogen requirement [kg]**
Scenario 1	11
Scenario 2	64

Table 3.1 Results from model

4. Hydrogen storage model for powertrain test laboratory

We know our hydrogen requirement for both laboratory scenarios we need storage for it. There are many methods for storing hydrogen but most commercially hydrogen in stored in compressed from in gas cylinders.

To estimate out hydrogen cylinder requirement, there are three models made to give an idea about the number of cylinders required accounting for various temperature and pressures. As discussed in literature review section of hydrogen storage.

4.1. Van Der Waals Model

The equation of state given by Van Der Waal is

$$P = \frac{RT}{V-b} - \frac{a}{V^2} \text{ [13]}$$

Where “a” and “b” are specific parameters related to fluid in this case our fluid is hydrogen. “a” and “b” are given by formulas [13].

$$a = \frac{27}{64} * \frac{(RT_c)^2}{P_c},\ b = \frac{1}{8} * \left(\frac{R*T_c}{P_c}\right) \text{ [13]}$$

In these formulas T_c and P_c denotes critical temperature and critical pressure for hydrogen respectively. Values of T_c and P_c taken into account in model are 32.98K and 12.93 bar [13] respectively, and R is universal gas constant.

The equation of compressibility factor Z for Van Der Waal gas model is given by

$$(1)Z^3 - (B'+1)Z^2 + (A')Z - (A'B') = 0 \text{ [13]}$$

Solving this cubic equation, we can get value of Z, thereby knowing the value of volume occupied by gas under given temperature and pressure conditions. where,

$$A' = \frac{aP}{(RT)^2},\ B' = \frac{bP}{RT} \text{ [13]}$$

To get our volume occupied by actual gas we can use the following relation

$$Z = \frac{V_{actual}}{V_{Ideal}} = \frac{V_{actual}}{nRT/P} \text{ [17].}$$

We assume that we will be storing gas in a 50L cylinder so we divide total volume occupied by gas by 50 to get number of cylinders required for storing our required H_2 gas

4.2. Soave Redlich Kwong Gas (SRK) Model

The equation of state given by SRK Model is

$$P = \frac{RT}{V-b} - \frac{a}{V\left(V+b\right)} \text{ [13]}$$

The specific fluid parameters “a” and “b” are given by

$$a = 0.42748\frac{\left(RT_c\right)^2}{P_c}\left(1+\Omega\left(1-\frac{T}{T_c}\right)^{1/2}\right)^2,\ b = 0.08664\frac{RT_c}{P_c} \text{ [13]}$$

The specific fluid parameters differ from Van Der Waal as these account for acentric factor for hydrogen, value of this acentric factor ω is -0.217 [13].

The equation of compressibility factor Z for SRK model is given by

$$\left(1\right)Z^3 + \left(-1\right)Z^2 + \left(A' - B' - B'^2\right)Z - \left(A'B'\right) = 0 \text{ [13]}$$

The equation of A’ and B’ are same as that defined in Van Der Waal Model, hence we have all the parameters required to predict the number of cylinders required. We solve this cubic equation and fine the volume occupied by hydrogen gas.

The accuracy of SRK is more than Van Der Waal gas Model as mentioned earlier in Literature Review hence we need to validate SRK Model and use the result given by SRK as our cylinder requirements for Scenario 1 and Scenario 2.

4.3. H_2 storage model validation

To validate our SRK model experimental data was found in literature [18] and was compared to SRK as well as Van Der Waal Model, the parameter for comparison was compressibility factor Z at constant temperature of 298.15K varying pressure and observing variation in compressibility factor. The result is shown in figure 4.4

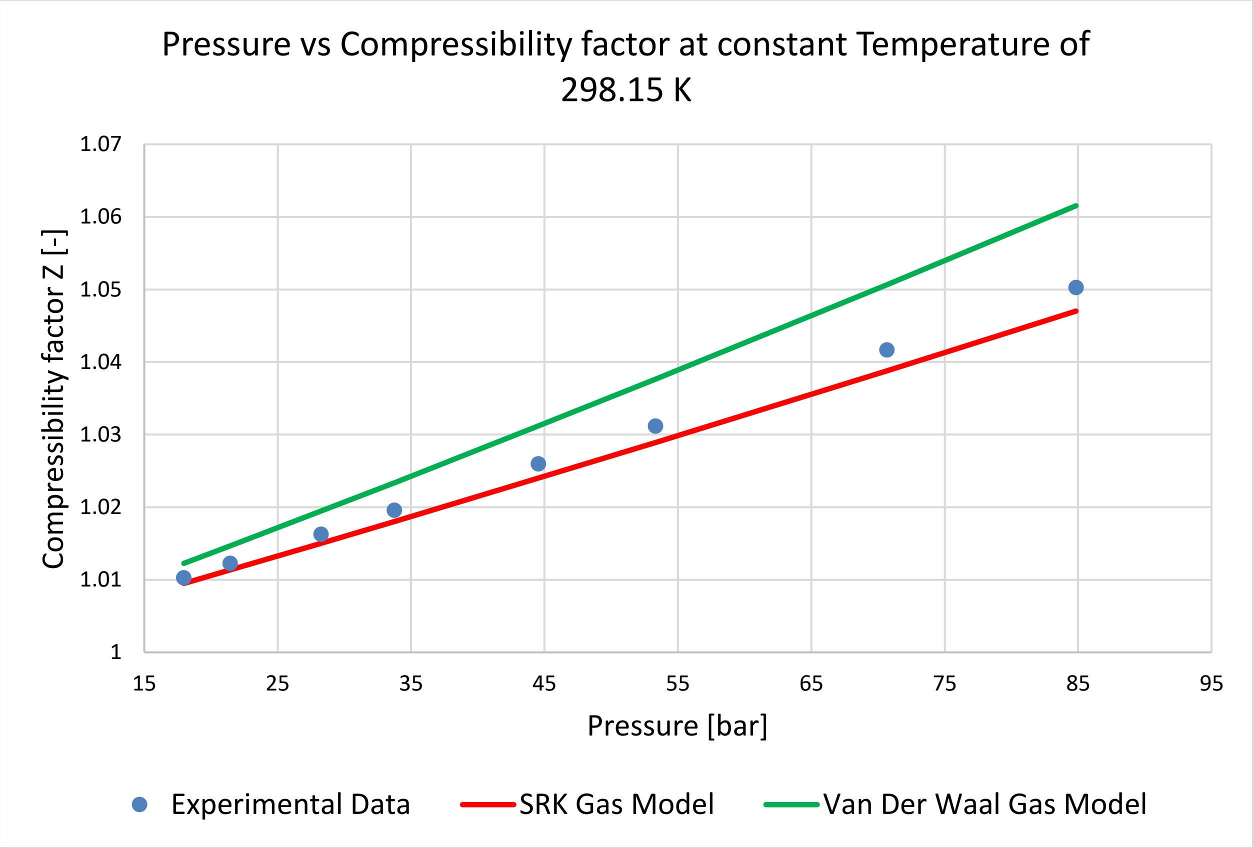


Figure 4.1 Experimental compressibility data comparisons with models

4.4. Results and conclusions from H_2 storage model

There are 3 models used to predict the cylinder requirements, out of these models SRK model gives most accurate results when compared to real experimental data but other models like Van Der Waal can give the upper limit or maximum number of cylinders required and Ideal gas Model give us the base line or minimum no of cylinders required for storage.

To get a good Idea on how each of these three models predict the volume occupied by H_2 gas as we change the pressure keeping temperature constant the results from three models is compared in the figure 4.2

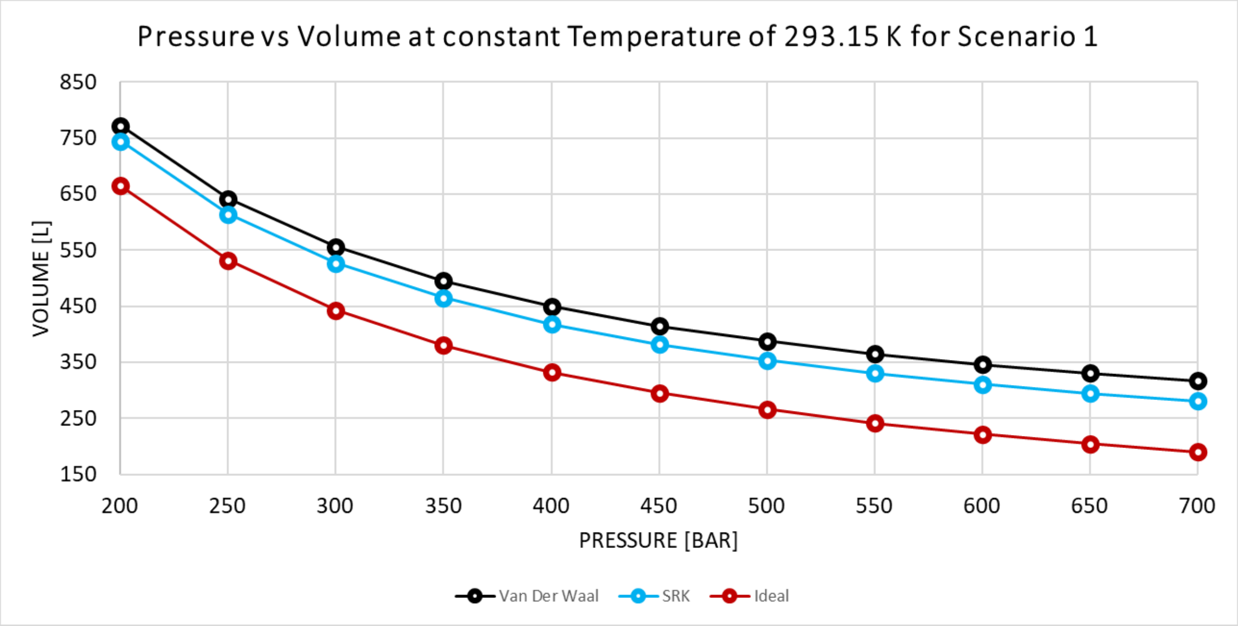


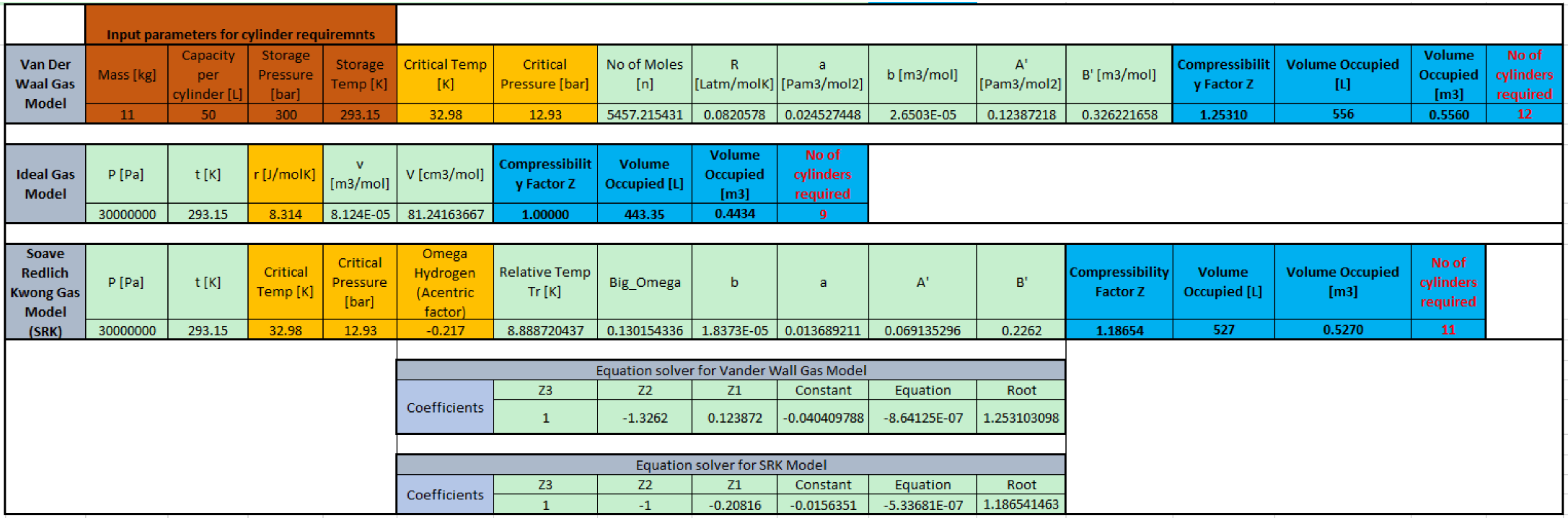
Figure 4.2 Comparison between H_2 storage models

For our powertrain laboratory testing Scenario 1 and Scenario 2, we assume that we will store H_2 at 300 bar pressure and 293.15K temperature, we also assume that each cylinder will have a storage capacity of 50L then results of number of cylinders required according to SRK Model is given in Table 4.1

