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Design of a fuel processor unit for PEM fuel cell via shortcut design method

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Abstract

The objective of this paper is to conceptually design a fuel processor system for a 5 kW proton electrolyte membrane fuel cell (PEMFC) system for mobile and portable application. The first section describes the auto-thermal reformer (ATR) system while the second section demonstrates the significance of the water gas shift (WGS) reaction in the system. Shortcut design methods are used for the process units and the characterization curve for each unit is also presented. Kinetic parameters for steam reforming and WGS reactions are also shown. The 5 kW PEMFC requires about 0.08 m^3/min (3.74 mol/min) of H_2 fuel at the fuel cell stack. The primary fuel source to the ATR system is methanol 0.1 m^3/min (4 mol/min), which is fed together with steam and oxygen with the ratio of S/C and O_2/C at 1.3:1 and 1:4, respectively. The conceptual design indicates that if the mole ratio of O_2/C is 0.20–0.25, then the hydrogen selectivity is around 2.5–2.6 for complete methanol. Steam is fed at excess condition in both units, ATR and WGS, to avoid reverse WGS reaction. The conceptual design also proved the significance of WGS reaction in the reduction of CO produced in the ATR and indicated the importance of pressure to reduce the bulk size of WGS reactor. Finally from the overall mass balance for fuel processor unit, the ATR product contains H_2: 73%, CO: 2%, and CO_2: 25%. The CO level is then further reduced to less than 2000 ppm after the WGS reactor. In addition, this paper also studied the performance of preferential oxidation (PROX) in removing the CO and it was observed that the PROX could reduce the CO to less than 100 ppm and performed better than WGS reaction in terms of water management. However, the main problem with PROX is to decide a good catalyst that can give a good selectivity for CO oxidation rather than water formation.

Keywords: PEMFC; Auto-thermal reformer; Water gas shift reaction; Reaction kinetics

1. Introduction

The choice of fuel and fuel processing technology will be the fundamental factor in the success of fuel cells vehicles. Linking fuel cell vehicle entry strategies with a specific alternative fuel with expensive infrastructure cost will ultimately create fuel cost burdens that exceed the cost targets for fuel cell power plants themselves. Hydrogen is the lightest, the simplest, abundant elements in nature and both production and utilization of hydrogen can be emission-free. Apart from unquestionable advantages of hydrogen, several problems also occur in developing the required technologies. The major obstacle of hydrogen as an energy carrier is the lack of safe, efficient and cost effective hydrogen storage system. Currently the key issue is to provide hydrogen to the fuel cell. There are two options: either to store it on board of the vehicle or to produce the hydrogen on the vehicle by means of a fuel processor. To store the hydrogen at cryogenic temperature results in high volumetric density, but the cost of cooling the hydrogen and the loss of hydrogen by evaporation make this mode only useful for special applications. In the near term, for light-duty vehicles, the hydrogen would still be produced on-board from conventional fuel (gasoline, methanol or cyclohexane), many experts considered methanol as an ideal hydrogen carrier among the different alcohols [1–7].

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Nomenclature

A_0	pre-exponential factor mol (min g cat kPa$^{0.22}$)$^{-1}$
C_i	concentration of component *i* (mol/m^3)
C_{i0}	feed concentration of component (mol/m^3)
E_a	activation energy (kJ/mol)
F_i	feed flow rate of component *i* to ATR (mol/min)
$F_i{}'$	feed flow rate of component *i* to WGS
k_1,k_2	rate constant for reactions 1, 2 in ATR (mol/kg cat s)
K_{eq}	rate constant equilibrium (mol/kg cat s)
n_1,n_2,n_3	degree of reaction
P'	pressure at inlet of WGS reactor (kPa)
P_0	pressure at inlet of ATR (kPa)
P_1	pressure after the ATR (kPa)
P_2	pressure after the WGS reactor (kPa)
P_i	molar flow rate after the ATR
$P_i{}'$	molar flow rate after the WGS reactor
$\bar{P}_i$	partial pressure of *i* (*i* = CO, H_2, CO_2, H_2O) (kPa)
P_r	pressure for recycle stream (kPa)
r_{ATR}	steam reforming rate (mol/kg cat s)
r_{WGS}	reaction rate for WGS reaction (mol/kg cat s)
R	ideal gas constant (8.314 kg m^2 s^{-2} mol^{-1} K^{-1})
R_i	molar flow rate for recycle stream (mol/min)
S/C	ratio of steam to methanol
S/CO	ratio of steam to carbon monoxide
$S_{H_2/M}$	selectivity of H_2 per mol methanol 2 = in WGS reactor (mol/kg cat s)
T'	temperature at inlet of WGS reactor (°C)
T_0	temperature at inlet of ATR (°C)
T_1	temperature after the ATR (°C)
T_2	temperature after the WGS reactor (°C)
T_r	temperature for recycle stream (°C)
V	volume (cm^3)
X_i	conversion for component *i* (*i* = M and CO)
y_i	mole fraction of component *i* (*i* = H_2, CO, CO_2, H_2O, M)

Greek symbols

ε	voidage of catalyst
ε_M	varying volume or density
λ	ratio of CO:O_2 in PROX
ρ	density of catalyst (g/m^3)
ψ	temperature changes

Subscripts

1,2	reactions 1 and 2
CO	carbon monoxide
CO_2	carbon dioxide
F	feed
H_2	hydrogen
H_2O	water
M	methanol
MO	methanol at initial stage
O_2	oxygen
O_2O	oxygen at initial stage
R	recycle
S	steam
SO	steam at initial stage

