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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.

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, H_2 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
a'_{ij}	stoichiometric coefficients of the reactants
a''_{ij}	stoichiometric coefficients of the products
C_F	quadratic drag factor
D	diffusion coefficient, $m^2\ s^{-1}$
D_λ	diffusivity of membrane, $m^2\ s^{-1}$
E_a	activation energy, kJ mol^{-1}
F	Faraday constant 96,487, C mol^{-1}
G	gas species (H_2, CH_3OH, H_2O, CO, O_2, CO_2)
H	channel high, cm
h_{fg}	latent heat of vaporization, J kg^{-1}
i	ionic/electronic current density, A m^{-2}
j	transfer current density, A m^{-3}
j^{ref}	reference current density, A m^{-2}
k_i	chemical reaction coefficients
L	channel length, cm
M	molecular weight, kg $kmol^{-1}$
M_m	membrane equivalent weight, kg $kmol^{-1}$
m	exponent on pressure dependency
N_{ch}	total number of channels
N_G	total number of gas spices
n	temperature exponent
n_d	electro-osmotic drag coefficient
P	pressure, Pa
P_c	capillary pressure head, Pa
$\dot{Q}$	volumetric flow rate, cc min^{-1}
R	universal gas constant, 8.314 J $mol^{-1}\ K^{-1}$
R'	surface reaction rate, kmol $m^{-2}\ s^{-1}$
S_c	sources term in species equation
S_L	source term accounting due to phase change of water
S_t	relative standard deviation
s	ratio of the liquid water volume to the pore volume
T	temperature, K
t	thickness, cm
U	velocity vector, m s^{-1}
V	cell voltage, V
W	width, cm
x	mole fraction
Y	mass fraction
x,y,z	Cartesian coordinates, cm

Greek symbols

α'	concentration exponent
α	charge transfer coefficients
ε	porosity
η	electrode over-potential, V
θ_c	contact angle
κ_p	permeability, m^2
κ_{rg}	relative permeability of the gaseous mixture
κ_{rl}	relative permeability of the liquid water
λ	effect thermal conductivity, W $m^{-1}\ K^{-1}$
λ_s	thermal conductivity of solid matrix in porous region, W $m^{-1}\ K^{-1}$
λ_f	thermal conductivity of fluid parts in porous region, W $m^{-1}\ K^{-1}$
μ	viscosity of the fluid, kg $m^{-1}\ s^{-1}$
ρ	density, kg m^{-3}
ρ_{dry}	membrane dry density, kg m^{-3}
σ^*	surface tension, N m^{-2}
σ_s	electronic conductivity, $\Omega^{-1}\ m^{-1}$
σ_m	membrane reference conductivity, $\Omega^{-1}\ m^{-1}$
Φ	electric potential, V

Subscripts

a	anode
avg	average
c	cathode
ch	channel
CL	catalyst layer
eff	effective
f	forward
g	gaseous phase
GDL	gas diffusion layer
H_2O	water
in	inlet
ion	ionic phase
l	liquid phase
m	membrane
ref	reference
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].

$$CH_3OH + H_2O \rightarrow 3H_2{+}CO_2 \qquad \Delta H_{298} = 49\ \text{kJ mol}^{-1} \qquad \text{(a)}$$

$$CH_3OH \rightarrow CO{+}2H_2 \qquad \Delta H_{298} = 92\ \text{kJ mol}^{-1} \qquad \text{(b)}$$

$$CO + H_2O \rightarrow CO_2{+}H_2 \qquad \Delta H_{298} = -41.1\ \text{kJ mol}^{-1} \qquad \text{(c)}$$

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.