Laboratory testing scenario	**Mass of hydrogen [Kg]**	**Cylinder requirement**
Scenario 1	11	11
Scenario 2	64	62

Table 4.1 Results from H_2 storage models

The hydrogen model to estimate cylinder requirement was made in Microsoft Excel with all formulas embedded in cells is shown in figure 4.3 and figure 4.4



	Input parameters for cylinder requiremnts															
Van Der Waal Gas Model	Mass [kg]	Capacity per cylinder [L]	Storage Pressure [bar]	Storage Temp [K]	Critical Temp [K]	Critical Pressure [bar]	No of Moles [n]	R [Latm/molK]	a [Pam3/mol2]	b [m3/mol]	A' [Pam3/mol2]	B' [m3/mol]	Compressibility Factor Z	Volume Occupied [L]	Volume Occupied [m3]	No of cylinders required
	11	50	300	293.15	32.98	12.93	5457.215431	0.0820578	0.024527448	2.6503E-05	0.12387218	0.326221658	1.25310	556	0.5560	12

Ideal Gas Model	P [Pa]	t [K]	r [J/molK]	v [m3/mol]	V [cm3/mol]	Compressibility Factor Z	Volume Occupied [L]	Volume Occupied [m3]	No of cylinders required
	30000000	293.15	8.314	8.124E-05	81.24163667	1.00000	443.35	0.4434	9

Soave Redlich Kwong Gas Model (SRK)	P [Pa]	t [K]	Critical Temp [K]	Critical Pressure [bar]	Omega Hydrogen (Acentric factor)	Relative Temp Tr [K]	Big_Omega	b	a	A'	B'	Compressibility Factor Z	Volume Occupied [L]	Volume Occupied [m3]	No of cylinders required
	30000000	293.15	32.98	12.93	-0.217	8.888720437	0.130154336	1.8373E-05	0.013689211	0.069135296	0.2262	1.18654	527	0.5270	11

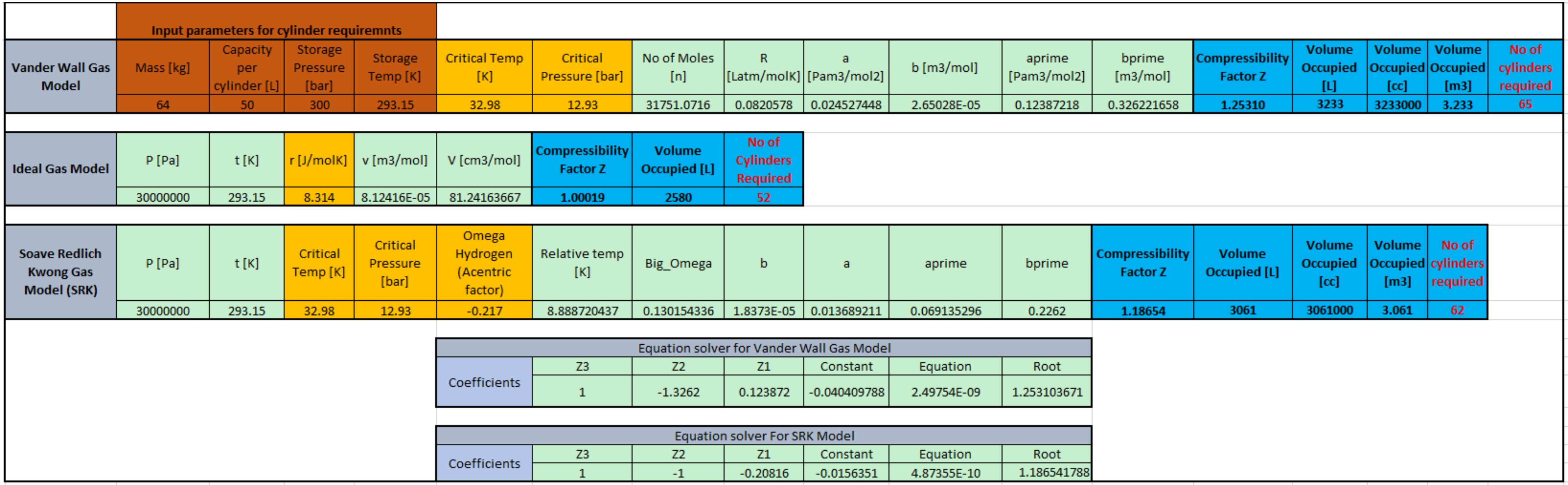
Equation solver for Vander Wall Gas Model

	Z3	Z2	Z1	Constant	Equation	Root
Coefficients	1	-1.3262	0.123872	-0.040409788	-8.64125E-07	1.253103098

Equation solver for SRK Model

	Z3	Z2	Z1	Constant	Equation	Root
Coefficients	1	-1	-0.20816	-0.0156351	-5.33681E-07	1.186541463

Figure 4.4 Hydrogen storage model Scenario 1



	Input parameters for cylinder requiremnts																
Vander Wall Gas Model	Mass [kg]	Capacity per cylinder [L]	Storage Pressure [bar]	Storage Temp [K]	Critical Temp [K]	Critical Pressure [bar]	No of Moles [n]	R [Latm/molK]	a [Pam3/mol2]	b [m3/mol]	aprime [Pam3/mol2]	bprime [m3/mol]	Compressibility Factor Z	Volume Occupied [L]	Volume Occupied [cc]	Volume Occupied [m3]	No of cylinders required
	64	50	300	293.15	32.98	12.93	31751.0716	0.0820578	0.024527448	2.65028E-05	0.12387218	0.326221658	1.25310	3233	3233000	3.233	65

Ideal Gas Model	P [Pa]	t [K]	r [J/molK]	v [m3/mol]	V [cm3/mol]	Compressibility Factor Z	Volume Occupied [L]	No of Cylinders Required
	30000000	293.15	8.314	8.12416E-05	81.24163667	1.00019	2580	52

Soave Redlich Kwong Gas Model (SRK)	P [Pa]	t [K]	Critical Temp [K]	Critical Pressure [bar]	Omega Hydrogen (Acentric factor)	Relative temp [K]	Big_Omega	b	a	aprime	bprime	Compressibility Factor Z	Volume Occupied [L]	Volume Occupied [cc]	Volume Occupied [m3]	No of cylinders required
	30000000	293.15	32.98	12.93	-0.217	8.888720437	0.130154336	1.8373E-05	0.013689211	0.069135296	0.2262	1.18654	3061	3061000	3.061	62

Equation solver for Vander Wall Gas Model

	Z3	Z2	Z1	Constant	Equation	Root
Coefficients	1	-1.3262	0.123872	-0.040409788	2.49754E-09	1.253103671

Equation solver For SRK Model

	Z3	Z2	Z1	Constant	Equation	Root
Coefficients	1	-1	-0.20816	-0.0156351	4.87355E-10	1.186541788

Figure 4.3 Hydrogen storage model Scenario 2

4.5. Proposed solutions for reducing number of cylinders

The number of cylinders required for both of these scenarios is too much we need to reduce this to reasonable amount. To do this there are two possible solutions.

4.5.1. Increasing cylinder pressure and cylinder capacity

First possible solution is to increase the pressure from 300 bar to 500 bar and increasing cylinder capacity from 50L to 300L such a combination is manufacture by MAHYTEC [19] company doing this we are able to reduce our cylinder requirement for Scenario 1 from 11 to 2, and for Scenario 2 from 64 to 7.

4.5.2. Decreasing pressure and Increasing the cylinder capacity

Second possible solution is to get single big H_2 tank with a high-volume capacity but at low storage pressure of 40 bar and assuming a storage temperature of 293.15 K which is a reasonable pressure output capacity of many PEM H_2 generators. Doing this we can eliminate the need to get a compressor and reduce costs. The model developed earlier can estimate this but needs to a few changes. The results for Scenario 1 we need a volume of 3398L and for Scenario 2 we would need 19766L. A single H_2 tank with such a high storage capacity can fulfill our requirements. Such a possible solution is given by a Vítkovice Cylinders Inc and Linde Gas company.

5. Hydrogen production models

The aim of the model is to provide the Input requirements for producing enough hydrogen to satisfy our powertrain testing scenario 1 and scenario 2. The two models are based on the most widely used techniques steam methane reforming and electrolysis for producing hydrogen as discussed earlier in literature review section.

For steam methane reforming model our aim is to get the natural gas and steam required to satisfy our demand for both scenarios of laboratory.

For electrolysis model our aim is to get the electrical energy and the water quantity that will be consumed to satisfy our hydrogen demand for powertrain laboratory scenarios.

5.1. Steam methane reforming modelling in Excel

There are many mathematical models for modelling SMR process but in this report, model that was made is a mathematical model made in Microsoft Excel.

Usually operating conditions of commercial SMR provide fast enough chemical kinetic rates that equilibrium conditions are approached closely [7]. Hence it makes sense to model SMR at equilibrium conditions for best results.

The relevant reactions considered in the SMR model are steam methane reforming reaction

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

And water gas shift reaction

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

This model works by equalising the reaction constants for steam reforming reaction and water gas shift reaction with the equilibrium reaction constant equations given in literatures [20] [7] [21] [22]

$$K_{SMR} = \exp\left(\frac{-26830}{T} + 30.114\right) \ [\mathrm{bar}^2] ----- (1)$$

$$K_{WGS} = \exp\left(\frac{4400}{T} - 4.036\right) \ [-] ----- (2)$$

From these above reactions we assume value of operating temperature of reformer and we get the values if these equilibrium reaction constants mentioned above.

Also, we know that

$$K_{SMR} = P^2 * \left(\frac{Y_{CO} * \left(Y_{H_2}\right)^3}{Y_{CH_4} * Y_{H_2O}} \right) -----(3)$$

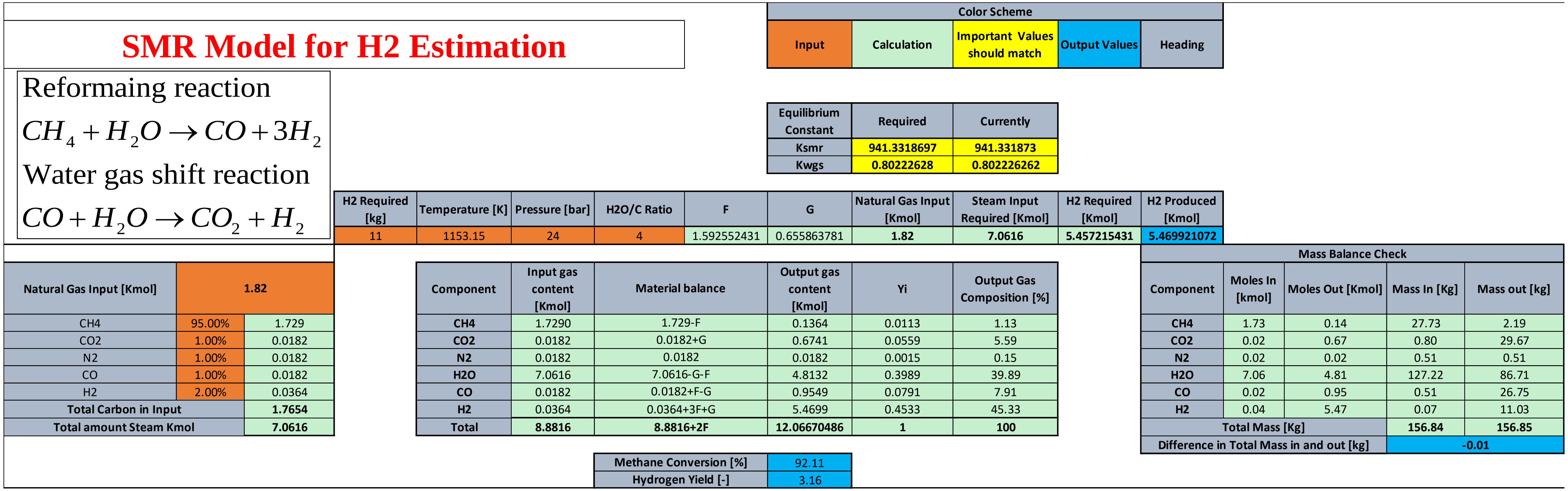
$$K_{WGS} = \left(\frac{Y_{CO_2} * Y_{H_2}}{Y_{CO} * Y_{H_2O}} \right) -----(4)$$

Where P [bar] is the operating pressure of reformer, Y is the mole fraction of the individual species in the subscript. The model tries to match the values of K_{SMR} and K_{WGS} from equation (1) and (2) to values of K_{SMR} and K_{WGS} in equation (3) and (4). Since we have all the required parameters performing mass balancing, we can estimate the output gas composition since we get the mole fraction of each species at output after these mass balance.