Methanol, like hydrogen is also capable of delivering power directly in fuel cell without the needs for reforming and this clearly simplifies hardware and response characteristics. Other alcohols, such as ethanol, ethylene glycol, propanol, etc. have also been considered for use in a fuel cell, but until now very few direct alcohol fuel cells (DAFC) [8], have been demonstrated, the most advanced system being the direct methanol fuel cell (DMFC) [9–11]. Nevertheless, their performances are still limited because of several problems namely: (1) the low activity of the state of the art electro catalysts, which can only be enhanced by increasing the operating temperature, (2) anode poisoning by strongly adsorbed intermediates (mainly CO) formed during methanol oxidation, (3) the high extent of methanol cross over through the Nafion® type membranes, which depolarizes the air cathode, and (4) the power density and efficiency are several times lower than for hydrogen (or methanol reforming) system because a large fraction of the input methanol crosses over the membrane and is oxidized at the cathode without producing useful power [3]. Moreover, methanol has particular disadvantages, e.g. it is relatively toxic, inflammable with a low boiling point (65 °C), and it is neither a primary fuel nor a renewable fuel [8]. The design of a fuel processor is an important technology for the deployment of PEMFCs. It produces hydrogen-rich streams from hydrocarbons like methanol in a multi-step process (fuel vaporizer, primary conversion reactor that produces synthesis gas, water gas shift reaction and CO clean-up reactor).

The purpose of this study is to conceptually design a fuel processor for 5 kW mobile and portable PEMFC. The main target is to produce the concentration of CO at less than 2000 ppm before entering the separation units. For a fuel other than hydrogen, the sensitivity of the PEMFC to CO requires the installation of at least two reformers at purification stages. Here, we use ATR as the primary hydrogen production and WGS reactor in series as secondary hydrogen production as well as primary CO clean-up units. This paper will also show the overall system design and the rate of reaction considering the volume expansion for both units, which are always neglected by most of the researcher. Besides that the authors will show the comparison between WGS and PROX in removing the CO. Finally the authors will present the selectivity of hydrogen for both systems and show the overall material balance to determine the efficiency of the system.

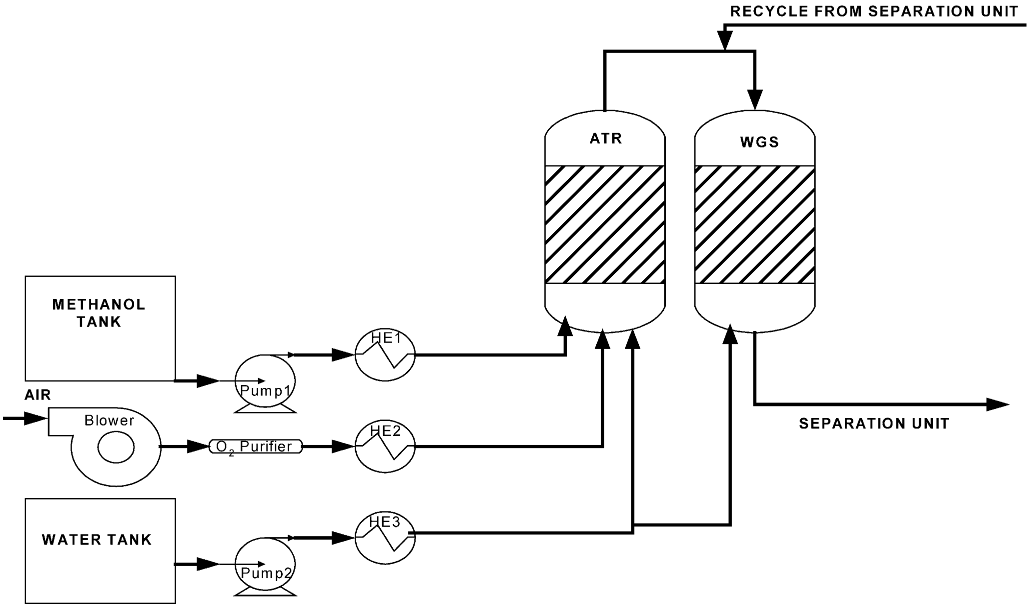


Fig. 1. Schematic diagram of fuel processor unit.

Fig. 1 shows the schematic diagram of the fuel processor unit proposed in this study. Beginning at the left-bottom, the water stream is pumped to HE3 to generate a superheated steam, while ambient air passed through an oxygen concentrator to separate the O_2 from N_2. The fuel flow circuits begin at the fuel tank (methanol). From the tank, it is pumped to HE1 where it is heated and vaporized. It is then fed to the ATR where it reacts with the preheated air by HE2 and superheated steam to yield the raw reformate. The hot reformate is used to superheat the ATR steam feed. It is then mixed with additional steam and fed to the WGS reactor. The fuel gas from WGS will go to the separation units for further treatment on the CO and hydrogen purification.

2. Auto-thermal reformer

In principle, there are three types of reforming processes: (1) partial oxidation (POX), (2) auto-thermal reforming (ATR), and (3) steam reforming (SR). Hydrogen produced from the SR process (a highly endothermic reaction) requires a large amount of energy [4,6,12,13], while the POX of methanol is an exothermal step produces water that offers compactness, fast start-up and rapid responses, is a co-reactant in the SR reaction. Thus, conceptually, coupling the POX and SR (POX–SR) in a single reaction unit so-called an auto-thermal reforming (stand-alone-reactor) could yield an energetically self-sufficient system for the production of H_2 [5,7,12,14–17]. The ATR involves in the production of H_2 from methanol and steam while co-feeding with oxygen can be represented in the following reactions:

$$CH_3OH + H_2O \rightarrow CO_2 + 3H_2 = r_1 \quad (1)$$

$$CH_3OH + 0.5O_2 \rightarrow CO_2 + 2H_2 + CO = r_2 \quad (2)$$

The ratio of the three reactants can vary and is often chosen such that the overall reaction is thermal-neutral or only modestly exothermic. It is observed that the stoichiometry of H_2O and O_2 effect significantly the moles of H_2 produced. Increasing S/C increases the total amount of water used in the fuel processor, with a resultant of decrease in the concentration of CO. Due to that the selection of the feed ratio is very important in order to produce a high purity of hydrogen with necessary heat supply for the endothermic SR process by exothermic POX.

