Available online at www.sciencedirect.com

SciVerse ScienceDirect

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

Numerical predictions of design and operating parameters of reformer on the fuel conversion and CO production for the steam reforming of methanol

Shiang-Wuu Perng [a], *Rong-Fang Horng* [a,*], *Hui-Wen Ku* [b]

[a] *Department of Mechanical Engineering, Kun Shan University, No. 949, Da Wan Rd., Yung-Kang District, Tainan 710, Taiwan*
[b] *Department of Systems and Naval Mechatronic Engineering, National Cheng Kung University, Tainan, Taiwan*

ARTICLE INFO

Article history:
Received 12 September 2012
Received in revised form
20 October 2012
Accepted 21 October 2012
Available online 17 November 2012

Keywords:
Methanol reforming
Reaction chamber
Catalyst bed
Carbon monoxide concentration

ABSTRACT

SIMPLE-C algorithm and Arrhenius form of reaction model were employed to simulate the three-dimensional laminar flow field and the chemical reaction in a cylindrical methanol reformer under steam reforming. The effects of geometrical and thermo-fluid parameters on the CO and CO_2 productions as well as the heat and mass transfer in a cylindrical methanol reformer with a constant-volume catalyst bed will be observed in the present study. Low CO concentration in hydrogen-rich gas denotes a low load of CO removal in purifying processes. The results indicate that the smaller diameter-to-length ratio of chamber with a thicker catalyst bed enhances the methanol conversion and reduces the overall CO concentration in the cylindrical methanol reformer. This is because that a lower temperature distribution restrains the reverse water–gas-shift reaction to reduce the production of CO with a thicker catalyst bed.

Copyright © 2012, Hydrogen Energy Publications, LLC. Published by Elsevier Ltd. All rights reserved.

1. Introduction

Owing to the high energy efficiency and low operating temperature, a proton exchange membrane fuel cell (PEMFC) has been regarded as a promising candidate of the power sources in the future. Applying PEMFC to the power sources needs enough hydrogen fuel. Accordingly, the hydrogen production is a major topic for PEMFC. Methanol clearly has obvious benefits as a fuel for hydrogen production by reforming because it has a higher hydrogen-to-carbon ratio, lower reforming temperature and greater environmental friendliness [1]. However, PEMFC performance would become worse as the carbon monoxide (CO) concentration gets up to 5–10 ppm [2]. In order to prevent the CO poisoning in a fuel cell system, controlling the CO concentration is an important issue.

Several published literature [3–8] focused on the experiments about the CO poisoning in the PEMFC. Various experimental methods of reducing the CO concentration have been utilized to improve the CO tolerance of a PEMFC system. Waszczuk et al. [3] performed electrochemical measurements to study adsorption and desorption of methanol-derived surface CO on fuel cell grade platinum and platinum–ruthenium alloy nanoparticle catalysts. Takeda et al. [4] investigated experimentally the chemical reaction rates of reforming and CO oxidation in a methanol reforming system, and then obtained the dynamic changes in CO concentration from the reformer. Abdollahi et al. [5] observed that the Pd membrane reactor system is capable of attaining almost complete CO conversion and full hydrogen recovery at realistic experimental conditions through the water-gas-shift (WGS) reaction. Chein et al. [6] observed experimentally that

* *Corresponding author*. Tel.: +886 62050496; fax: +886 6 2050509.
E-mail address: hong.rf@msa.hinet.net (R.-F. Horng).

0360-3199/$ – see front matter Copyright © 2012, Hydrogen Energy Publications, LLC. Published by Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ijhydene.2012.10.070