To get the output gas composition we assume a certain mole of CH_4 that will be converted denoted by “F” in the model, we also assume “G” which is amount of mole of CO_2 that will be formed at end of equilibrium. The Excel model will vary these “F” and “G” parameters until the equilibrium mole fraction gas composition will be obtained.

The model has also a check for mass balance which sums up the mass that was input in reformer and the mass of output gas composition and the difference between them gives us a check if the mass balance is calculated accurately.

The excel model has its limitations it can only run 500 iterations with a reasonable accuracy but the results obtained from this model are very promising and very close to other models and also to experimental data from H_2 generation plant. The model is shown in figure 5.1



SMR Model for H2 Estimation

Reforming reaction

$CH_4 + H_2O \rightarrow CO + 3H_2$

Water gas shift reaction

$CO + H_2O \rightarrow CO_2 + H_2$

Color Scheme				
Input	Calculation	Important Values should match	Output Values	Heading

Equilibrium Constant	Required	Currently
Ksmr	941.3318697	941.331873
Kwgs	0.80222628	0.802226262

H2 Required [kg]	Temperature [K]	Pressure [bar]	H2O/C Ratio	F	G	Natural Gas Input [Kmol]	Steam Input Required [Kmol]	H2 Required [Kmol]	H2 Produced [Kmol]
11	1153.15	24	4	1.592552431	0.655863781	1.82	7.0616	5.457215431	5.469921072

Natural Gas Input [Kmol]	1.82	
CH4	95.00%	1.729
CO2	1.00%	0.0182
N2	1.00%	0.0182
CO	1.00%	0.0182
H2	2.00%	0.0364
Total Carbon in Input		1.7654
Total amount Steam Kmol		7.0616

Component	Input gas content [Kmol]	Material balance	Output gas content [Kmol]	Yi	Output Gas Composition [%]
CH4	1.7290	1.729-F	0.1364	0.0113	1.13
CO2	0.0182	0.0182+G	0.6741	0.0559	5.59
N2	0.0182	0.0182	0.0182	0.0015	0.15
H2O	7.0616	7.0616-G-F	4.8132	0.3989	39.89
CO	0.0182	0.0182+F-G	0.9549	0.0791	7.91
H2	0.0364	0.0364+3F+G	5.4699	0.4533	45.33
Total	8.8816	8.8816+2F	12.06670486	1	100

Methane Conversion [%]	92.11
Hydrogen Yield [-]	3.16

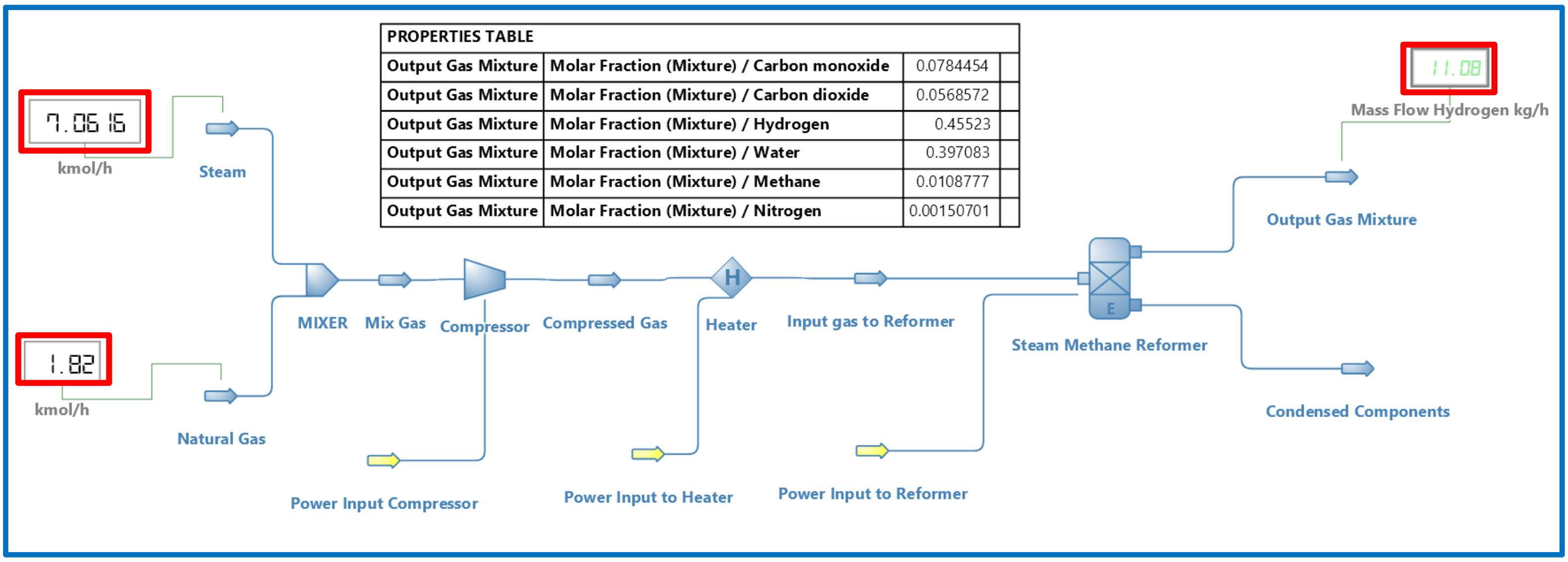
Mass Balance Check				
Component	Moles In [kmol]	Moles Out [Kmol]	Mass In [Kg]	Mass out [kg]
CH4	1.73	0.14	27.73	2.19
CO2	0.02	0.67	0.80	29.67
N2	0.02	0.02	0.51	0.51
H2O	7.06	4.81	127.22	86.71
CO	0.02	0.95	0.51	26.75
H2	0.04	5.47	0.07	11.03
Total Mass [Kg]			156.84	156.85
Difference in Total Mass in and out [kg]			-0.01	

Figure 5.1 SMR Excel model

5.2. Steam methane reforming modeling in DWSIM software

DWSIM is an open-source process simulation software which makes it easy to estimate the hydrogen production it is advantageous over Excel model that whenever there is any change in mixture of natural gas contents it is easy to change and calculate H_2 output, but to account for this change there will be a need to recalculate the mass balance and then H_2 production can be estimated in Excel model.

The hydrogen model for Scenario 1 is shown in fig 5.2, there is a small difference in the hydrogen output from Excel model and DWSIM Model for Scenario 1. This can mainly due to the fact that the DWSIM is running with 2000 Iterations with a low tolerance compared to Excel model. The SRK equation property package was used in this model.

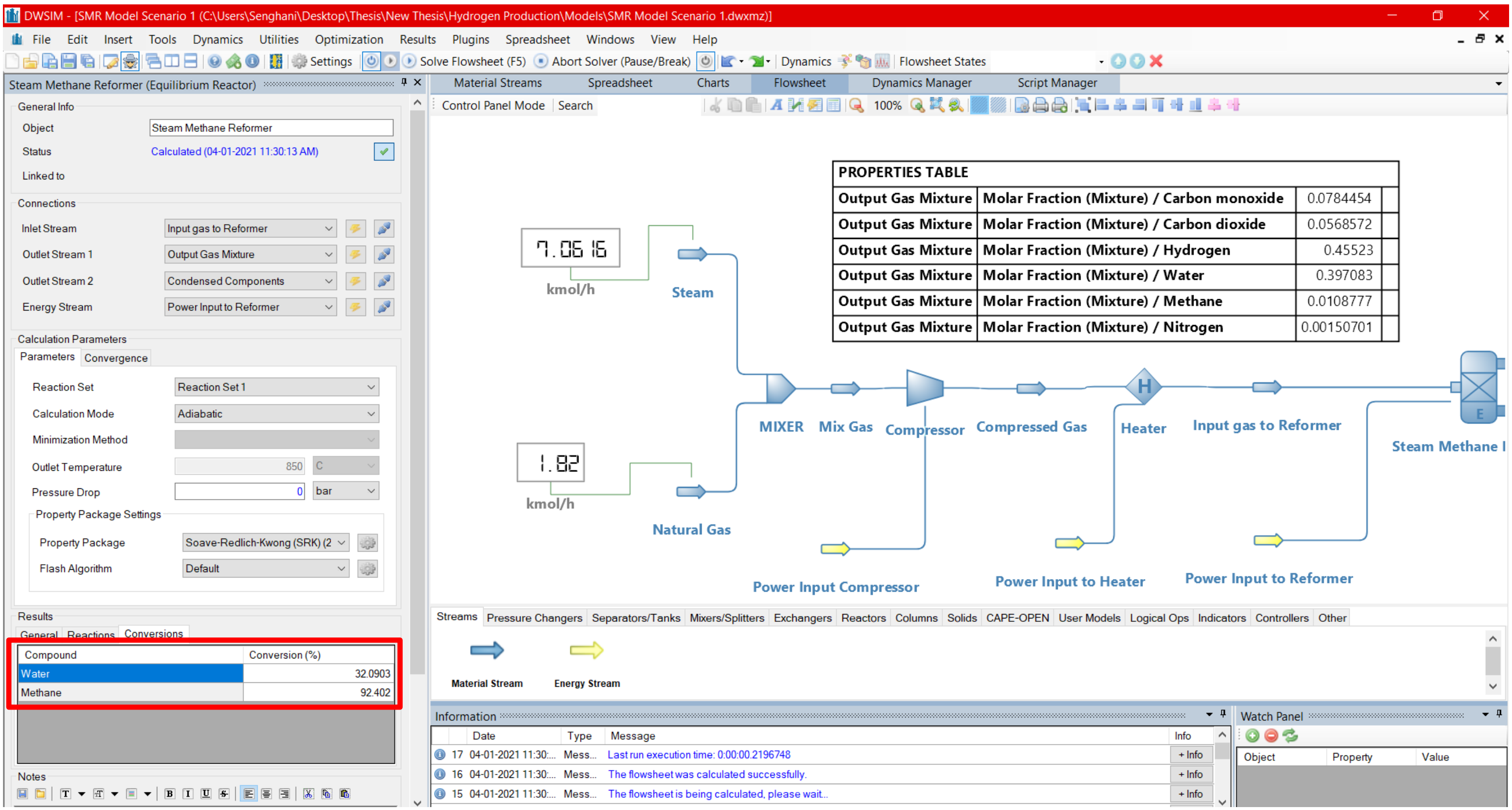


PROPERTIES TABLE

Output Gas Mixture	Molar Fraction (Mixture) / Carbon monoxide	0.0784454
Output Gas Mixture	Molar Fraction (Mixture) / Carbon dioxide	0.0568572
Output Gas Mixture	Molar Fraction (Mixture) / Hydrogen	0.45523
Output Gas Mixture	Molar Fraction (Mixture) / Water	0.397083
Output Gas Mixture	Molar Fraction (Mixture) / Methane	0.0108777
Output Gas Mixture	Molar Fraction (Mixture) / Nitrogen	0.00150701

Figure 5.2 DWSIM model for Scenario 1

The input parameters and the operating parameters for both Excel and DWSIM model are kept same. It should be noted that only our main aim and only concern is to get the mass balance accurately and get the hydrogen output, Hence the energy input parameters such as “Power Input Compressor” “Power Input to Heater” and “Power Input to Reformer” were not validated.