2.1. Hydrogen selectivity

Calculation of hydrogen selectivity is presented as below

$$-\frac{dC_M}{dt} = -r_M = r_1 + r_2 \quad (3)$$

$$-\frac{dC_{O_2}}{dt} = -r_{O_2} = 0.5r_2 \quad (4)$$

$$-\frac{dC_S}{dt} = -r_S = r_1 \quad (5)$$

Thus, from the stoiciometrics, it is known that

$$r_H = 3r_1 + 2r_2 = 3r_M - 2r_{O_2} = r_S + 2r_M \quad (6)$$

$$C_{H_2} = 3C_{M0}X_M - 2C_{O_20}X_{O_2} = C_{S0}X_S + 2C_{M0}X_M \quad (7)$$

The selectivity of hydrogen, $S_{H_2/M}$ is given by Eq. (8) assuming the partial oxidation reaction is extremely fast [18] and all the oxygen is consumed in the initial stage of the reaction:

$$S_{H_2/M} = \frac{C_{H_2}}{C_{M0}X_{M0}} = \left(3 - 2\frac{M_O}{X_{M0}}\right) \quad (8)$$

where $M_O = C_{O_2 0}/C_{M0}$, is the ratio of initial concentration of oxygen to methanol, X_{M0} the mole fraction of methanol in the feed flow and C_{H_2} is the concentration of H_2.

The selectivity of hydrogen for S/C is given as

$$S_{H_2/M} = \frac{M_S X_S}{X_M} + 2 \tag{9}$$

where the initial ratio concentration of steam to methanol, $M_S = C_{S0}/C_{M0}$, X_S and X_M are the mole fraction of steam and methanol in the flow.

2.2. Reactor design

Cu-based is used as a catalyst in the design calculation as it is active for the simultaneous reactions of steam reforming and partial oxidation. The design of the reactor volume is based on the methanol steam reforming reaction, as the partial oxidation reaction is extremely fast. The volume of catalytic plug flow reactor obtained from the material balance is given by [22]:

$$V = \frac{F_{M0}}{\rho(1-\varepsilon)} \int_0^{X_M} - \frac{dx}{r_{ATR}} \tag{10}$$

Here, F_{M0} is the feed flow rate of methanol, ρ the catalyst density, ε the voidage of catalyst and r_{ATR} is the rate of reaction for methanol in ATR. Assuming the pressure is constant in the ATR during the reaction and considering the varying-volume, ε_M (or varying density), the temperature changes from T_0 to T gives the volume, V of ATR is linearly related to the conversion of methanol, X_M or

$$V = V_0(1 + \varepsilon_M X_M)\left(\frac{T}{T_0}\right) \tag{11}$$

The kinetic rate of ATR is expected as below

$$-r_{ATR} = k_1 C_M C_S^{0.5} C_{O_2}^{0.25} \tag{12}$$

with $C_M = C_{M0}((1 - X_M)/(1 + \varepsilon_M))$, and $\psi = T/T_0$ than Eq. (12) can be rewritten in term of C_{M0} as

$$-r_{ATR} = k_1 C_{M0}^{1.75} \frac{(1 - X_M)(M_S - X_M)^{0.5}(M_O - X_M)^{0.25}}{\psi(1 + \varepsilon_M X_M)^{1.75}} \tag{13}$$

where the rate constant, $k_1 = A_0 e^{-(E_a/RT)}$, E_a the activation energy and A_0 the pre-exponential factor.

Substituting Eqs. (10)–(13), the volume of ATR is expected as

$$V = \frac{F_{M0}}{\psi\rho(1-\varepsilon)k_1} \times \int_0^X \frac{(1 + \varepsilon_V X_M)^{1.75} dx}{C_{M0}^{1.75}(1 - X_M)(M_S - X_M)^{0.5}(M_O - X_M)^{0.25}} \tag{15}$$

3. Water gas shift reaction

The other step of processing is water gas shift reaction (WGS). The reaction is given as below

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \tag{16}$$

The carbon monoxide in the presence of steam will be converted to carbon dioxide and hydrogen. This reaction is exothermic and thermodynamically favoured at lower temperatures. WGS provides primary CO clean-up as well as secondary H_2 production. A target CO conversion of 90–95% in the WGS unit would translate into a CO level of 30 000–100 000 ppm being reduced to 1000–10 000 ppm [17,20]. The kinetic reaction for WGS is taken as below [16]

$$r_{WGS}\ (\text{mol/g cat s}) = 2.25E - 3 \exp\left(\frac{-50\,000}{RT}\right) P_{CO} P_{H_2O} x \text{Eq}_{WGS} \tag{17}$$

where the pressure are in kPa, and

$$\text{Eq}_{WGS} = 1 - \frac{\overline{P}_{CO_2} \overline{P}_{H_2}}{K_{eq,WGS} \overline{P}_{CO} \overline{P}_{H_2O}} \tag{18}$$

with

$$K_{eq,WGS} = 9.543E - 3 \exp\left(\frac{39\,876}{RT}\right) \tag{19}$$

The volume for WGS reactor with recycle stream can be expressed as below

$$V = (R+1)\frac{F_{CO0}}{\rho(1-\varepsilon)} \int_{(R/(R+1))X_{C,F}}^{X_{CO,F}} - \frac{dx}{r_{ATR}} \tag{20}$$

$$V = (R+1)\frac{F_{CO0}}{\rho(1-\varepsilon)[2.25E - 3e^{-(50\,000/RT)} \overline{P}_{CO} \overline{P}_{H_2O} x \text{Eq}]} \times \int_{(R/(R+1))X_{C,F}}^{X_{CO,F}} - \frac{dx}{r_{WGS}} \tag{21}$$

where R is referred to recycle stream, F_{CO0} the feed flow rate of CO to WGS, ρ the catalyst density, ε the voidage of catalyst and r_{WGS} is the rate of reaction in WGS reactor.

4. Overall material

The overall material balance for a fuel processor unit is as depictured in Fig. 2.

