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Numerical analysis of performance enhancement and non-isothermal reactant transport of a cylindrical methanol reformer wrapped with a porous sheath under steam reforming

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ABSTRACT

This paper accomplished a three-dimensional computational analysis of the methanol reformer with steam reforming by the Arrhenius form of reaction model and SIMPLE-C algorithm. The performance enhancement and non-isothermal reactant transport of the cylindrical reformer wrapped with a porous sheath were investigated. The parameters, including temperature of internal heater (T_H), porosity (ϵ), and thickness of porous sheath (R_p), on methanol conversion, hydrogen, carbon monoxide, carbon dioxide productions, temperature and velocity fields with the same inlet conditions have been investigated. The results present that higher methanol conversion and richer hydrogen production occur as temperature of heater, porosity, and porous sheath thickness increase. As temperature of internal heater is equal to 250 °C, employing a porous sheath with $\epsilon = 0.9$ and $R_p = 10$ mm to wrap a reformer results in the maximum enhancements of 35.71% in methanol conversion and 21.18% in hydrogen production. Besides, a porous sheath with $\epsilon = 0.5$ and $R_p = 10$ mm leads to the maximum reduction of 2.23% in carbon monoxide produced from the reformer at $T_H = 300$ °C.

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Introduction

Proton exchange membrane (PEM) fuel cell has presently become the important power sources in the future because of its clean exhaust gas, low-operating temperature and high efficiency under consuming oxygen and hydrogen [1–3]. Accordingly, hydrogen must be fed into PEMFC as the fuel. Methanol (CH_3OH) intelligibly has apparent advantages as fuel for producing hydrogen through reforming due to lower

reforming temperature (about 200–300 °C), larger hydrogen-to-carbon ratio (about 4.0) as well as better environmental friendliness [4,5]. Besides, CH_3OH augments the hydrogen production and diminishes the CO selectiveness of the water-gas-shift (WGS) reaction under lower operating-temperature. Therefore, the carbon monoxide (CO) production from hydrogen-rich gas can be low at low temperature, and then avoids poisoning the catalyst on the anode to decline the PEMFC performance [6,7]. The methanol steam reformer (MSR) connected with PEMFC is considered as a promising

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Nomenclature	
c_i	concentration of species i (mol m^{-3})
C_p	specific heat ($\text{kJ kg}^{-1} \text{K}^{-1}$)
D	diameter of cylindrical reactor (m)
D_{eff}	effective diffusivity ($\text{m}^2 \text{s}^{-1}$)
D_H	diameter of internal heater (m)
D_k	coefficient of mass diffusion ($\text{m}^2 \text{s}^{-1}$)
D_p	diameter of porous pellets (m)
E_{a1}, E_{a2}, E_{a3}	activation energy of reaction (kJ mol^{-1})
h_i^0	enthalpy (kJ mol^{-1})
k_1	reaction rate constant for steam reforming
k_2	reaction rate constant for reverse water-gas shift
k_3	reaction rate constant for water-gas shift
K_{eff}	effectual thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)
K_f	thermal conductivity in fluid phase ($\text{W m}^{-1} \text{K}^{-1}$)
K_s	thermal conductivity in solid phase ($\text{W m}^{-1} \text{K}^{-1}$)
L	length of cylindrical reactor (m)
L_C	distance from entrance to catalyst bed (m)
L_{CB}	length of catalyst bed (m)
L_H	length of internal heater (m)
M_i	mole fraction
$M_{w,i}$	molecular weight (kg mol^{-1})
n	normal vector along the reformer wall
N	species number
p	pressure (N m^{-2})
r, θ, z	cylindrical coordinates in the computational model (m)
R	universal gas constant ($\text{kJ kg}^{-1} \text{K}^{-1}$)
R_p	thickness of porous sheath (m)
$R_{i,r}$	Arrhenius reaction rate coefficient of species i in the reaction r ($\text{mole m}^{-3} \text{s}^{-1}$)
R_{SMR}	Arrhenius reaction rate coefficient of steam methanol reforming ($\text{mole m}^{-3} \text{s}^{-1}$)
$R_{r\text{WGS}}$	Arrhenius reaction rate coefficient of reverse water-gas-shift ($\text{mole m}^{-3} \text{s}^{-1}$)
S_t	energy source term in the chemical reaction
T	temperature ($^{\circ}\text{C}$)
T_0	fuel temperature at the entrance ($^{\circ}\text{C}$)
T_H	temperature of internal heater ($^{\circ}\text{C}$)
\vec{u}	velocity (m s^{-1})
u_r, u_θ, u_z	velocity components along the r, θ and z directions, respectively (m s^{-1})
Greek	
β	coefficient of inertial loss
ε	porosity for porous media
κ	permeability for porous media
μ	dynamic viscosity ($\text{kg m}^{-1} \text{s}^{-1}$)
μ_{mix}	viscosity of the fluid mixture ($\text{kg m}^{-1} \text{s}^{-1}$)
ϕ_{ij}	a term employed for evaluating the viscosity of the fluid mixture
ρ_f	density of fluid (kg m^{-3})
τ	tortuosity for porous media
Superscript	
i	species i
in	entrance

