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Simulation and Analysis of Hydrogen Production by Dimethyl Ether Steam Reforming for PEMFC

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Abstract

Energy crisis has become a serious global problem, and Proton exchange membrane fuel cell (PEMFC) has played an important role in the solution of the energy crisis. The hydrogen production process by dimethyl ether steam reforming for PEMFC was studied. The yield of H_2 and energy efficiency of system with different mass ratios (0.3:0.7, 0.35:0.65, 0.4:0.6) of dimethyl ether (DME) and steam were analyzed, and both of yield of H_2 and energy efficiency of system increased with the increase of the mass ratio of DME and steam. The energy efficiency of hydrogen production system using reactor as heat source and hydrogen production system using engine exhaust gas as heat source is compared, and energy efficiency of using reactor as heat source (57.96117%, 63.89651%, 69.0002%) is higher than that using engine exhaust gas as heat source (54.4913%, 60.11311%, 66.25342%).

Keywords

Steam Reforming, Dimethyl Ether, Proton Exchange Membrane Fuel Cell

1. Introduction

An increase in energy consumption that results from human-related activities causes the depletion of fossil fuel and the global warming problem. Thus, searching for clean and sustainable energy source is necessary for the future. Hydrogen is an important alternative fuel that is expected to replace fossil fuels because it is clean and environmentally friendly energy source [1]. Currently, hydrogen is commonly used as a reactant in chemical industries. In addition, hydrogen-based fuel cells have the advantages of zero emission, high energy conversion efficiency, low noise, etc. It will become a significant fuel in the near future [2] [3].

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Dimethyl ether (DME) is an excellent resource for hydrogen production with its high H/C ratio and high-energy volume density. DME does not contain harmful materials and it burns without producing NO_x, and particulates. DME was liquid in the low pressure similar to liquefied petroleum gas (LPG), thus could be stored and transported using the facilities providing LPG. DME is an ideal vehicle fuel, but also has capability of chemical hydrogen storage. Therefore, many scholars have been studied to the DME reforming processes. Steam Reforming (SR) is the most commonly used process of hydrocarbon reforming techniques of DME because it provides high yields of hydrogen production. However, it also requires a large amount of external heat source. The exhaust gas of the vehicle is wasted after clarification by an after-treatment system, but the heat resource and steam from the exhaust gas can be efficient by SR reaction [4]-[9].

PEMFC exhibits special advantages including fast start-up, low working temperature, high specific energy density, simple structure, convenient operation and great durability [3]. These characteristics are precisely that the automotive engine needs to be satisfied, so the PEMFC is recognized as the main source of energy of electric vehicles in the future. The working principle of proton exchange membrane fuel cell is same as the ordinary fuel cell. Platinum carbon or platinum ruthenium as an electro catalyst, hydrogen as fuel, air or pure oxygen as the oxidant and graphite or surface of the gas flow passage change of sheet metal is a bipolar plate.

In this paper, the hydrogen production system for PEMFC was studied. The hydrogen production process and operating parameters were calculated and simulated by using commercial process simulation software Aspen Plus. The effects of mass ratio of DME and steam and energy efficiency of the PEMFC power system are analyzed.

2. Simulation

2.1. Reactions of System

The system of hydrogen production mainly includes the following reactions:

Overall reaction of steam reforming of DME:

$$CH_3OCH_3 + 3H_2O(g) = 6H_2 + 2CO_2 \triangle H_{298} = 122 \text{ kJ/mol} \quad \text{(Equation 1)}$$

And steam reforming of DME process involves following four main reactions:

Water-gas shift:

$$CO_2 + H_2 = CO + H_2O(g) \triangle H_{298} = 41.2 \text{ kJ/mol} \quad \text{(Equation 2)}$$

DME hydrolysis:

$$CH_3OCH_3 + H_2O(g) = 2CH_3OH \triangle H_{298} = 37 \text{ kJ/mol} \quad \text{(Equation 3)}$$

Steam reforming of methanol:

$$CH_3OH + H_2O = 3H_2 + CO_2 \triangle H_{298} = 49 \text{ kJ/mol} \quad \text{(Equation 4)}$$

Methanol decomposition:

$$CH_3OH(g) = 2H_2 + CO \triangle H_{298} = 91 \text{ kJ/mol} \quad \text{(Equation 5)}$$