The primary fuel source to ATR is methanol combines with water and oxygen to produce hydrogen, carbon dioxide and carbon monoxide. Referring to Eqs. (4) and (5), let n_1 and n_2 = degree of first and second reaction, respectively.

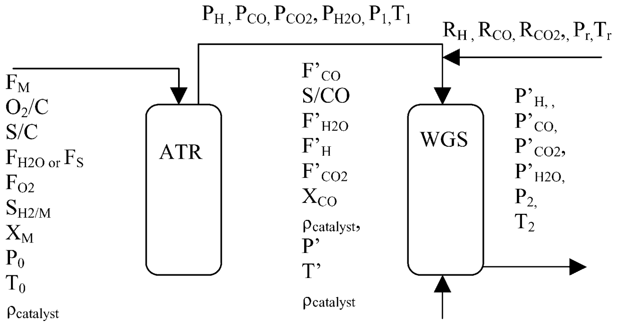


Fig. 2. Design parameters for ATR and WGS.

The mass balance for methanol:

$$F_M = X_M(n_1 + n_2) = F_S - y_S\, P_G + 2F_{O_2} = \frac{P_H}{X_M S_H} \quad (22)$$

The mass balance for steam:

$$\begin{aligned} F_S &= X_M n_1 + y_S P_G \\ &= F_M - 2F_{O_2} + (1 - y_{H_2} - y_{CO_2} - y_{CO})P_G \end{aligned} \quad (23)$$

The mass balance for oxygen:

$$F_{O_2} = 0.5X_M n_2 = 0.5X_M(F_M - F_S + y_S P_G) \quad (24)$$

The mass balance for hydrogen:

$$P_H = X_M(3n_1 + 2n_2) = F_M X_M S_H \quad (25)$$

The mass balance for carbon dioxide:

$$P_{CO_2} = n_1 + n_2 = F_M = \frac{P_H}{X_M S_H} \quad (26)$$

The mass balance for carbon monoxide:

$$P_{CO} = 0.2P_{CO_2} \quad (27)$$

With that the total product gas from ATR:

$$P_G = \frac{2S_H F_S + P_H}{S_H(5y_H - 4(1 - y_{CO_2} - y_{CO}))} \quad (28)$$

For WGS reaction, the mass balance is referred to Eq. (16) and assumed no reverse WGS reaction occurs at excess steam condition. With that let n_3 = degree of reaction.

The mass balance for CO:

$$\begin{aligned} P'_{CO} &= y_{CO,P} P_G + y_{CO,R} R'_G - X_{CO} n_3 \\ &= y_{CO,P} P_G + y_{CO,R} R'_G + P'_S - F''_S \end{aligned} \quad (29)$$

The mass balance for steam:

$$P'_S = F''_S - X_{CO} n_3 = y_{S,P'} F''_G \quad (30)$$

The mass balance for H_2:

$$\begin{aligned} P'_H &= X_{CO} n_3 + y_{H,P} P_G + y_{H,R} R_G \\ &= F''_S - y_{S,P''} F''_G + y_{H,P} P_G + y_{H,R} R_G \end{aligned} \quad (31)$$

The mass balance for CO_2:

$$\begin{aligned} P'_{CO_2} &= X_{CO_2} n_3 + y_{CO_2,P} P_G + y_{CO_2,R} R_G \\ &= F''_S - y_{S,P'} F''_G + y_{H,P} P_G + y_{H,R} R_G \end{aligned} \quad (32)$$

The total product gas at the outlet of WGS:

$$F''_G = \frac{F''_S \pm y_{H,P} P_G + y_{H,R} R_G - P'_H}{y_{S,P''}} \quad (33)$$

5. Result and discussion

Fig. 3 is plotted based on Eq. (8) and the ratio of O_2/C is found to be between 0.20 and 0.25 for complete conversion of methanol. The hydrogen selectivity at this point is around 2.5–2.6. Similar method was used to obtain for S/C as given in Eq. (9) and Fig. 4. From Fig. 4, the minimum value for S/C is taken as 0.5 to yield a 2.5–2.6 of hydrogen. However, steam

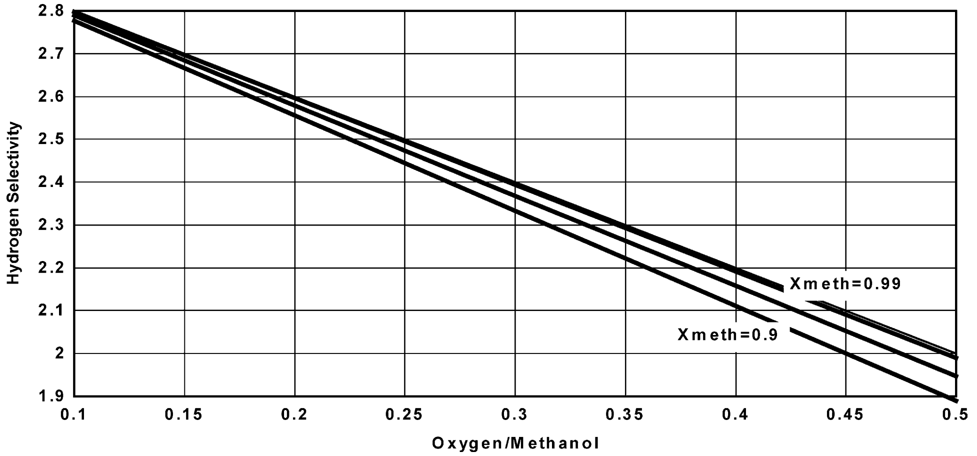


Fig. 3. The hydrogen selectivity for different oxygen/methanol ratio.