Nomenclature

c_i	concentration of species i, mol m^{-3}
C_P	specific heat at constant pressure, kJ kg^{-1} K^{-1}
D	flow channel diameter of reformer chamber, m
D_{eff}	effective diffusivity, m^2 s^{-1}
D_k	mass diffusion coefficient, m^2 s^{-1}
D_P	diameter of the catalyst particles, m
E_a	activation energy, kJ mol^{-1}
h_i^0	enthalpy of species i, kJ mol^{-1}
k_1	pre-exponential factor for steam reforming
k_2	pre-exponential factor for reverse water–gas shift
k_3	pre-exponential factor for water–gas shift
K_{eff}	effective thermal conductivity, W m^{-1} K^{-1}
K_{eq}	equilibrium constant of the water–gas shifting reaction
K_f	thermal conductivity of fluid, W m^{-1} K^{-1}
K_S	thermal conductivity of solid, W m^{-1} K^{-1}
L	flow channel length of reformer chamber, m
L_C	distance between inlet and catalyst bed, m
L_{CB}	catalyst bed thickness, m
M_i	mole fraction of species i
$M_{w,i}$	molecular weight of species i, kg mol^{-1}
N	number of species in the chemical reaction
p	pressure, N m^{-2}
r, θ, z	coordinates, m
R	universal gas constant, J mol^{-1} K^{-1}
$R_{i,r}$	Arrhenius reaction mole rate of creation and destruction of species i in the reaction r, mol m^{-3} s^{-1}
R_{SR}	Arrhenius reaction mole rate for the steam reforming reaction, mol m^{-3} s^{-1}
R_{rWGS}	Arrhenius reaction mole rate for reverse water–gas-shift reaction, mol m^{-3} s^{-1}
S_t	energy source term for chemical reaction
T	temperature, °C
T_0	inlet fuel temperature, °C
T_W	wall temperature, °C
$\vec{u}$	velocity vector, m s^{-1}
u_r, u_θ, u_z	velocity components in the r, θ and z directions, respectively, m s^{-1}

Greek symbols

β	inertial loss coefficient
ε	porosity of the catalyst bed
κ	permeability of the catalyst bed
μ	dynamic viscosity, kg m^{-1} s^{-1}
μ_{mix}	viscosity of the gas mixture, kg m^{-1} s^{-1}
φ_{ij}	a term used in calculating the viscosity of the gas mixture
ρ_f	fluid density, kg m^{-3}
τ	tortuosity of the catalyst bed

Superscript

in	inlet

the CO methanation, CO_2 methanation, and reversed water-gas-shift reactions took place simultaneously with a higher reaction temperature. Besides, an increase in the H_2 consumption causes a decrease in the CO conversion. Fukahori et al. [7,8] applied a papermaking approach to create the pore paper-structured catalysts (so-called catalyst paper). Methanol steam reforming was performed over pieces of catalyst paper to produce hydrogen for fuel cell applications. Their results displayed that higher heat conductivity leads to a lower CO concentration.

In the past decade, for saving the experimental cost, many researches and engineering applications utilized extensively numerical simulations to investigate the CO poisoning in the fuel cell. Hao et al. [9] performed a numerical analysis of a micro methanol steam reformer with eight non-parallel channels. Their results indicated that the catalyst thickness can affect CO concentration in the product gases indirectly. Yan et al. [10] investigated numerically the effects of CO and CO_2 poisoning on the degradation of PEM fuel cell performance. The results showed that, the performance drop was only 18% as the CO concentration is 50 ppm. Consequently, CO_2 poisoning became much more significantly when the CO content in the reactant gas was small. Suh et al. [11,12] investigated mass and heat transport phenomena in a methanol reformer by using a cylindrical mathematical modeling of a packed bed reactor. Their results presented that the CO concentration increases by the internally heated reformer. Jang et al. [13] built a three-dimensional numerical model to predict the effects of channel patterns and the inlet and outlet manifold configuration with a fixed inlet flow rate on a reformer in a PEMFC system. The numerical results presented that a CO mole fraction can be reduced through the preferential oxidation reaction effectively. Wang and Wang [14] utilized FLUENT to investigate the influences of pressure, temperature, oxygen-to-carbon molar ratio, and steam-to-carbon molar ratio on the auto-thermal reforming of methanol. Chein et al. [15] performed a numerical analysis of a micro-scale cylindrical packed bed reformer. In the low-temperature zone of the reformer, the forward water-gas-shift reaction was clearly demonstrated to decrease the CO concentration selectivity. On the basis of the above reasons, it is important to develop a suitable numerical model of the methanol reformer for investigating the mass and heat transport phenomena and the control of CO concentration.

Although many papers have focused on developing a numerical model of the cylindrical methanol steam reformer, few reports on the CO and CO_2 productions with various thermo-fluid parameters and diameter-to-length ratios applied to the reaction chamber in the reformer. Moreover, our previous studies [16–18] developed the numerical program to simulate the heat and mass transport in the fuel channel of a PEMFC for obtaining the cell performance enhancement. A good agreement between numerical and experimental results is presented in the results of our studies, so the numerical program is proved to deal properly with the physical problem which involves the continuity, momentum, energy and species equations with chemical reaction in a PEMFC system.

In general, SIMPLE-C method [19] integrating with the preconditioned conjugate gradient method [20,21] costs less computer storage and CPU computation time than the

Download English Version:

https://daneshyari.com/en/article/1282050

Download Persian Version:

https://daneshyari.com/article/1282050

Daneshyari.com