In addition, Partial oxidation reaction (PROX):

$$CO + 0.5O_2 = CO_2 \triangle H_{298} = -283 \text{ kJ/mol} \quad \text{(Equation 6)}$$

$$H_2 + 0.5O_2 = H_2O(g) \triangle H_{298} = -241.8 \text{ kJ/mol} \quad \text{(Equation 7)}$$

2.2. Describe of Model

Figure 1 shows the flowchart of hydrogen production system for PEMFC. The correspond steam and abbreviations are defined in **Table 1**. And H_2/CO indicate H_2 and CO produced by steam reforming, H_2_rest indicates rest H_2 of PEMFC, Electric Power represent power generated by PEMFC, Q_rest indicates rest energy of engine exhaust gas, Q_lost indicate energy consumption of engine work.

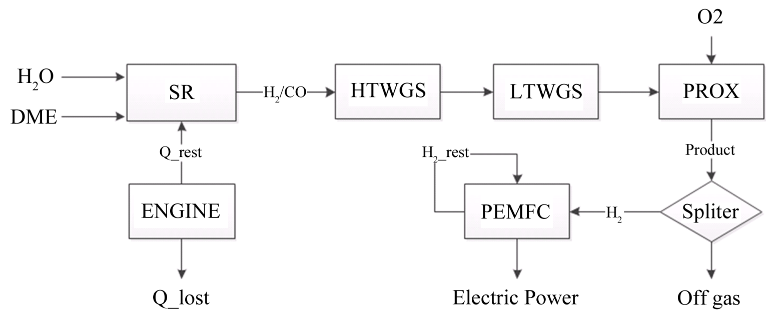

Figure 1. Flowchart of hydrogen production system.

Table 1. Steam and block abbreviations.

Streams	
DME	DME for reforming process
H_2O	Deionized water for reforming process
ENGINE	Engine for reforming process
O_2	Oxygen for PROX reaction
PEMFC	Product for PEMFC
OFFGAS	Off gas of system
Blocks	
MIXER	Mixer for DME and steams
SPLITER	Spliter for H_2 and Off gas
SR	Yield reactor used for isothermal SR reaction
HTWGS	Gibbs reactor used for isothermal HTWGS reaction
LTWGS	Gibbs reactor used for isothermal LTWGS reaction
PROX	Stoic reactor used for isothermal PROX reaction
HEATER1	Heater preheating deionized water
HEATER2	Heater preheating DME
HEATER3	Cooler between SR and HTWGS reactors
HEATER4	Cooler between HTWGS and LTWGS reactors
HEATER5	Cooler between LTWGS and PROX reactors
HEATER6	Heater preheating O_2
HEATER7	Cooler between PROX and Spliter

Q_rest can provide heat for reaction of dimethyl ether steam reforming, and H_2_rest can be reused by PEMFC. It indicates that the system has a good energy cycle, and the energy can be used to the maximum extent. This can also improve the energy efficiency of the whole system.

Figure 2 shows the simulation diagram of hydrogen production process by Aspen Plus software. **Figure 2(a)** represents model A that illustration a hybrid system by using engine exhaust gas as heat source for hydrogen production. **Figure 2(b)** represents model B which indicates a hydrogen production system using reactor as heat source. The model A and model B is based on a zero-dimensional approach with steady and isothermal operation condition and all working fluid are simulated by using the Peng-Robinson equation.

The hydrogen production process mainly consists of three parts: SR part, purification part and supply part. SR part is the core part of the hydrogen production process, it mainly include DME stream reforming reaction (Equation 1) and water-gas reaction (Equation 2). These two reactions occur simultaneously in the reactor and their conversions are considered to be close the equilibrium. H_2O and DME are preheated by heater 1 and heater 2.

Their temperature must be up to the temperature of the SR reaction. The SR reactor temperature is constant, so the external heat supply should be maintain isothermal. Purification part includes high-temperature water-gas reaction (HTWGS), low-temperature water-gas reaction (LTWGS) and PROX (Equation 6-7). HTWGS and LTWGS use the Gibbs reactor and PROX uses the Stoic reactor. Those three reactions also should be maintained constant temperature. The isothermal conditions mean that the heat produced by the reactions must be removed and can be used as hot streams for energy recovery [10]. CO is converted to H_2 and CO_2 during the HTWGS and LTWGS reactions, with outlet streams containing about 5% - 12% and 0.5% - 1.0% CO, respectively. The high CO concentration can cause the deactivation of PEMFC catalysts. This means a further CO