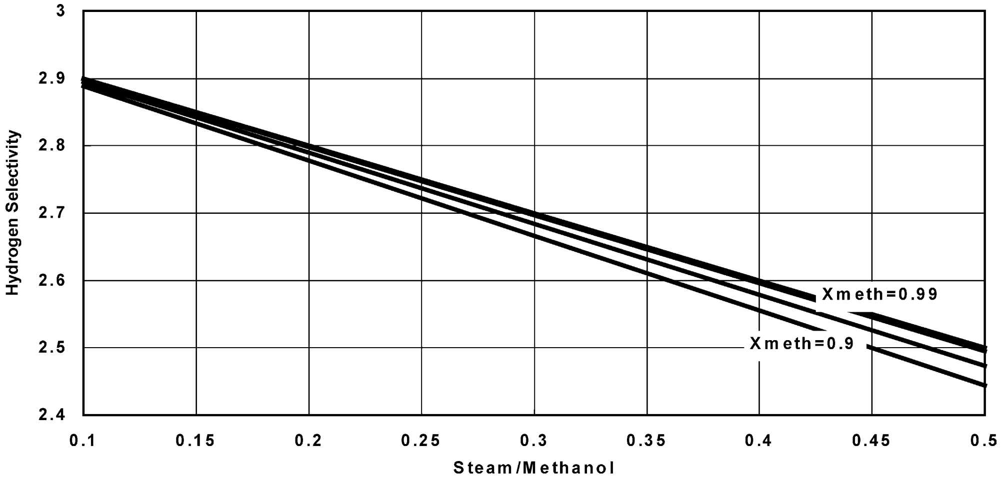


Fig. 4. The hydrogen selectivity for different steam/methanol ratio.

is fed in excess into the system in order to avoid the reverse WGS reaction and inhibit the CO production. With that the overall reaction for ATR in this study is taken as below

$$CH_3OH + 0.5\,H_2O + 0.25\,O_2 \rightarrow 2.5H_2 + CO_2 + (CO) \tag{34}$$

Taking the activation energy, E_a and pre-exponential factor, A_0 as 100.9 kJ/mol and 1.9×10^{12} mol (min g cat kPa$^{0.22}$)$^{-1}$ [19], respectively, with a 100% conversion of methanol, Figs. 5 and 6 are plotted. Two different flow rates of methanol are considered in this study, that is at 6 and 4 mol/min. From Figs. 5 and 6, it observed that the optimum operating temperature falls at the range of 220–250 °C. Although, at higher temperature, the rate of reaction is high, the production of CO is also rapid [18]. However, an operating temperature lower than 220 °C also is not suitable neither for mobile and portable applications, as this will require a large volume (more than 2000 cm^3) of reactor and a large amount of catalyst.

From Fig. 7, it was observed that for temperature higher than 220 °C, the operating pressure did not significantly affect the volume of ATR reactor; however, for lower operating temperature the volume of reactor decreased exponentially as the pressure increased up to 10 bar. Nevertheless, the latter is not recommended for mobile and portable applications of fuel cell system. Therefore, ambient pressure is best used as the operating pressure. Besides that, from Fig. 8, it can be concluded that the ratio of O_2:MeOH in the feed neither affect the reactor volume.

Fig. 9 is plotted based on Eqs. (17)–(21). From Fig. 9, it is observed that the CO equilibrium in WGS is very dependent on temperature and the ratio of S/CO. As a result, lower operating temperature conditions and higher amount of water steam favour CO_2 over CO, which are desired and inhibit the

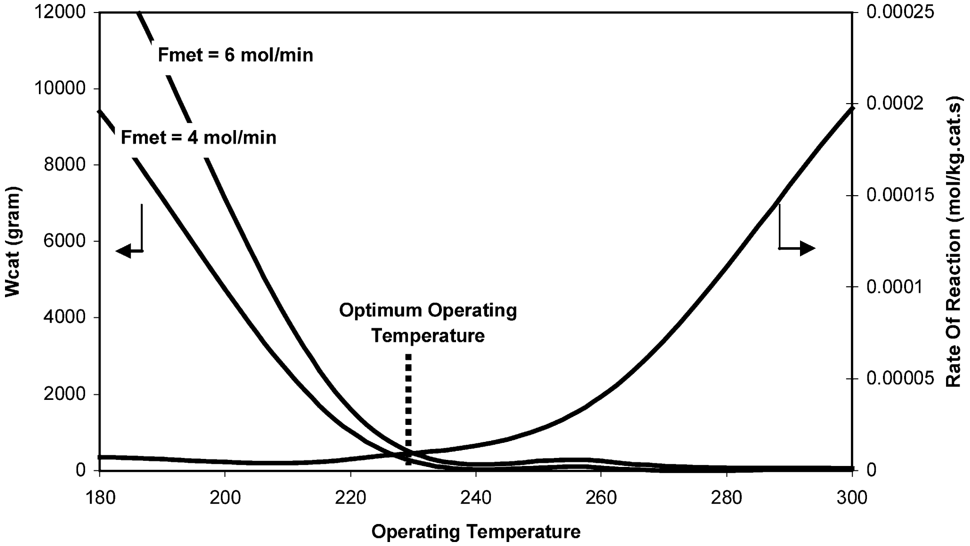


Fig. 5. The reaction rate and the amount of catalyst required for different operating temperature.

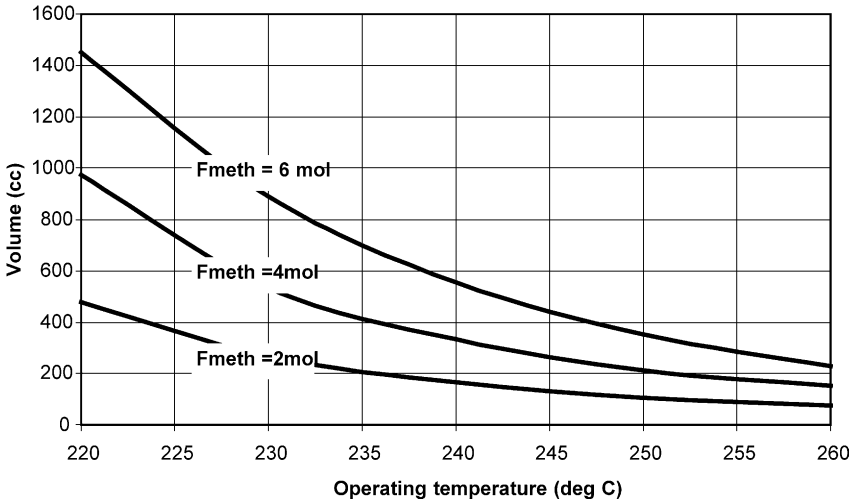


Fig. 6. Reactor volume for various flow rate of methanol at different selected temperature.

