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The three-dimensional simulation and optimization of an integrated power system for reformer–PrOx–fuel cell modeling

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ABSTRACT

The present study is aimed at integrating a power system for reformer, PrOx and PEM fuel cells using a simulation model. A three-dimensional numerical model is established for predicting the effects of channel patterns and the inlet and outlet manifold configuration with a fixed inlet flow rate on a reformer. Distributions of velocity, gases concentrations and current density are predicted, and the methanol conversion ratios are evaluated as well. In addition, the mole fraction of CO is contained and removed in the reformer and PrOx reactions, respectively. The solution model is used to improve the design of both the micro reformer and the fuel cell. Results showed that a CO mole fraction can be decreased through the PrOx reaction effectively; furthermore, the methanol conversion ratio and the concentration of hydrogen can be improved from 83% to 99% and from 67.11% to 74.4%, respectively. Additionally, the relative standard deviations of velocity in channels are decreased from 58.68% to 0.048%, according to the manifold configuration design; from the point of view of a fuel cell, high fuel usage and current density are obtained using a z-serpentine channel pattern. The current density is increased by 184% on the basis of inlet flow rate for a steam reformer from Design 1 to Design 2.

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1. Introduction

In recent years, the proton exchange membrane fuel cell (PEMFC) has received increased attention with regard to portable applications. However, before this system becomes competitive with traditional internal combustion engines, its performance and costs must be further optimized. Numerous numerical optimization investigations have been conducted on PEMFCs in recent years [1–9]. A PEMFC with clean fuel sources of hydrogen and an oxygen supply is considered to be

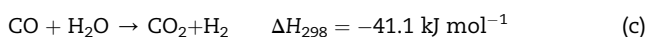
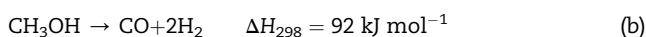
a promising power source [10,11]. Thus, H₂ storage problems, refueling, generation and safety are concerns that still have to be overcome in the future [12–14]. Hydrogen gas can be produced from the reforming of hydrocarbon fuel, which can be converted into hydrogen-rich gas through steam reforming (STR) or autothermal reforming (ATR), followed by a water gas shift (WGS) reaction and a preferential oxidation (PrOx) reaction. According to the available hydrocarbon fuels, methanol is a unique sulfur-free fuel that can be activated at relatively low temperatures (under 300 °C).

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Nomenclature			
A	pre-exponential constant	Y	mass fraction
a'_{ij}	stoichiometric coefficients of the reactants	x,y,z	Cartesian coordinates, cm
a''_{ij}	stoichiometric coefficients of the products	<i>Greek symbols</i>	
C_F	quadratic drag factor	α'	concentration exponent
D	diffusion coefficient, $m^2 s^{-1}$	α	charge transfer coefficients
D_λ	diffusivity of membrane, $m^2 s^{-1}$	ε	porosity
E_a	activation energy, $kJ mol^{-1}$	η	electrode over-potential, V
F	Faraday constant 96,487, $C mol^{-1}$	θ_c	contact angle
G	gas species (H_2 , CH_3OH , H_2O , CO , O_2 , CO_2)	κ_p	permeability, m^2
H	channel high, cm	κ_{rg}	relative permeability of the gaseous mixture
h_{fg}	latent heat of vaporization, $J kg^{-1}$	κ_{rl}	relative permeability of the liquid water
i	ionic/electronic current density, $A m^{-2}$	λ	effect thermal conductivity, $W m^{-1} K^{-1}$
j	transfer current density, $A m^{-3}$	λ_s	thermal conductivity of solid matrix in porous region, $W m^{-1} K^{-1}$
j^{ref}	reference current density, $A m^{-2}$	λ_f	thermal conductivity of fluid parts in porous region, $W m^{-1} K^{-1}$
k_i	chemical reaction coefficients	μ	viscosity of the fluid, $kg m^{-1} s^{-1}$
L	channel length, cm	ρ	density, $kg m^{-3}$
M	molecular weight, $kg kmol^{-1}$	ρ_{dry}	membrane dry density, $kg m^{-3}$
M_m	membrane equivalent weight, $kg kmol^{-1}$	σ	surface tension, $N m^{-2}$
m	exponent on pressure dependency	σ_s	electronic conductivity, $\Omega^{-1} m^{-1}$
N_{ch}	total number of channels	σ_m	membrane reference conductivity, $\Omega^{-1} m^{-1}$
N_G	total number of gas species	Φ	electric potential, V
n	temperature exponent	<i>Subscripts</i>	
n_d	electro-osmotic drag coefficient	a	anode
P	pressure, Pa	avg	average
P_c	capillary pressure head, Pa	c	cathode
\dot{Q}	volumetric flow rate, $cc min^{-1}$	ch	channel
R	universal gas constant, $8.314 J mol^{-1} K^{-1}$	CL	catalyst layer
R'	surface reaction rate, $kmol m^{-2} s^{-1}$	eff	effective
S_c	sources term in species equation	f	forward
S_L	source term accounting due to phase change of water	g	gaseous phase
S_t	relative standard deviation	GDL	gas diffusion layer
s	ratio of the liquid water volume to the pore volume	H_2O	water
T	temperature, K	in	inlet
t	thickness, cm	ion	ionic phase
U	velocity vector, $m s^{-1}$	l	liquid phase
V	cell voltage, V	m	membrane
W	width, cm	ref	reference
x	mole fraction	s	electronic phase

The three main reactions of a methanol reformer for combination of reactants and products can be written by the following equations [15–18].



Eq. (a) is the algebraic summation of Eqs. (b) and (c). Eq. (b) represents methanol decomposition. Eq. (c) represents

a water gas shift reaction (WGS). It is also necessary to consider the reverse water gas shift reaction, Eq. (c), in the kinetic model of the reformer reactor. Although the equilibrium constant of the water gas shift reaction is about 225 at 200 °C, the concentrations of H_2 and CO_2 are approximately 75% and 25%, respectively, which are high enough to influence the reverse WGS reaction. Pan et al. [19] carried out optimal design of complex manifold geometries for even flow distribution between microchannels by means of a flow network method. Balaji and Lakshminarayanan [20] also designed a novel structure so as to produce an even velocity distribution. In this design, the model was equipped with one inlet and two outlets to yield a uniform pressure drop in the channels.

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