Steam Methane Reformer (Equilibrium Reactor)

General Info

Object: Steam Methane Reformer
Status: Calculated (04-01-2021 11:30:13 AM)
Linked to

Connections

Inlet Stream: Input gas to Reformer
Outlet Stream 1: Output Gas Mixture
Outlet Stream 2: Condensed Components
Energy Stream: Power Input to Reformer

Calculation Parameters

Parameters | Convergence

Reaction Set: Reaction Set 1
Calculation Mode: Adiabatic
Minimization Method:
Outlet Temperature: 850 C
Pressure Drop: 0 bar

Property Package Settings

Property Package: Soave-Redlich-Kwong (SRK) (2
Flash Algorithm: Default

Results

General | Reactions | Conversions

Compound	Conversion (%)
Water	32.0903
Methane	92.402

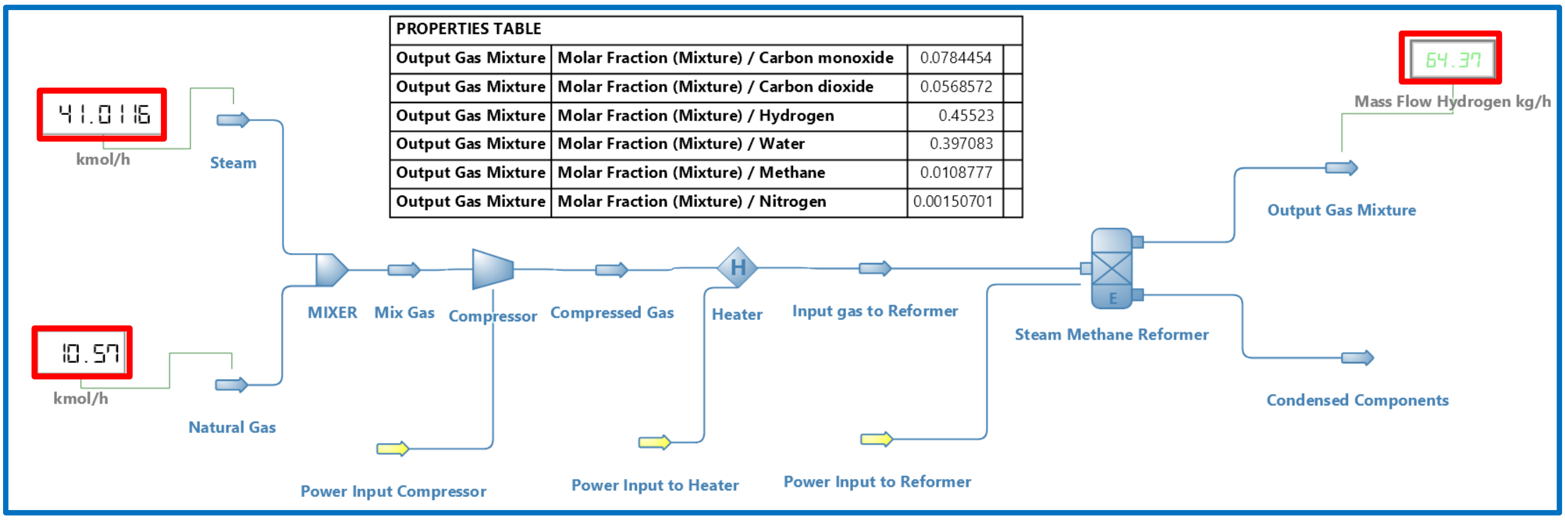
PROPERTIES TABLE		
Output Gas Mixture	Molar Fraction (Mixture) / Carbon monoxide	0.0784454
Output Gas Mixture	Molar Fraction (Mixture) / Carbon dioxide	0.0568572
Output Gas Mixture	Molar Fraction (Mixture) / Hydrogen	0.45523
Output Gas Mixture	Molar Fraction (Mixture) / Water	0.397083
Output Gas Mixture	Molar Fraction (Mixture) / Methane	0.0108777
Output Gas Mixture	Molar Fraction (Mixture) / Nitrogen	0.00150701

Information

	Date	Type	Message	Info
17	04-01-2021 11:30:...	Mess...	Last run execution time: 0:00:00.2196748	+ Info
16	04-01-2021 11:30:...	Mess...	The flowsheet was calculated successfully.	+ Info
15	04-01-2021 11:30:...	Mess...	The flowsheet is being calculated, please wait...	+ Info

Figure 5.3 Methane conversion as per DWSIM model

The methane conversion was found to be 92.402 % while in Excel model it was 92.11 %. It was assumed the steam in the input was assumed was 120˚C and 2 bar pressure. Natural gas at input was assumed to be at 100˚C and 1 bar pressure. And with use of compressor and heater The mixture was heated and pressurized to 880˚C and 24 bar pressure. There is no pressure drop across Steam Reformer.



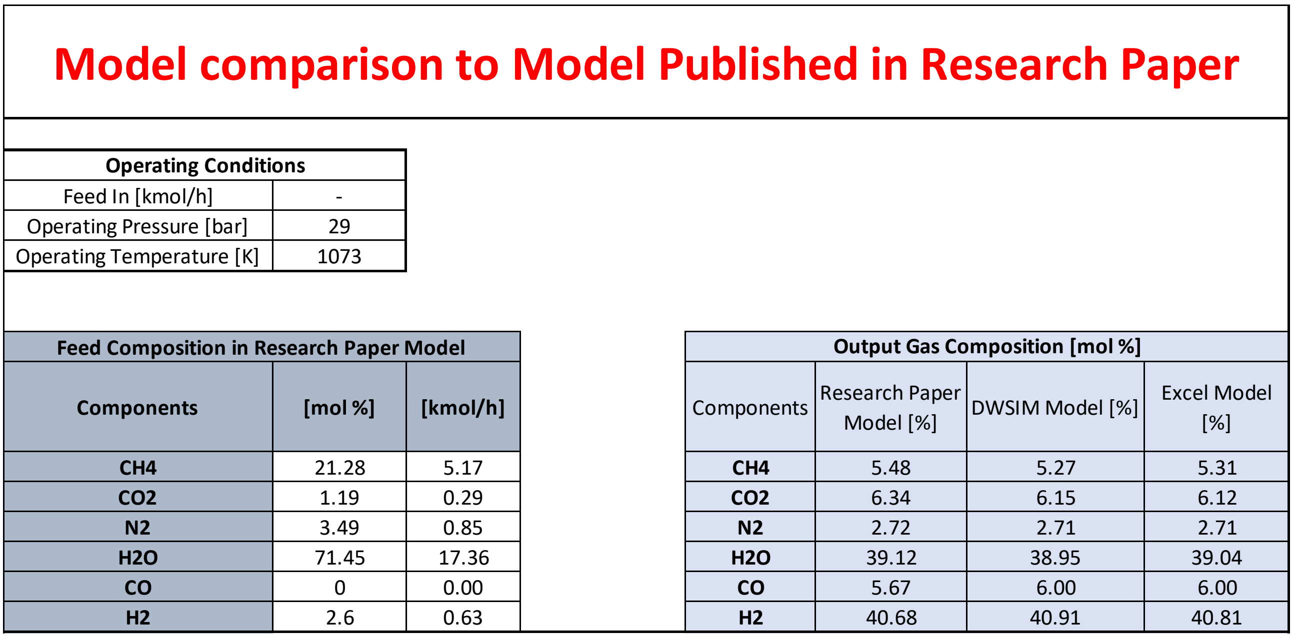
PROPERTIES TABLE		
Output Gas Mixture	Molar Fraction (Mixture) / Carbon monoxide	0.0784454
Output Gas Mixture	Molar Fraction (Mixture) / Carbon dioxide	0.0568572
Output Gas Mixture	Molar Fraction (Mixture) / Hydrogen	0.45523
Output Gas Mixture	Molar Fraction (Mixture) / Water	0.397083
Output Gas Mixture	Molar Fraction (Mixture) / Methane	0.0108777
Output Gas Mixture	Molar Fraction (Mixture) / Nitrogen	0.00150701

Figure 5.4 DWSIM model for Scenario 2

According to this model to generate 64 kg of hydrogen approximately 10.57 kmol of natural gas and 41.01 kmol of Steam is required. Using this data, we can calculate the cost of fuel for scenario 2, Similarly for Scenario 1 to generate 11 kg of hydrogen 1.82 kmol of natural gas and 7.06 kmol of Steam will be required.

5.3. SMR model validation

To validate the Excel model and DWSIM model the output gas composition results from models were compared with the output gas composition from H_2 production plant and other models published in literature [23]. The difference between them is reasonable.



Model comparison to Model Published in Research Paper

Operating Conditions	
Feed In [kmol/h]	-
Operating Pressure [bar]	29
Operating Temperature [K]	1073

Feed Composition in Research Paper Model		
Components	**[mol %]**	**[kmol/h]**
CH4	21.28	5.17
CO2	1.19	0.29
N2	3.49	0.85
H2O	71.45	17.36
CO	0	0.00
H2	2.6	0.63

Output Gas Composition [mol %]			
Components	Research Paper Model [%]	DWSIM Model [%]	Excel Model [%]
CH4	5.48	5.27	5.31
CO2	6.34	6.15	6.12
N2	2.72	2.71	2.71
H2O	39.12	38.95	39.04
CO	5.67	6.00	6.00
H2	40.68	40.91	40.81

Figure 5.5 Comparison between literature model, DWSIM model and Excel model

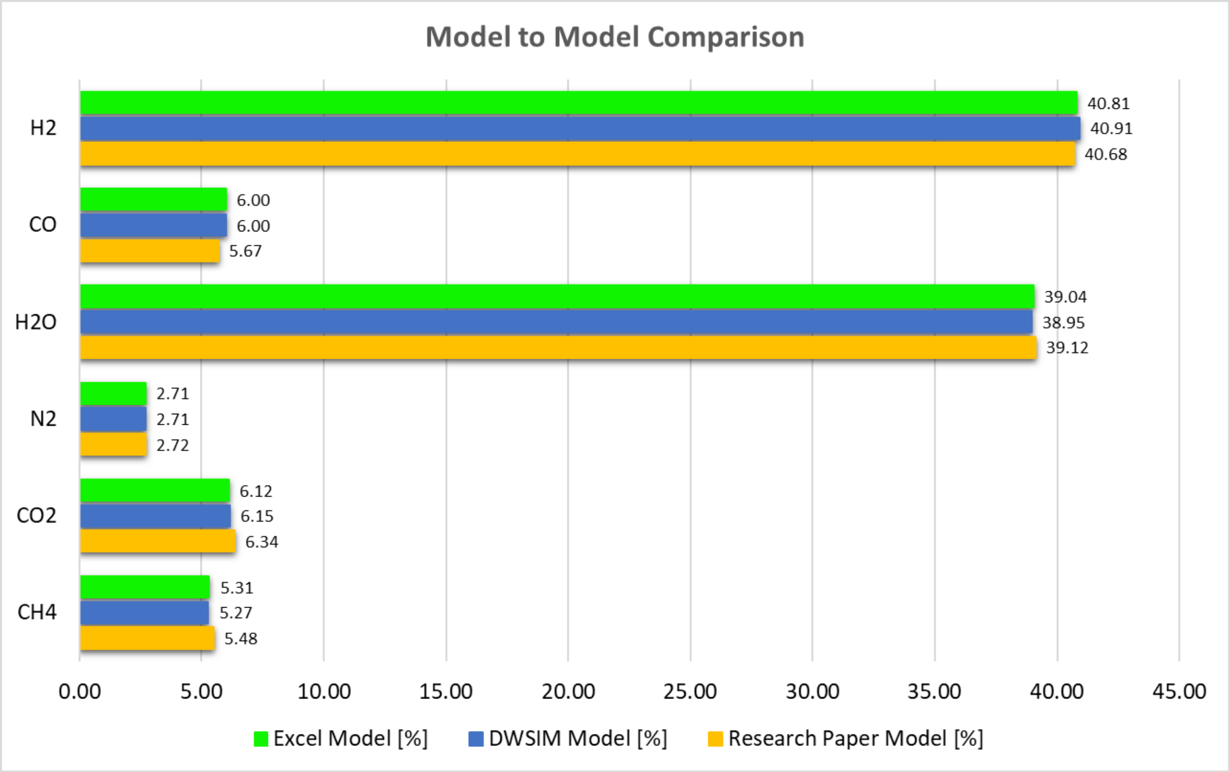
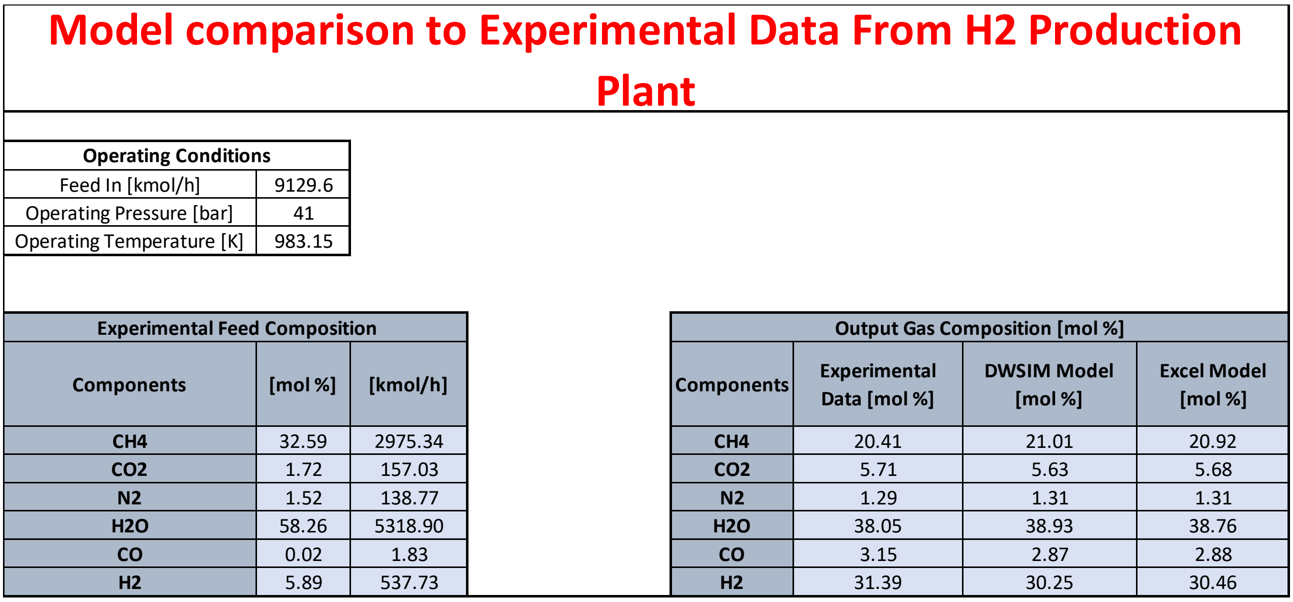


Figure 5.6 Graphical representation of model-to-model comparison

It is clear from the graph that the difference between the gas composition from the excel model and the model in literature is around 1 %.