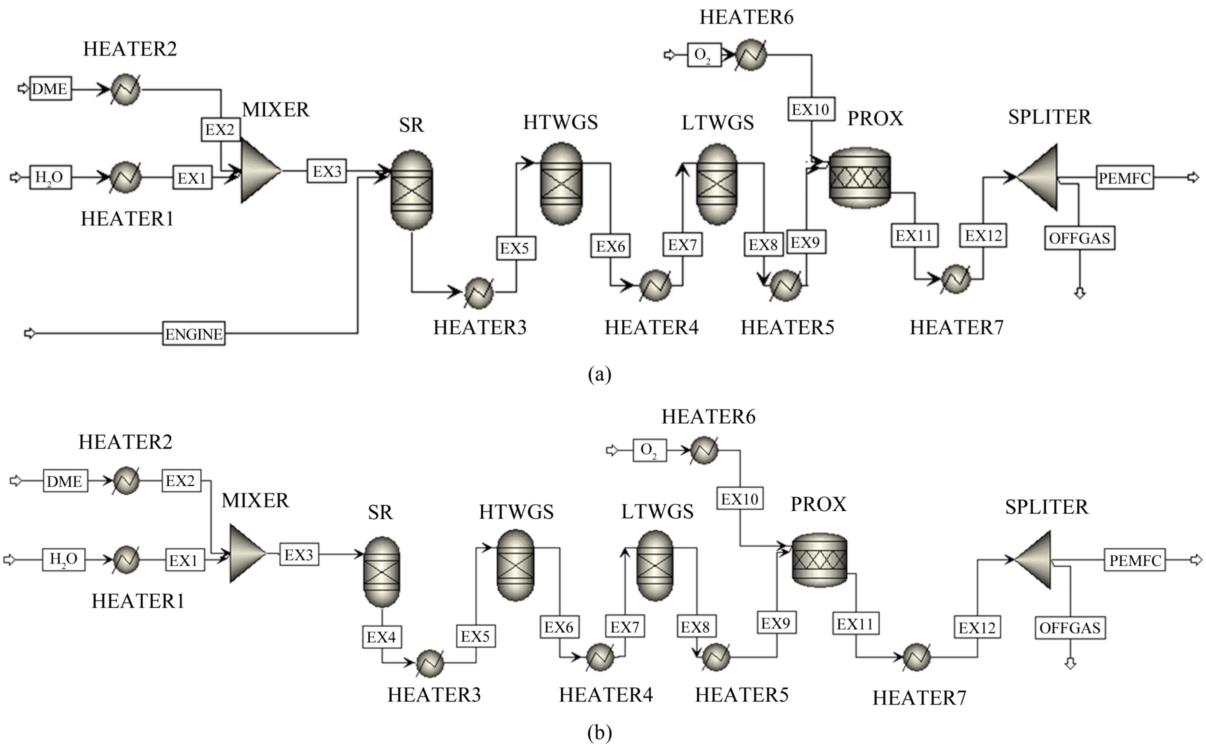

Figure 2. Simulation diagram of hydrogen production process: (a) model A: hybrid power by using engine exhaust gas as heat source, (b) model B: using reactor as heat source.

reduction unit needed to decrease CO to levels below 10 ppm [11]-[13]. In the Supply part, the purified hydrogen by Purification part is supplied directly to the PEMFC through the heater and separator.

2.3. Parameters

Table 2 shows the parameters initial value of this simulation. Some of the parameters of hydrogen production system are based on typical parameters reported for literature. SR block was used in Yield reactor, the reaction temperature is 750 K. And kinetic data were measured by the experiment, as shown in **Table 3**.

3. Result and Analysis

Table 4 illustrates the yield of H_2 of system while the inlet flow rate of DME is 0.30 kg/s, 0.35 kg/s, 0.4 kg/s. It indicates that the yield of H_2 increases with the increase of the mass ratio of DME and steam, because the increasing in DME can promote the production of H_2. The yield of H_2 achieves a maximum (186.878333 kmol/hr) while mass ratio is 4:6 of DME and steam.

Table 5 shows the heat duty of hydrogen production process for PEMFC of model A and model B. In order to evaluate the performance of the DME steam reforming system for PEMFC, the energy efficiency of the system were defined by the relationship:

$$\text{Energy efficiency}(\%) = \left(P_{\text{H2,PEMFC}}\right) / \left(Q_{\text{LHV,DME}} F_{\text{DME,in}} + Q_{\text{in}}\right) \times 100 \qquad \text{(Equation 8)}$$

$F_{\text{DME,in}}$ is the molar flow rates of DME at the inlet. $Q_{\text{LHV,DME}}$ is the low heat values of DME. $P_{\text{H2,PEMFC}}$ is the energy produced of PEMFC with supplying hydrogen.