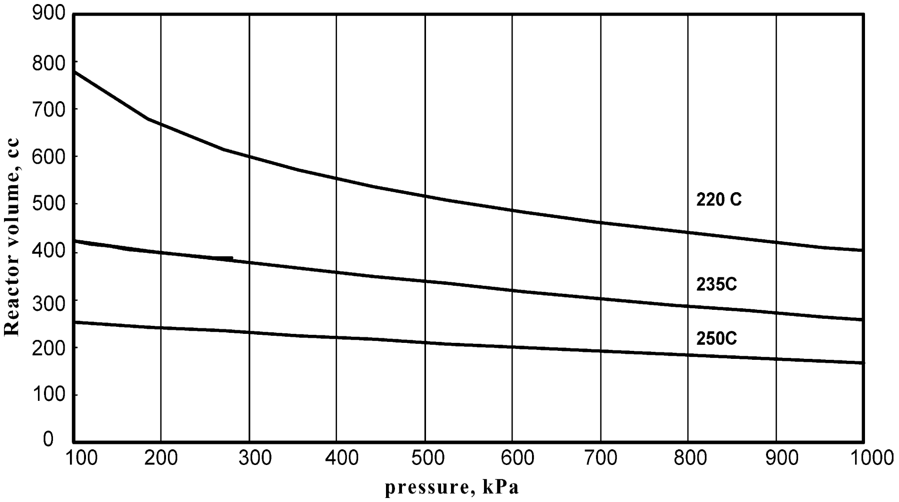


Fig. 7. The effect of pressure to the volume of ATR at different temperature.

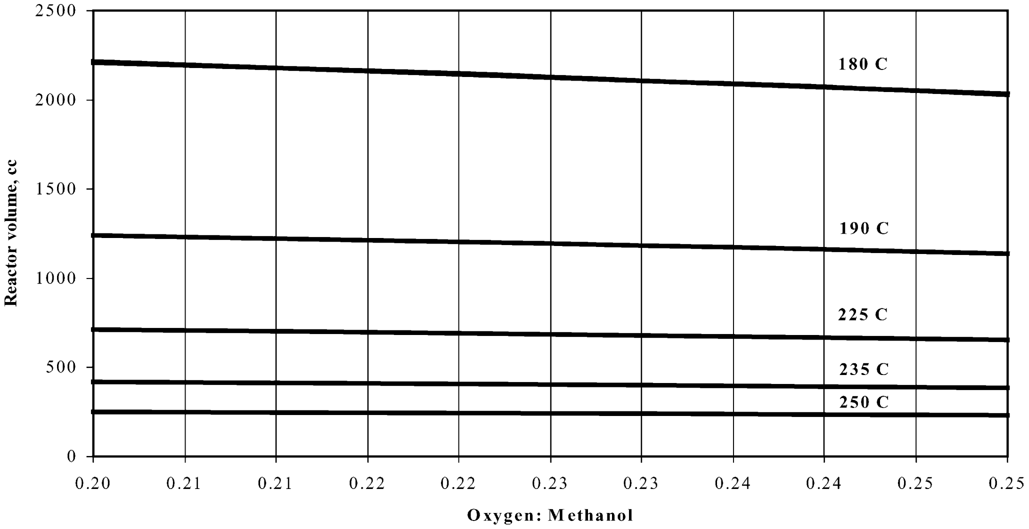


Fig. 8. The effect of oxygen:methanol to the volume of ATR at different temperature.

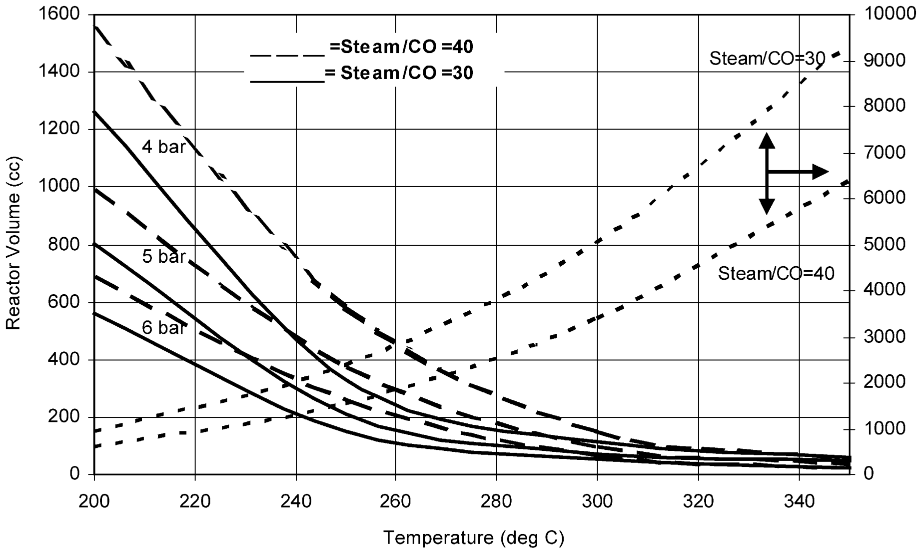


Fig. 9. The equilibrium of CO vs. the ratio of steam/CO, temperature and pressure.

reverse WGS reaction to occur. However, this will end-up with a large unit of WGS reactor. Hence, pressure plays an important role in the WGS reactor design so as to overcome the problem. As can been seen in Fig. 9, the volume of the reactor reduces with pressure increment. Moreover, the CO formation also decreases at high operating pressure.