The model was also compared to experimental data from H_2 production plant [21] [22].The Excel model and DWSIM were inputted with same feed gas composition and the operating temperature and pressure as the data from this plant for this comparison.



Model comparison to Experimental Data From H2 Production Plant

Operating Conditions	
Feed In [kmol/h]	9129.6
Operating Pressure [bar]	41
Operating Temperature [K]	983.15

Experimental Feed Composition		
Components	**[mol %]**	**[kmol/h]**
CH4	32.59	2975.34
CO2	1.72	157.03
N2	1.52	138.77
H2O	58.26	5318.90
CO	0.02	1.83
H2	5.89	537.73

Output Gas Composition [mol %]			
Components	**Experimental Data [mol %]**	**DWSIM Model [mol %]**	**Excel Model [mol %]**
CH4	20.41	21.01	20.92
CO2	5.71	5.63	5.68
N2	1.29	1.31	1.31
H2O	38.05	38.93	38.76
CO	3.15	2.87	2.88
H2	31.39	30.25	30.46

Figure 5.7 Comparison between experimental data and Excel model

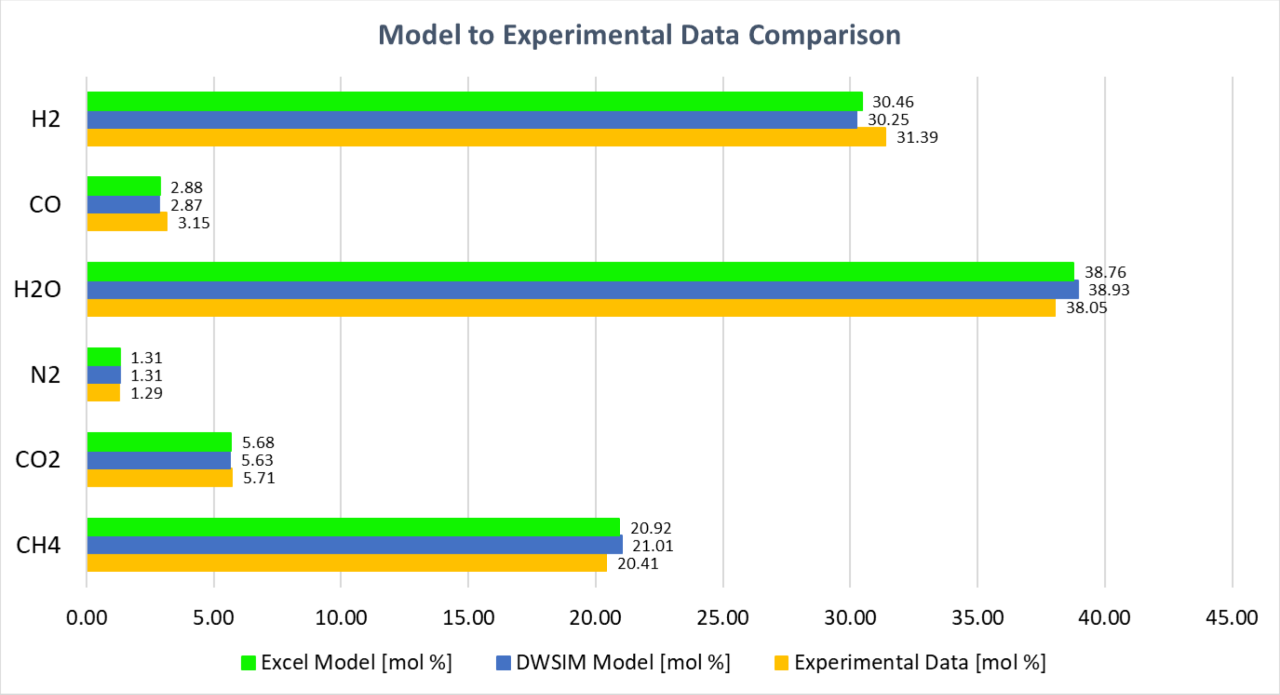


Figure 5.8 Graphical representation model to experimental data comparison

The graph gives us the visual representations of comparison, it is clear from the results that the difference between the experimental data and the model predictions is also around 1%. Thereby validating the model.

5.4. Result discussion and conclusions for SMR models

Considering the two-laboratory scenario 1 and scenario 2 we consider the operating of reformer at standard typical operating parameters stated in Table 2.1 with feed composition of 95% CH_4, 1% CO, 1% CO_2, 1% N_2 and 2% H_2. To get our required amount of H_2 for both Scenarios the natural gas content required for both these scenarios is given in Table 5.1 and 5.2

Components	Feed Input	Output Gas (Excel Model)	Output Gas (DWSIM Model)
Natural gas content [Kmol]	1.82	-	-
CH_4 [Kg]	27.73	2.19	2.10
CO_2 [Kg]	0.80	29.67	30.21
N_2 [Kg]	0.51	0.51	0.51
CO [Kg]	0.51	26.75	26.53
H_2 [Kg]	0.07	**11.03**	**11.08**
H_2O [Kg]	127.22	86.71	86.39

Table 5.1 Feed composition to generate required H_2 for Scenario 1

Components	Feed Input	Output Gas (Excel Model)	Output Gas (DWSIM Model)
Natural gas content [Kmol]	10.57	-	-
CH_4 [Kg]	161.07	12.71	12.23
CO_2 [Kg]	4.65	172.29	175.50
N_2 [Kg]	2.96	2.96	2.96
CO [Kg]	2.96	155.34	154.11
H_2 [Kg]	0.43	**64.03**	**64.36**
H_2O [Kg]	738.84	503.59	501.74

Table 5.2 Feed composition to generate required H_2 for Scenario 2

It is observed from the Excel model that when we keep the S/C ratio and temperature to be constant and increase the pressure of reformer, the methane conversion decreases as pressure increases, this behavior is shown in figure 5.9. It should be noted that the Fig 5.9, 5.10, 5.11 are made for 2.48 kmol of natural gas as input keeping the rest of the parameters same as for scenario 1.

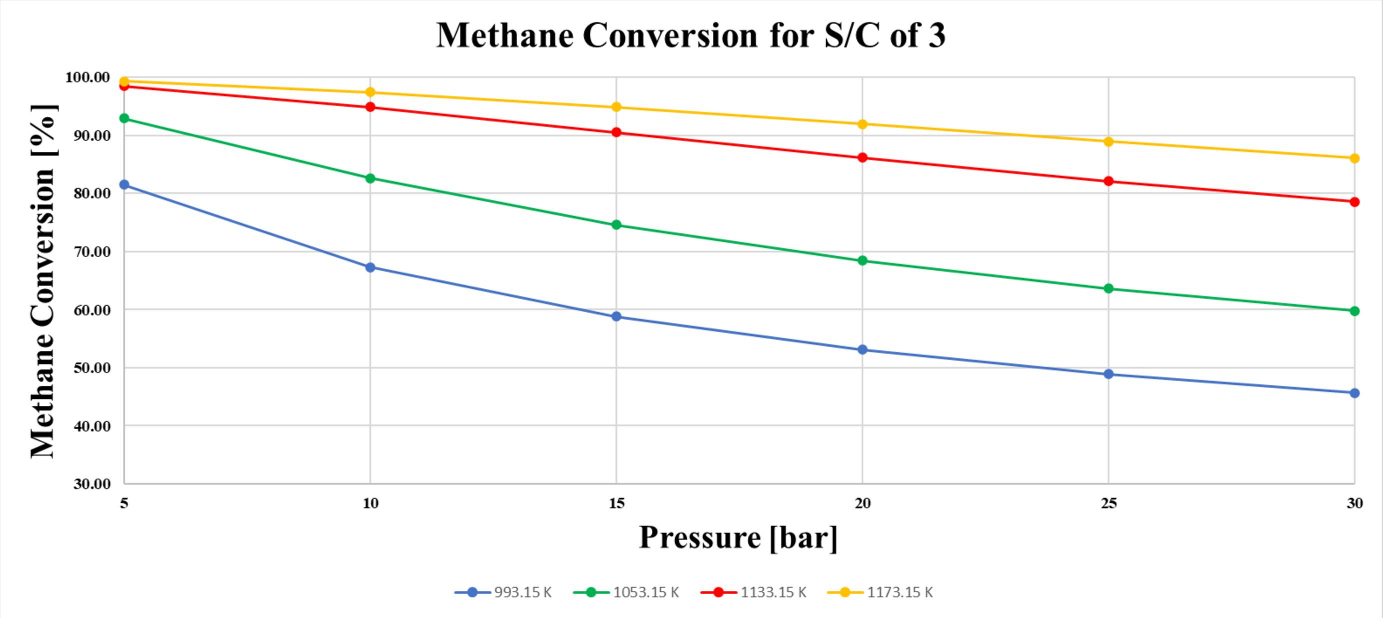


Figure 5.9 Conversion of methane as a function of pressure for different temperatures

From model, it is also observed that methane conversion increases with increasing temperature for a constant pressure figure 5.10 describes such behavior.

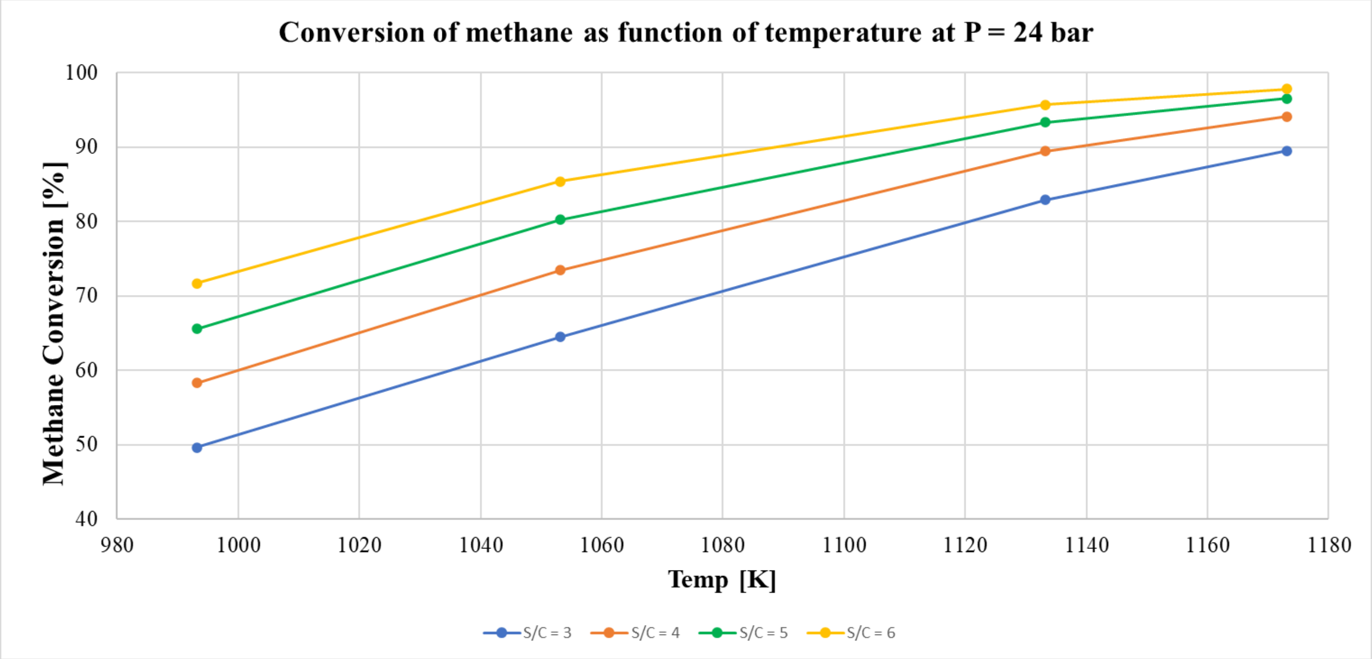


Figure 5.10 Conversion of methane as a function of temperature for different steam to carbon ratio

It is also observed from the model results that keeping the S/C ratio and pressure constant the H_2 composition increases with increase in temperature. The behavior of each species in output gas composition with varying in temperature is shown in figure 5.11

