INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2018) 1–11

Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he

Dynamic analysis of a PEM fuel cell hybrid system with an on-board dimethyl ether (DME) steam reformer (SR)

Tieqing Zhang, Kai Ou, Seunghun Jung, Byungchul Choi, Young-Bae Kim *

Department of Mechanical Engineering, Chonnam National University, Gwangju, Republic of Korea

ARTICLE INFO

Article history:
Received 24 March 2018
Received in revised form
11 May 2018
Accepted 15 May 2018
Available online xxx

Keywords:
Catalytic reactions
DME reformer
Dynamic simulation
PEMFC
Simulink
Hybrid system

ABSTRACT

Low-temperature polymer electrolyte membrane fuel cell (PEMFC) acts as a promising energy source due to the non-pollution and high-energy density. However, as hydrogen supply is a major constraint limiting the wide spread of fuel cell vehicles, a dimethyl ether (DME)-steam on-board reformer (SR) based on catalytic reforming via a catalytic membrane reactor with a channel structure is a possible solution to a direct hydrogen supply. The DME-SR reaction scheme and kinetics in the presence of a catalyst of CuO/ZnO/Al_2O_3+ZSM-5 are functions of the temperature and hydrocarbon ratio in the hydrogen-reforming reaction. An electric heater is provided to keep the temperature at a demanded value to produce hydrogen. As there is no available analysis tool for the fuel cell battery hybrid vehicle with on-board DME reformer, it is necessary to develop the tool to study the dynamic characteristics of the whole system. Matlab/Simulink is utilized as a dynamic simulation tool for obtaining the hydrogen production and the power distribution to the fuel cell. The model includes the effects of the fuel flow rate, the catalyst porosity, and the thermal conductivity of different subsystems. A fuel cell model with a battery as a secondary energy storage is built to validate the possible utilization of on-board reformer/fuel cell hybrid vehicle. In consideration of time-delay characteristic of the chemical reactions, the time constant obtained from the experiment is utilized for obtaining dynamic characteristics. The hydrogen supplied by the reformer and the hydrogen consumed in the PEMFC prove that DME reformer can supply the adequate hydrogen to the fuel cell hybrid vehicle to cope with the required power demands.

Introduction

An alternative and recyclable energy sources is becoming more and more indispensable as the consumption of the fossil energy increases. Nowadays an increasing attention is currently paid to the hydrogen energy as the alternative energy source. Significant effort has been made to commercialize the hydrogen fuel cell vehicles worldwide for the last 20 years [1]. The current energy efficiency of the internal combustion engine is approximately 20%–35% [2], and the conversion efficiency of the fuel cell can reach 60%, which is much higher than the internal combustion engine. Therefore, hydrogen fuel cell vehicles are thought as one of the right

* Corresponding author.
E-mail address: ybkim@chonnam.ac.kr (Y.-B. Kim).

https://doi.org/10.1016/j.ijhydene.2018.05.098
0360-3199/

Nomenclature

R	universal gas constant (8.3145 $Jmol^{-1}K^{-1}$)
r_i	rate of reaction i ($molm^{-3}s^{-1}$)
ΔH	heat of protonation ($kJmol^{-1}$)
C_i	concentration of surface species i ($molm^{-3}$)
k_i	rate coefficient of step i (molg-cat^{-1}s^{-1})
MeOH	methanol
DME	dimethyl ether
T	temperature (°C)
L	length of reactor (m)
pi	partial pressure of gas-phase species i (bar)
Ei	activation energy of reaction type i($Jmol^{-1}$)
J	permeation rate of gas-phase species i

Greek symbols

ε	porosity of the catalyst (0.3)
ρ	density of the catalyst 1300 kg m^{-3}(CuO-ZnO-Al_2O_3) 720 kg m^{-3}(ZSM-5)
Φ	steam to methanol ratio
δ	steam to CO molar ratio
δ_t	the thickness of the membrane

subscripts

H	DME hydrolysis
R	methanol reforming
WGS	water-gas shift
D	decomposition
H_2	hydrogen

directions to replace the internal combustion engine due to its absence of emission, fast start-up, low temperature, and capability of longer distance trip compared with pure electrical vehicle. Methods for fault diagnosis in PEM fuel cells are considered in Ref. [3]. Despite some commercial hydrogen vehicles have been on the market for more than 10 years, its full penetration to the market remains a long way to go. One of the major hindrances to the full penetration is the great scarcity of hydrogen station to supply hydrogen. As Alazemi et al. reviewed the comprehensive hydrogen station supply for automotive application, the number of the available hydrogen stations in the world is not more than 200 since 2015 [4]. This finding indicates that only limited number of fuel cell vehicle can be on the road due to the great shortage of hydrogen supply. Therefore, the primary challenge to popularize the fuel cell vehicle is how to produce and supply a large amount of hydrogen rapidly. As the hydrogen station number is very limited and costly to build, the on-board hydrogen reformer is an alternative way to supply hydrogen to the hydrogen vehicle.