The hydrogen consumption in the fuel cell stack is taken as 1000 l/h of hydrogen for every power output of 1 kW$_e$ [5]. With that the total hydrogen required at the stack for a power output of 5 kW is calculated as 0.08 m^3/min (3.74 mol/min). Taking the primary fuel source to the ATR system as 0.1 m^3/min (4 mol/min) which is fed together with steam and oxygen with the ratio for H_2O:MeOH and O_2:MeOH at 1.3:1 and 1:4 respectively, Figs. 10 and 11 are plotted.

Finally from the overall mass balance, as the result from Fig. 10, the products from ATR are determined as: H_2: 73%, CO: 2%, and CO_2: 25%. While Fig. 11 shows the changes of H_2, CO, CO_2 in terms of mole fraction (dry basis) before and after the WGS. It is observed that the hydrogen recovery after the WGS is only about 0.3–0.6% but the mole fraction of CO is found to decrease from 2% to about 0.2%. Although this is a very small drop but it is very significant in the PEMFCs system because the concentration of CO reduces from 20 000 ppm (after the reformer) to less than 2000 ppm (after the WGS) assuming no reverse WGS reaction occurs due to the excess steam. However, if CO is being produced thermodynamically by the reverse water gas shift reaction, it will only be in the range of 20–50 ppm [20,21]. As a result, it denied the acquisition by [14,17,18], that the WGS was not needed in the fuel processor as one of the CO clean-up systems. Although the main problem in WGS process is the low temperature of catalyst activity and expected to be the largest component in the system, but this paper proves that WGS

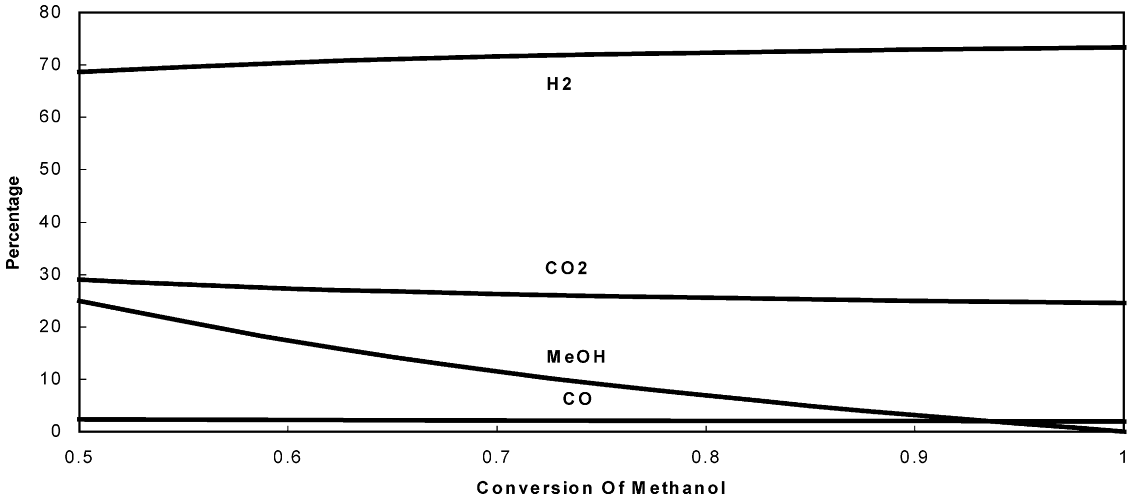


Fig. 10. The percentage of H_2, CO_2 and CO (dry basis) produced from ATR.

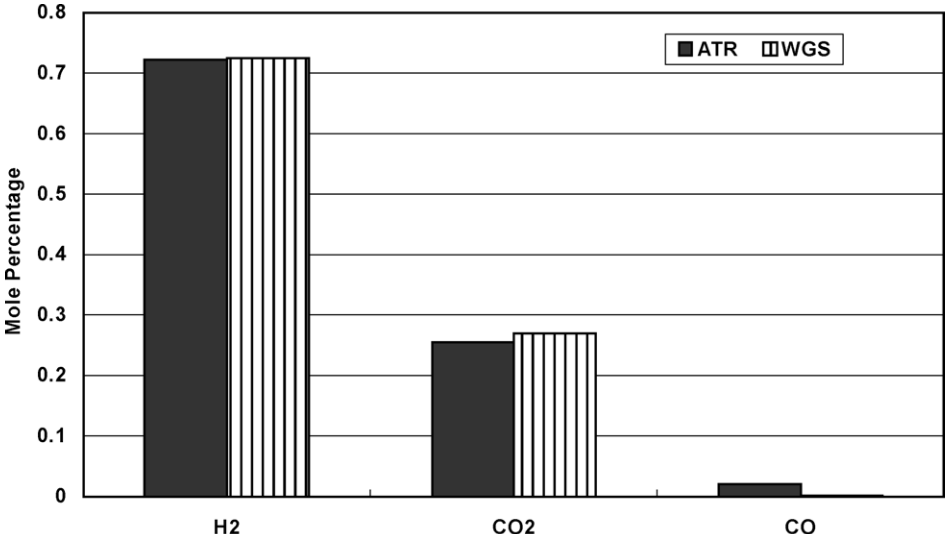


Fig. 11. Mole fraction of H_2, CO and CO_2 (dry basis) before and after WGS reactor.

reaction is very important in PEMFC unit as secondary hydrogen source and primary CO clean-up unit. Furthermore, the conceptual design also proves that pressure can be used as a control parameter to reduce the size of the WGS reactor.