candidate of the power sources at the moment [8–13]. Accordingly, the design of methanol reformer plays a major role for enhancing the MSR performance.

In an MSR, the utilization of thermal energy is the host to some transport mechanisms in the chamber of reformer, so the thermal insulation of a reformer plays the important role in the performance of hydrogen production by methanol reforming. Generally, the heat is transferred toward the shell form the heater on the center line in the reformer. If the thermal energy couldn't be kept effectively in the reformer, the thermal energy would be wasted to reduce the reforming efficiency and hydrogen generation performance of a reformer. Lo and Wong [14] used a catalytic methanol combustor to heat a unique thermally-controlled MSR system. The efficiency of CH_3OH conversion surpassed 98% as the operating temperature was over 292°C and the $\text{H}_2\text{O}/\text{CH}_3\text{OH}$ ratio (S/C) was larger than 1.0. Chein et al. [15] addressed numerically the effect of heat transfer on the MSR performance for three various heat-supplied mechanisms. For heat provided from the internal heat generation and from the wall of reformer, it was presented that the axial thermal conduction plays a principal role in both heat transport and performance of an MSR. Hotz et al. [16] proposed a union of solar-powered parts (an evaporator, an MSR, and two heaters) with PEMFC to create a power plant that converts CH_3OH to electrical power. The density of electrical power more than 920 Wm^{-2} was gained for a solar heat supply of 1000 Wm^{-2} .

Pan and Wang [17] studied numerically the effect of thermal transport on the hydrogen production in a compact plate-fin reformer. The internal plate-fins and external catalytic combustion enhance heat transfer of the reformer to obtain both low CO concentration and high methanol conversion. The above literature [14–17] showed that the internal temperature obviously influences the efficiency of CH_3OH conversion and hydrogen generated from an MSR. Therefore, how to keep the thermal energy generated from the internal heater is the major motive of the present study.

Hao et al. [18] theoretically analyzed the influences of temperature, pressure and porosity on the thermal insulation performance of porous materials, and then obtained the optimal porosity distribution with the best insulation performance. Korin et al. [19] employed a porous phase-change material (PCM) to maintain the temperature of catalyst for off-working duration. Under operating conditions of an engine, some thermal energy generated from the exhaust was kept in the porous PCM. As the vehicles were not in operation, the porous PCM was in a state of partial solidification. Therefore, a better conversion efficiency occurred because the latent heat was used to keep the temperature of catalyst within the wanted range. Horng et al. [20,21] used a porous heat-stored material to develop a four-stroke engine with an electrically-heated catalyst, and then explored the influence of heat-stored material length, operating temperature and pre-heated time on the efficiency of CO conversion after a cold

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