Several reforming techniques are available for hydrogen production, including steam reforming, partial oxidation, and auto-thermal reforming [5–7]. Considering multiple sources to produce hydrogen, dimethyl ether (DME) is a preferable fuel to be applied for hydrogen production. DME contains higher mass fraction of hydrogen (13 wt%), and reforming process can be carried out under low temperature (200 °C–450 °C) compared with other options, including natural gas or diesel [8–11].

The reforming process also provides much safer and easier hydrogen storage mean with relatively low temperature and pressure compared with other processes, because storing hydrogen in tanks in the form of liquid or compressed hydrogen is not suitable for everyday applications due to low-energy density and serious safety issues. To produce hydrogen through DME/SR, the mixture of DME and vapor is utilized as the fuel, and four reactions are involved in the reactor: the DME hydrolysis to obtain methanol, the steam reforming of methanol, the methanol decomposition, and the water-gas shift reaction (WGSR). Four different catalysts are utilized for the different four reactions with following equations [1].

$$CH_3OCH_3 + H_2O \leftrightarrow 2CH_3OH \qquad \Delta H = +24.5kJmol^{-1} \tag{1}$$

$$CH_3OH + H_2O \rightarrow CO_2 + 3H_2 \qquad \Delta H = +49.1\ kJ\ mol^{-1} \tag{2}$$

$$CH_3OH \rightarrow CO + 2H_2 \qquad \Delta H = +90\ kJ\ mol^{-1} \tag{3}$$

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad \Delta H = -41.17\ kJ\ mol^{-1} \tag{4}$$

However, one of the largest issues for hydrogen reforming process is that it contains inevitable by-products of CO_2 and CO. Depending on the catalysts utilized and the reaction parameters, some side reactions that include WGSR and DME decomposition may occur [12]. The influence of the CO_2 on the fuel cell stack is negligible when DME reformer is utilized to feed hydrogen to the fuel cell, but the CO is poisonous to the fuel cell stack because the fuel cell catalyst is inactivated even on a very low order of magnitude concentration. Therefore, some measures should be taken to eliminate CO, which is partially consumed by WGS. A hydrogen permeation membrane is added into the reactor to improve the purity of the hydrogen produced in this study. It is reported that pure hydrogen was obtained with a micro-reactor with a Pd-Ag membrane, which offers an efficient method of the hydrogen purification [13].

As PEMFC is hybridized with battery for reducing fuel cell size and providing instant power delivery due to rapid power increase of a fuel cell vehicle, the dynamic characteristics of the hybrid vehicle equipped with an on-board hydrogen reformer are important to validate the total fuel cell/reformer system that can provide enough power to the rapid load change. The dynamic model for a hybrid fuel cell and battery vehicle has been developed by many researchers. However, publications to study the dynamic simulation model for hydrogen reformer are very few. Hedayadi et al. developed a dynamic simulation model to produce pure hydrogen via the ethanol-steam reforming in a catalytic membrane reactor [14]. However, the operating temperature of the ethanol-steam reforming is much higher than the DME steam reforming (i.e., the DME steam reforming is operated at about 300 °C, whereas ethanol-steam reforming is operated at 630 °C). They applied a hydrogen permeate membrane in the reactor, and the application of catalytic membrane reactors (CMRs) is beneficial in which the production and separation of hydrogen from the mixture of produced gases take place in the same reactor vessel simultaneously. However, the reformer volume is larger than DME reformer. In the case of

Please cite this article in press as: Zhang T, et al., Dynamic analysis of a PEM fuel cell hybrid system with an on-board dimethyl ether (DME) steam reformer (SR), International Journal of Hydrogen Energy (2018), https://doi.org/10.1016/j.ijhydene.2018.05.098