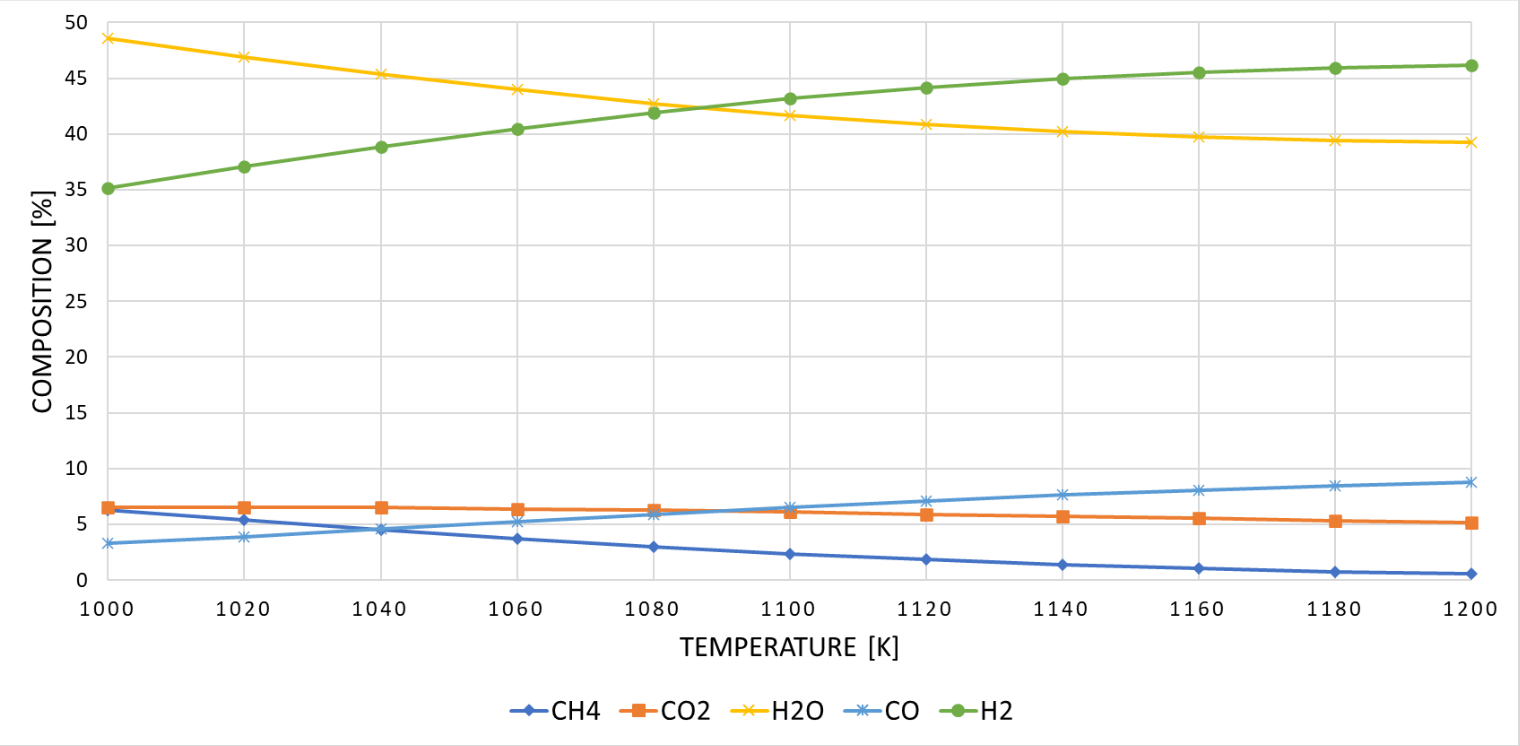


Figure 5.11 Effect of temperature on outlet gas composition at P = 24 bar and S/C of 4

These behaviors mentioned in graphs above is found in consistence with behavior mentioned in literature [24].

5.5. H_2 generation by electrolysis

Electrolyser are generally bi-polar as stated earlier in literature review so it is reasonable that model to be bi-polar. The H_2 production from electrolysis can be estimated by Faraday's Law of Electrolysis, from which it can be concluded that the hydrogen production rate in electrolyser is directly proportional to transfer rate of electrons at electrodes, which is equivalent to electric current in external circuit [25].

$$Q_{H_2} = (80.69 * \eta_F) * \left(\frac{n_c * I}{z * F} \right) \; [\mathrm{Nm}^3 / h] \quad [25]$$

From this equation we can estimate the hydrogen flow rate, where "η_F" is the faraday efficiency, "z" is the number of charges transferred per hydrogen molecule, "F" is the Faraday's constant, the value of faraday efficiency is close to 99% but to be more accurate it can be estimated by equation

$$\eta_F = f_2 * \left(\frac{(I/A)^2}{(I/A)^2 + f_1} \right) \quad [26]$$

Where, f_1 and f_2 are faraday's coefficient and are experimental values, these parameters are dependent on temperature but the relation between them is not known [26] therefore it needs to be estimated from experimental values.

Therefore, the parameters f_1 and f_2 are estimated by relation

$$\begin{aligned} f_1(T) &= a_{f1} * T + b_{f1} \\ f_2(T) &= c_{f2} * T^2 + d_{f2} * T + e_{f2} \end{aligned} \quad [26]$$

The values of the parameters to calculate f_1 and f_2 are also provided in literature

$$a_{f1} = 2.5 \frac{mA^2}{cm^4 \, °C},\ b_{f1} = 50 \frac{mA^2}{cm^4},\ c_{f2} = -1.25e-5 °C^{-2},\ d_{f2} = 0.001 °C^{-1},\ e_{f2} = 0.97 \quad [26]$$

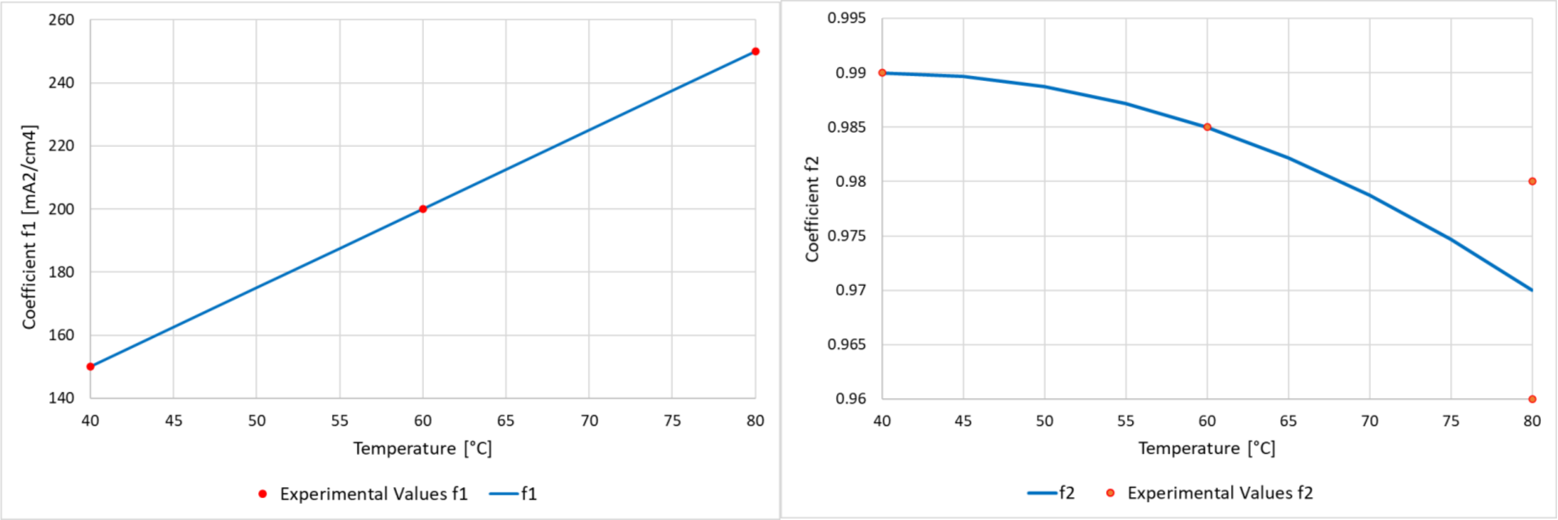
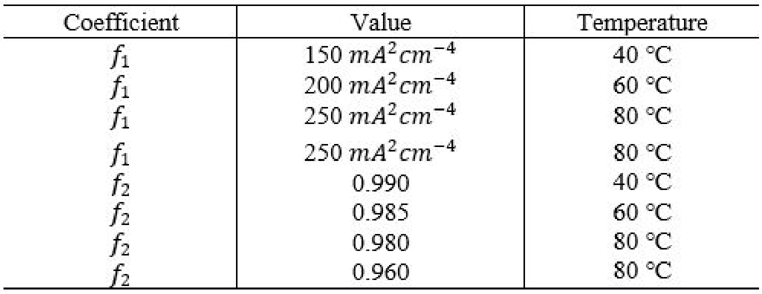


Figure 5.12 Tuned faraday efficiency parameters graph to experimental values

The f_1 and f_2 parameters mentioned above are curve fitted to experimental values depending on temperature these experimental coefficients are mentioned in Table 5.3. From these we are able to estimate faraday efficiency at different temperatures.



Coefficient	Value	Temperature
f_1	$150\ mA^2cm^{-4}$	40 °C
f_1	$200\ mA^2cm^{-4}$	60 °C
f_1	$250\ mA^2cm^{-4}$	80 °C
f_1	$250\ mA^2cm^{-4}$	80 °C
f_2	0.990	40 °C
f_2	0.985	60 °C
f_2	0.980	80 °C
f_2	0.960	80 °C

Table 5.3 Coefficient values f1 and f2 [26]

For each kilomole of H_2 produced, half a kilomole of O_2 is produced since molecular mass of O_2 is 16 times that of H_2. Thus, we can conclude that the gases are produced in 8:1 ratio therefore if we have total amount of H_2 produced in kg we can multiply by 8 to get amount of oxygen that will be produced.

To get the total water consumption in kg we know that the total mass output from the system is amount of H_2 and O_2 produced, hence the mass Input i.e. The water required is sum of amount of H_2 and O_2 produced in kg.

The values from the model should be compared to reference values mentioned in literature [11] [27] to ensure the input parameters are reasonable values.

The input parameters required to run the model are the electrode area, power input, the current input, the total no cells in electrolyser, the operating temperature of system, the operation time of the electrolyser.

$$Operational\ voltage\ [V] = \frac{Power\ Input\ [kW]*1000}{Current\ Input\ [A]}$$

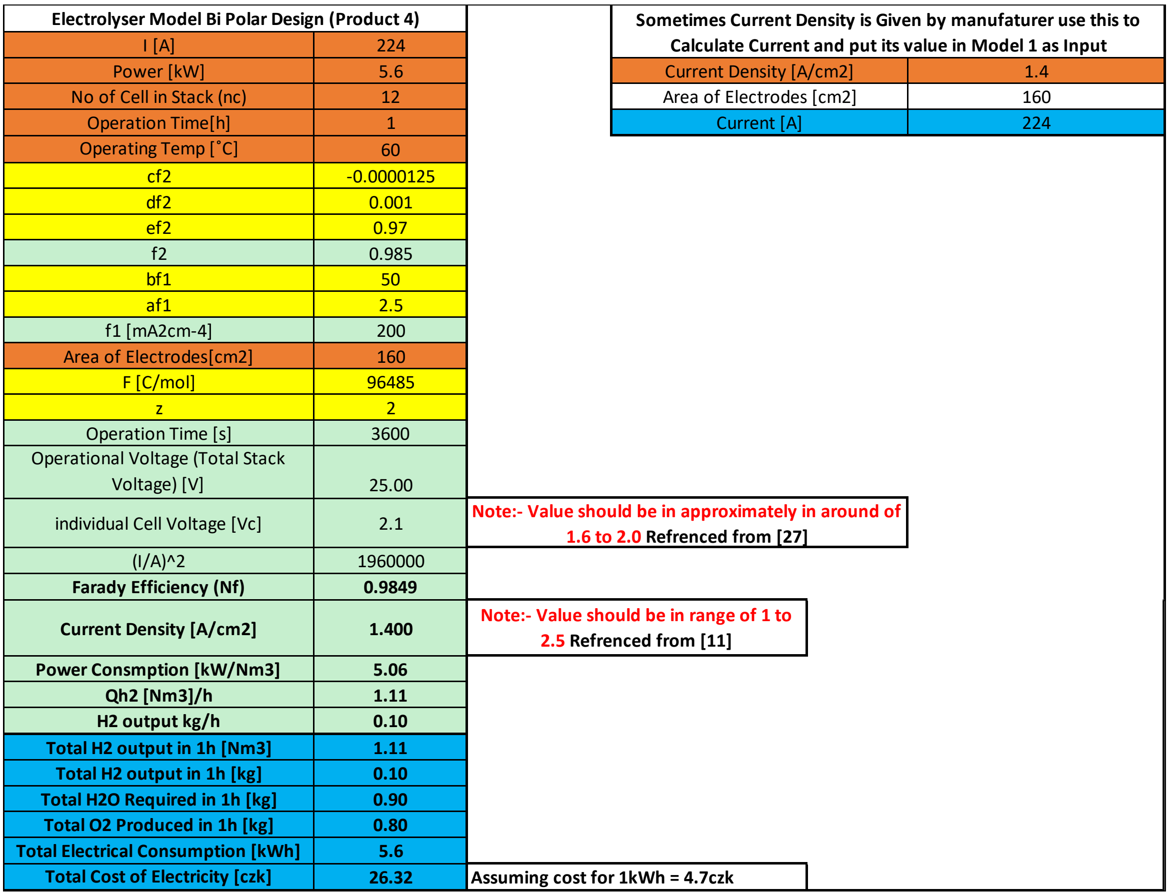
$$Individual\ cell\ voltage\ [V] = \frac{Operational\ Voltage\ [V]}{no\ of\ cell\ in\ stack}$$

$$Current\ density\ [A/cm^2] = \frac{Current\ Input\ [A]}{Electrode\ Area\ [cm^2]}$$

$$Power\ consumption\ [kWh/Nm^3] = \frac{Power\ Input\ [kW]}{H_2\ produced\ [Nm^3/h]}$$

$$Total\ electrical\ comsumption\ [kWh] = Power\ Input\ [kW]*operation\ time\ [h]$$

$$Total\ \cos t\ of\ electricity\ [czk]\ = Total\ electrical\ comsumption\ [kWh]*4.7$$