Besides that comparison is also made for a preferential oxidation (PROX) to replace the WGS reaction as a second alternative. The preferential oxidation reactor is used to eliminate the CO from the ATR. It uses pure oxygen in the process with the following reaction:

$$CO + O_2 \rightarrow CO_2 \quad (35)$$

Unfortunately, the selectivity of the catalyst will not avoid the combustion of some hydrogen in the gas stream with the following reaction [23,24]:

$$H_2 + 0.5O_2 \rightarrow H_2O \quad (36)$$

Taking the selectivity of Eq. (35) as 0.4 and 100% conversion of CO, the results for PROX are illustrated in Figs. 12 and 13.

In Fig. 12, it is observed that the production of CO is inversely proportional to the ratio of CO:O_2, λ in PROX. This concludes that the production of CO is very dependent on the value of λ. While Fig. 13 shows the comparison of the output stream of WGS reactor and PROX as alternatives 1 and 2, respectively. As a result, it can be seen that the PROX performs better than WGS reactor in terms of water and CO production in outlet stream. However, the flow rate of hydrogen decreases from 10.4 to 9.92 mol/min in PROX at $\lambda = 2.5$. Whereby in WGS reactor, it increases from 10.4 to 10.65 mol/min. Due to that, the feed flow rate of MeOH to the ATR is expected to be slightly higher for PROX than WGS reaction. However, the main advantage of PROX is from the water management point of view whereby it produces less water in the system while WGS reactor produces at about

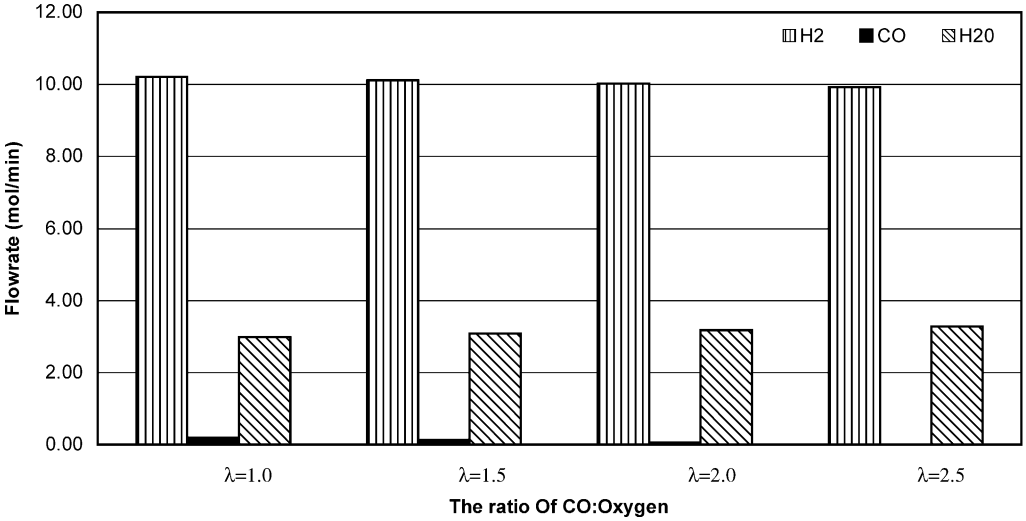
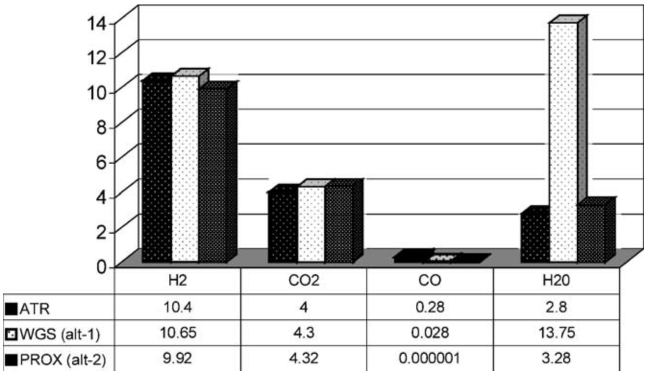


Fig. 12. The ratio of CO:O_2, for different flow rate in PROX.



	H2	CO2	CO	H20
■ATR	10.4	4	0.28	2.8
◘WGS (alt-1)	10.65	4.3	0.028	13.75
■PROX (alt-2)	9.92	4.32	0.000001	3.28

Fig. 13. Flow rate (mol/min) of outlet stream for WGS and PROX.

48% of water in the product stream. Water management is very important in the secondary hydrogen separation unit because water can be the main obstacle for separating the CO from hydrogen in membrane unit that is not explained in this paper. Nevertheless the main problem with PROX is to select a good catalyst that can yield a good selectivity for CO oxidation reaction.

6. Conclusion

In conclusion the main task of the study to conceptually design a fuel processor system and CO clean-up system for fuel cell has been achieved. The formula for kinetic reaction rate and volume for both units are derived by the authors by taking the expansion of volume during reaction into consideration. In particular, through the conceptual design, this paper proves that the WGS is very significant as a primary CO clean-up system and pressure can be used to reduce the size of WGS.

From the result, it is also observed that the temperature and the ratio of steam:MeOH are also important in reducing the production of CO mainly in the WGS system. Indeed, low-temperature catalyst activity and stability are the main issues related to WGS reactor. This is because most of the industrial WGS reaction catalysts have been developed for operation at higher temperature that is not viable for automotive fuel processor. Due to that, the selection of suitable catalyst for both processes in ATR and WGS reactor are also very important.

Besides that, this paper also highlights that PROX can be used as a CO clean-up unit replacing WGS reactor and it performs better than WGS in terms of water management. Catalysts for PROX owe their selectivity to the fact that H_2 oxidation is blocked by CO adsorption. However, H_2 oxidation will begin to predominate at low partial pressure of CO, when relatively a few catalytic-active sites are blocked. In practice, this means that the preferential oxidation of CO can become increasingly difficult as the CO concentration declines, which will in turns yield more CO_2 rather than H_2O formation. Moreover, the main problem with PROX is to select a good catalyst that can yield a good selectivity for CO oxidation reaction, due to the fact that the catalyst is so expensive.

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