Selection of a certain type of 1.8 L engine, power 80 kW, indicated thermal efficiency of 35%, fuel consumption 8.0 L/100 km. And Selection of ChaoYue 3 PEMFC fuel cell vehicle, power 50 KW, fuel consumption 1.12 kg/100 km.

The calculated results are as shown in **Table 6**. It indicates that the energy efficiency is also increased with the increase of the mass ratio of DME and steam. And the efficiency of model B (57.96117%, 63.89651%,

Table 2. Parametervalues in calculations.

Variables	Initial value
SR temperature	750 K
Pressure of all Reactors	1 atm
DME/Steam mass ratio of SR	0.3/0.7, 0.35/0.65, 0.4/0.6
HTWGS	723 K
LTWGS	423 K
PROX	400 K
HEATER1	373 K
HEATER2	750 K
HEATER3	723 K
HEATER4	423 K
HEATER5	400 K
HEATER6	400 K
HEATER7	343 K

Table 3. Kinetic data of DME steam reforming reaction.

Mass ratio of DME and steam	Conversion rate of DME
DME:Steam = 0.3:0.7	50%
DME:Steam = 0.35:0.65	43.14286%
DME:Steam = 0.4:0.6	14.57143%

Table 4. Yield of H_2.

	H_2 (kmol/hr)		
	0.3:0.7	0.35:0.65	0.4:0.6
Model A	140.538726	163.859110	186.871870
Model B	140.538783	163.859577	186.878333

Table 5. Heat duty of hydrogen production process.

(a)

REACTOR	Enthalpy (Gcal/hr)		
	0.3:0.7	0.35:0.65	0.4:0.6
SR	0	0	0
HEATER1	1.61658318	1.50111295	1.38564273
HEATER2	0.24175101	0.28204284	0.32233468
HEATER3	−0.055205	−0.0562453	−0.0548379
HEATER4	−0.6259349	−0.6417521	−0.6562922
HEATER5	−0.0465996	−0.0480511	−0.0494898
HEATER6	4.26E−05	8.38E−05	1.97E−04
HEATER7	−0.1141745	−0.1176629	−0.1211142
HTWGS	0.55356551	0.67638246	1.13663565
LTWGS	−0.0804862	−0.1259303	−0.1887269
PROX	−0.0080375	−0.0158039	−0.0368286

(b)

REACTOR	Enthalpy (Gcal/hr)		
	0.3:0.7	0.35:0.65	0.4:0.6
SR	0.87764865	0.84802104	0.55390332
HEATER1	1.61658318	1.50111295	1.38564273
HEATER2	0.24175101	0.28204284	0.32233468
HEATER3	−0.0556454	−0.0562449	−0.0548373
HEATER4	−0.6259289	−0.6417473	−0.6562884
HEATER5	−0.0465988	−0.0480505	−0.0494898
HEATER6	4.26E−05	8.38E−05	1.97E−04
HEATER7	−0.1140853	−0.1175975	−0.1211137
HTWGS	0.49594954	0.67637782	1.13662693
LTWGS	−0.0804862	−0.1259284	−0.1886922
PROX	−0.0079886	−0.0157064	−0.0368286

Table 6. Energy efficiency of hydrogen production process for PEMFC.

DME/steam mass ratio	Model A	Model B
0.3:0.7	54.4913%	57.96117%
0.35:0.65	60.11311%	63.89651%
0.4:0.6	66.25342%	69.0002%

69.0002%) is higher than that of model A (54.4913%, 60.11311%, 66.25342%), because the engine has energy losses of model A, while model B has no energy loss by engine working.

4. Conclusion

In this study, the simulation of hydrogen production via dimethyl ether steam reforming for PEMFC was studied by using Aspen Plus software. It shows that the whole system has good energy cycle utilization. Both of yield of H_2 and energy efficiency of system increased with the increase of the mass ratio of DME and steam, and the energy efficiency of hydrogen production system using reactor as heat source is higher than that hydrogen production system using engine exhaust gas as heat source. Finally, this article can provide important theoretical references to the hydrogen production process for PEMFC.

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