Electrolyser Model Bi Polar Design (Product 4)	
I [A]	224
Power [kW]	5.6
No of Cell in Stack (nc)	12
Operation Time[h]	1
Operating Temp [˚C]	60
cf2	-0.0000125
df2	0.001
ef2	0.97
f2	0.985
bf1	50
af1	2.5
f1 [mA2cm-4]	200
Area of Electrodes[cm2]	160
F [C/mol]	96485
z	2
Operation Time [s]	3600
Operational Voltage (Total Stack Voltage) [V]	25.00
individual Cell Voltage [Vc]	2.1
(I/A)^2	1960000
Farady Efficiency (Nf)	**0.9849**
Current Density [A/cm2]	**1.400**
Power Consmption [kW/Nm3]	**5.06**
Qh2 [Nm3]/h	**1.11**
H2 output kg/h	**0.10**
Total H2 output in 1h [Nm3]	**1.11**
Total H2 output in 1h [kg]	**0.10**
Total H2O Required in 1h [kg]	**0.90**
Total O2 Produced in 1h [kg]	**0.80**
Total Electrical Consumption [kWh]	**5.6**
Total Cost of Electricity [czk]	**26.32**

Sometimes Current Density is Given by manufaturer use this to Calculate Current and put its value in Model 1 as Input	
Current Density [A/cm2]	1.4
Area of Electrodes [cm2]	160
Current [A]	224

Note:- Value should be in approximately in around of 1.6 to 2.0 Refrenced from [27]

Note:- Value should be in range of 1 to 2.5 Refrenced from [11]

Assuming cost for 1kWh = 4.7czk

Figure 5.13 Electrolyser model layout

5.6. Electrolyser model validation

The electrolyser model is validated by comparing the hydrogen flow rates from H_2 generators by manufacturers and the H_2 flow rate estimated by electrolyser model. To compare these flow rates the model is inputted with same parameters as claimed by manufacturers.

Parameters (Product 1) [28]	Values
Active electrode area [cm2]	490
Number of cells	45
H_2 production rate [Nm3/h]	20
Operating temperature [˚C]	80
Power [kW]	100.45
Current [A]	1063

Parameters (Product 2) [11]	Values
Active electrode area [cm2]	1400
Number of cells	250
H_2 production rate [Nm3/h]	225
Operating temperature [˚C]	80
Power [kW]	1250
Current Density [A/cm2]	1.7

Parameters (Product 3) [11]	Values
Active electrode area [cm2]	680
Number of cells	100
H_2 production rate [Nm3/h]	50
Operating temperature [˚C]	58
Power [kW]	250
Current density[A/cm2]	1.85

Parameters (Product 4) [29]	Values
Active electrode area [cm2]	160
Number of cells	12
H_2 production rate [Nm3/h]	1.1
Operating temperature [˚C]	60
Power [kW]	5.6
Current [A]	224

Parameters (Product 5) [30]	Values
Active electrode area [cm2]	20100
Number of cells	480
H_2 production rate [kg/h]	72.02
Operating temperature [˚C]	85
Power [kW]	3491.72
Current [A]	4021.12

The data of these 5 products stated in literature or claimed by manufacturers was inputted in the electrolyser model in Excel to validate the hydrogen flow rate and thereby aiming to validate the model.

The results of the H_2 flow rates comparison and the percentage difference between flow rates is stated in Table 5.4

Electrolysers	H_2 flow rate from model [Nm3/h]	H_2 flow rate by manufacturers [Nm3/h]	**Percentage difference [%]**
Product 1	19.4	20	**3.09**
Product 2	241.3	225	**6.76**
Product 3	51.86	50	**3.59**
Product 4	1.11	1.1	**0.90**
Product 5	801.11	773.51	**3.45**

Table 5.4 Electrolyser model validation results

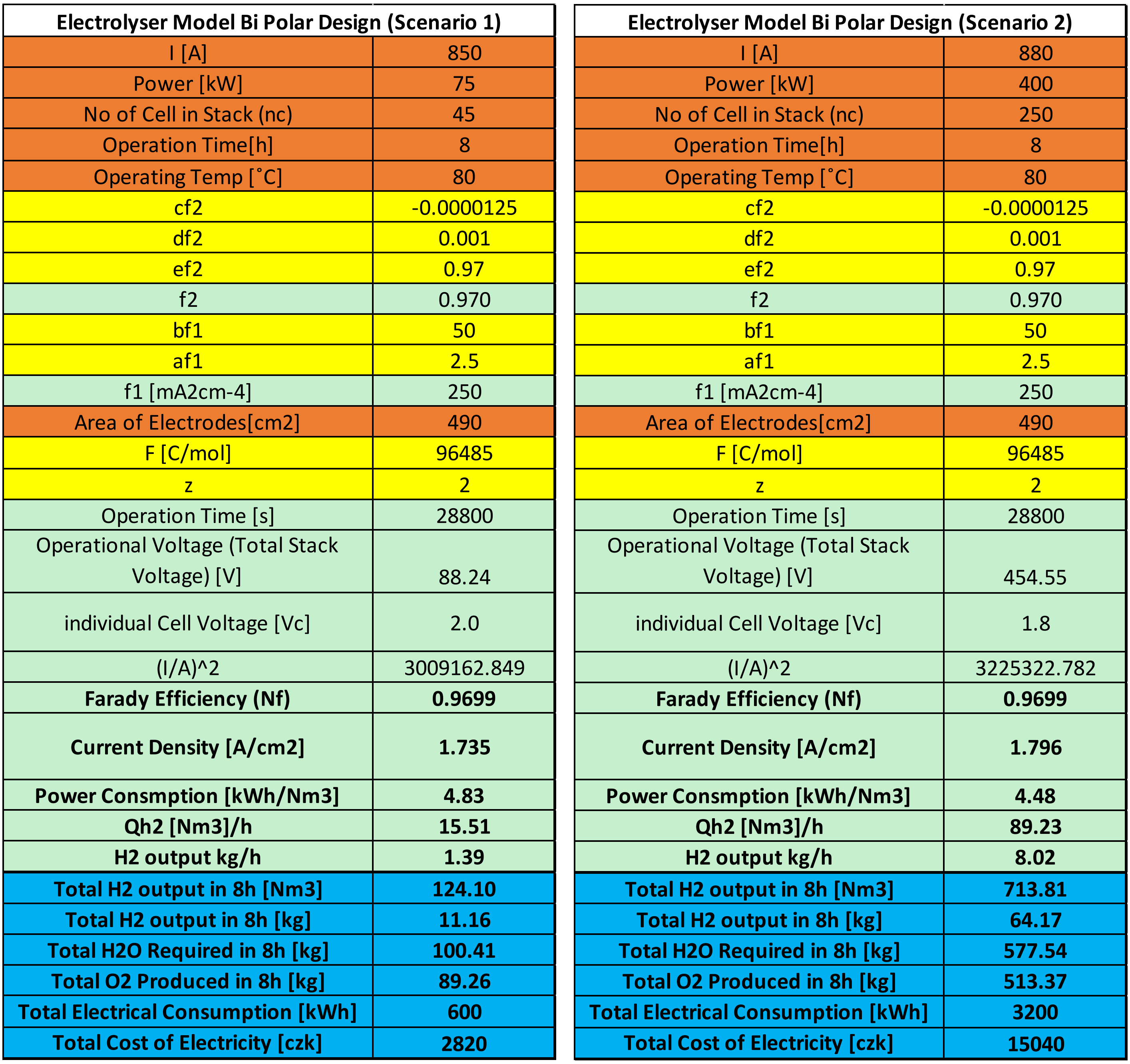
It can be concluded from the results that the H_2 flow rates given by the model are comparable to the data stated in literature or claimed by manufacturers, the percentage difference between values ranging from 0-7% is reasonable thereby validating the model.

5.7. Results and conclusion for electrolyser model

For our powertrain testing scenario 1 and scenario 2 we need to calculate the electrical consumption to generate the required hydrogen. The operating temperature for both the cases is assumed to be 80˚C. The electrode area is also kept constant at 490cm^2 in both the cases.

It is also assumed that the electrolyser will be running for 8 hours in both the cases, so by end of time it should satisfy the H_2 requirement in both our testing scenarios the no of cell in stacks and the amount of current and power requirement are varied until we get our required result by ensuring the limits of individual cell voltage and current density to be within reasonable values as mentioned in literature references.

The results from the model are described in figure 1 and 2 below, it should be noted that the values of the individual cell voltage and the current density criteria is being satisfied in both the results.



Electrolyser Model Bi Polar Design (Scenario 1)	
I [A]	850
Power [kW]	75
No of Cell in Stack (nc)	45
Operation Time[h]	8
Operating Temp [˚C]	80
cf2	-0.0000125
df2	0.001
ef2	0.97
f2	0.970
bf1	50
af1	2.5
f1 [mA2cm-4]	250
Area of Electrodes[cm2]	490
F [C/mol]	96485
z	2
Operation Time [s]	28800
Operational Voltage (Total Stack Voltage) [V]	88.24
individual Cell Voltage [Vc]	2.0
(I/A)^2	3009162.849
Farady Efficiency (Nf)	**0.9699**
Current Density [A/cm2]	**1.735**
Power Consmption [kWh/Nm3]	**4.83**
Qh2 [Nm3]/h	**15.51**
H2 output kg/h	**1.39**
Total H2 output in 8h [Nm3]	**124.10**
Total H2 output in 8h [kg]	**11.16**
Total H2O Required in 8h [kg]	**100.41**
Total O2 Produced in 8h [kg]	**89.26**
Total Electrical Consumption [kWh]	**600**
Total Cost of Electricity [czk]	**2820**

Electrolyser Model Bi Polar Design (Scenario 2)	
I [A]	880
Power [kW]	400
No of Cell in Stack (nc)	250
Operation Time[h]	8
Operating Temp [˚C]	80
cf2	-0.0000125
df2	0.001
ef2	0.97
f2	0.970
bf1	50
af1	2.5
f1 [mA2cm-4]	250
Area of Electrodes[cm2]	490
F [C/mol]	96485
z	2
Operation Time [s]	28800
Operational Voltage (Total Stack Voltage) [V]	454.55
individual Cell Voltage [Vc]	1.8
(I/A)^2	3225322.782
Farady Efficiency (Nf)	**0.9699**
Current Density [A/cm2]	**1.796**
Power Consmption [kWh/Nm3]	**4.48**
Qh2 [Nm3]/h	**89.23**
H2 output kg/h	**8.02**
Total H2 output in 8h [Nm3]	**713.81**
Total H2 output in 8h [kg]	**64.17**
Total H2O Required in 8h [kg]	**577.54**
Total O2 Produced in 8h [kg]	**513.37**
Total Electrical Consumption [kWh]	**3200**
Total Cost of Electricity [czk]	**15040**

Figure 5.14 Electrolyser model results for Scenario 1 and Scenario 2

The conclusion that can be drawn is that there for Scenario 1 approximately 100 Kg of water will be required to generate 11 kg of H_2. And for Scenario 2 the amount of water required is 577 kg to generate 64 kg of H_2.

It can also be noted that the number of cells required, current and power required for scenario 1 requirement is 45,850 A,75 kW respectively. And for scenario 2 the number of cells required, current and power required 250,880 A,400 kW respectively.

6. Market survey

The survey was done for hydrogen generators, hydrogen compressors and hydrogen storage cylinder suppliers. Hyperlinks to all the products mentioned in this survey is added in product name.

6.1. Hydrogen generator supplier comparison

This was further was classified into two sub categories depending on their H_2 output. low H_2 output generators and high H_2 output generators. This low H_2 output products are sufficient to full out requirement for out Scenario 1 and High H_2 output products can fulfill our requirement for Scenario 2.

6.1.1. Low H_2 output generator supplier comparison

The information in Table 6.1 is referenced from the website of the manufacturer the price of the product was directly quoted and provided by the company representative. Any of these products from Table 6.1 will satisfy our requirement for Scenario 1.

Product Name	**PEM Electrolyser C30**	**ELYTE 20**	**Mercury Advance G32**	**H210v.2**	**HYP40**	**HySTAT®-30-10**
Company	Nelhydrogen (Norway)	Areva H_2 Gen (Germany)	ErreDueGas (Italy)	Oxymat (Slovakia)	HIAT GGMBH (Germany)	Hydrogenics (Germany)
H_2 Flow Rate [Nm^3/h]	30	20	21.33	21.33	20	30
Power Consumption	5.8 kWh/Nm^3	5.2 kWh/Nm^3	114kW	-	102 kW	5.2 kWh/Nm^3
Purity [%]	99.9998	99.999	99.995	99.9995	-	99.9
Delivery Pressure [barg]	30	35	5	30	40	
Technology	PEM	PEM	ALKALINE	PEM	PEM	ALKALINE
O_2 Flow Rate [Nm^3/h]	-	10	10.66	-	10	
Coolant Flow [m^3/h]	10.02	4	-	-	-	-
Water Consumption [L/h]	26.9	<40	18.2	-		60
Weight [Kg]	3241	-	2800	-	-	16000
Dimensions [m]	2.5W x 1.2D x 2H	6.10L x 2.44W x 2.59H	1.65 x 2.4 x 2.15	1.7 x 2.6 x 2.4	-	6.10L x 2.44W x 2.90H
Cost in Million [CZK]	13.4	-	5.14	-	2.73	15.07

Table 6.1 Low H_2 flow rate generators

From this data we can calculate the running costs and the cost which can be recovered from selling O_2 the price for O_2 is assumed to be 2 CZK/kg

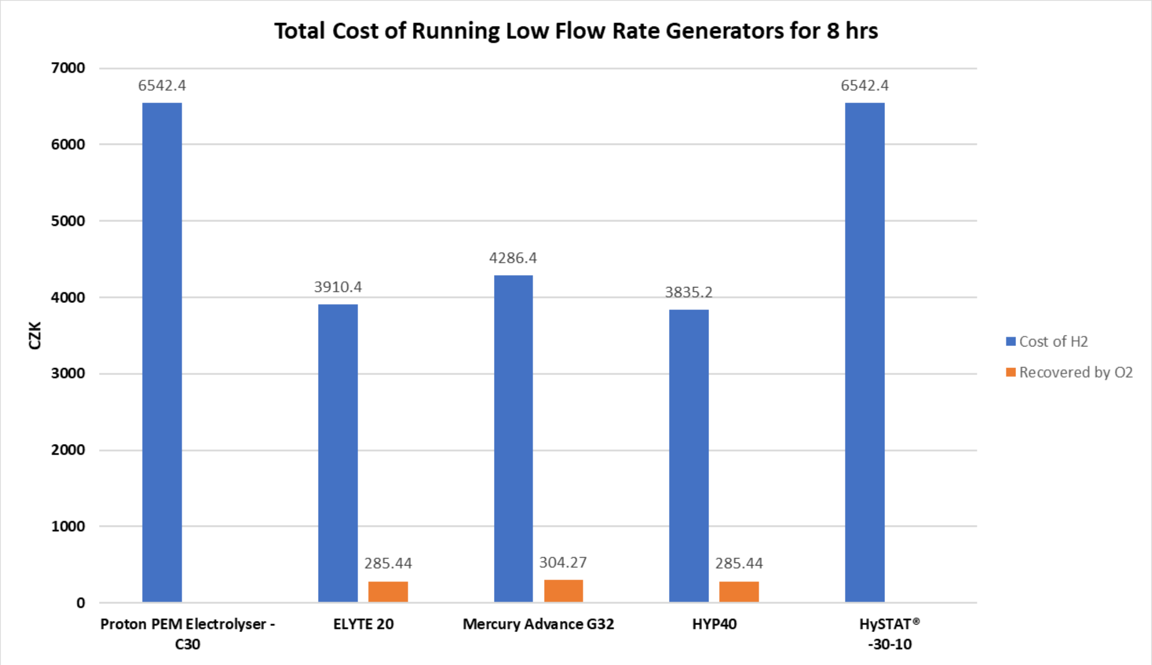


Figure 6.1 Running cost of low H_2 flow rate generators

6.1.2. High H_2 output generator supplier comparison

The information was referenced from the manufacturer's website and the price of the product was quoted by the company representative. Any of the product listed in Table 6.2 is sufficient to fulfill out requirement of Scenario 2.

Product Name	**MC250**	**ELYTE 200**	**PHG250**	**HGAS1SP**
Company	Nelhydrogen (Norway)	Areva H_2 Gen (Germany)	Air Products (Italy)	ITM Power (UK)
H_2 Flow Rate	246 [Nm^3/h]	200 [Nm^3/h]	250 [Nm^3/h]	11.25 kg/h
Power Consumption	4.5 kWh/Nm^3	4.4 kWh/Nm^3	-	700 kW
Purity [%]	99.9995	99.999	>99.5	99.999
Delivery Pressure [barg]	30	35	-	20
Technology	PEM	PEM	SMR	PEM
O_2 Flow Rate [Nm^3/h]	-	100	-	-
Coolant Flow [m^3/h]	-	40	-	-
Water Consumption [L/h]	222	<400	-	-
Dimensions [m]	12.2W x 2.5D x 3H	12.02L x 2.35W x 2.70H	-	20ft & 30ft ISO container
Cost in Million [CZK]	49.83	-	-	-

Table 6.2 High H_2 flow rate generators

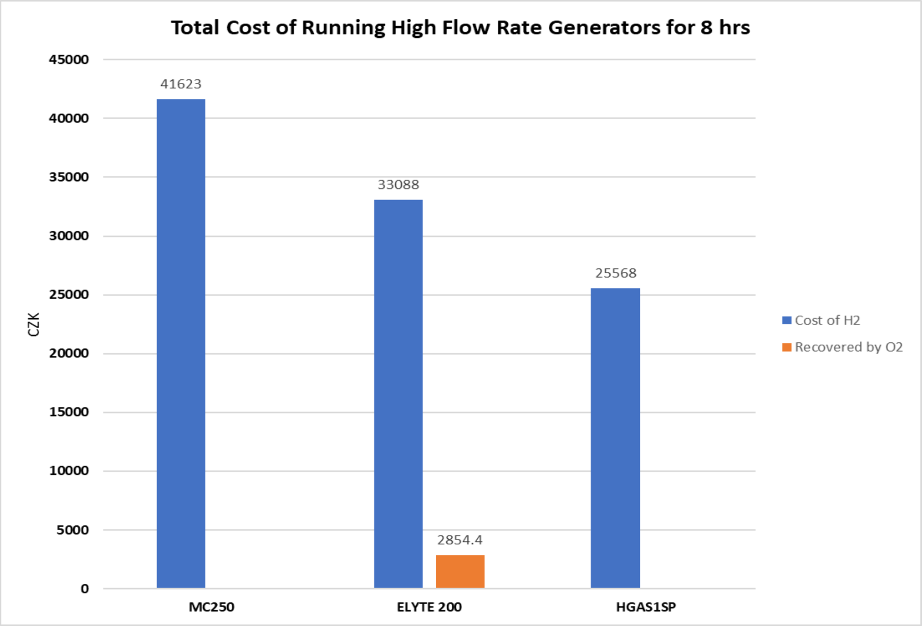


Figure 6.2 Running cost of high H_2 flow rate generators

6.2. Hydrogen compressor supplier comparison

If we want to store our H_2 at high pressure we would need compressors in this section the products capable of delivering H_2 at high pressure are discussed and the running cost are calculated based on the manufacturer data.

Product/Company Name	PureEnergyCentre	HAUG.Sirius NanoLoc	API618	LW 1300 EG
Discharge Pressure [bar]	200-900	451	600	350
Flow Rate [Nm^3/h]	400	60	Up to 90000	78
Power Consumption	200	11-30	-	37
Oil Requirements	Oil free	Oil free	Oil free	Oil Lubrication
Suction pressure [bar]	-	31	-	1-150
Dimensions [m]	-	1.9 x 1.2 x 1	-	1.6 x 1.21 x 1.275
Weight [kg]	-	950	-	1000

Table 6.3 Compressor suppliers comparison

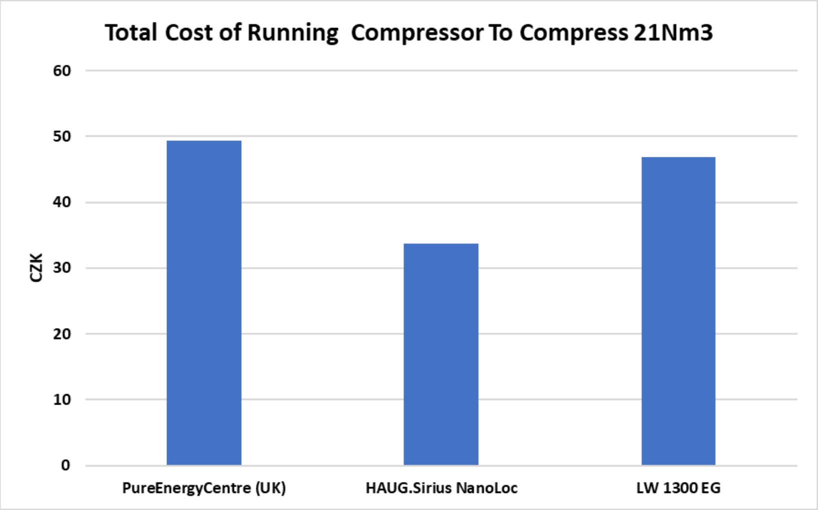


Figure 6.3 Running cost of compressors

6.3. Compressed hydrogen cylinder supplier comparison

In this section the need to avoid all the hydrogen generators and get our hydrogen directly in hydrogen bottles in compressed form is addressed. The number of cylinders required is already known. The manufacturers capable of delivering this kind of products is discussed in this section. The information and price mentioned is directly quoted by the manufacturer and mentioned in their website.

Company Name	Wystrach (Germany)	Linde Gas (Czech Republic)
Pressure [bar]	**300**	200
Cylinder per pack	6,8,9,12,16,**18**	12
Steel Rack Material	Galvanised steel	-
Available Capacity per cylinder [L]	20,30,40,**50**	50
Cost	7899 EUR	21750 CZK

Table 6.4 Hydrogen cylinder supplier comparison

6.4. Total fuel costs of both scenarios

In this section the total fuel costing of both scenarios is estimated, it should be noted only the fuel costs for SMR are considered the energy costs required to heat the steam and other related costs are not considered in this section.

The cost of electricity is assumed to be 4.7 CZK/kWh and natural gas requirement is considered from DWSIM model.

Hydrogen generator type	SMR
Scenario 1 natural gas requirement [kg]	29.63
Scenario 2 natural gas requirement [kg]	172.09
Cost of natural gas [€/kg]	0.97
Scenario 1 natural gas cost [CZK]	767
Scenario2 natural gas cost [CZK]	4455

Hydrogen generator type	Electrolyser
Scenario 1 electricity requirement [kWh]	600
Scenario 2 electricity requirement [kWh]	3200
Cost of electricity [CZK/kWh]	4.7
Scenario 1 electricity cost [CZK]	2820
Scenario 2 electricity cost [CZK]	15040

Table 6.5 Fuel cost comparison for SMR and electrolyser technologies

7. Conclusion and future prospects

From this thesis work and the results from the various models it can be concluded that the fuel costs of SMR are very low compared to hydrogen production by electrolysis.

However, SMR is only suitable if requirements of H_2 production rates are too for high because for SMR various additional components are required, such as for removing Sulphur contents, for separating the hydrogen gas from syngas. And steam requirement is too high because we need to keep S/C ratio high in order to avoid coke formation. Due to these reasons, it can be concluded that the investment cost will be much higher than for electrolysis-based hydrogen production methods.

Electrolysis based hydrogen production methods are ideal for low investment and low hydrogen production rate demands, but their running costs will be much higher than for SMR.

Storing hydrogen is a challenge due to its very low density. Currently technologies such as storing hydrogen in metal hydride are being researched for storing hydrogen more effectively but this is still not available for commercial use.

Based on current commercially available technologies and our hydrogen demands it can be concluded that it will be advantageous if we use electrolysis-based hydrogen production methods to procure our hydrogen and store it at same pressure output as given by hydrogen generator in a large single tank, this way we will be able to produce hydrogen most economically.

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