Effects of key factors on solar aided methane steam reforming in porous medium thermochemical reactor

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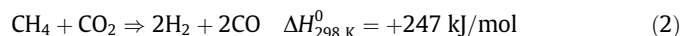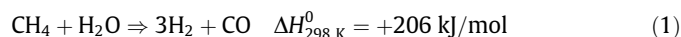
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ABSTRACT

With the aid of solar energy, methane reforming process can save up to 20% of the total methane consumption. Monte Carlo Ray Tracing (MCRT) method and Finite Volume Method (FVM) combined method are developed to establish the heat and mass transfer model coupled with thermochemical reaction kinetics for porous medium solar thermochemical reactor. In order to provide more temperature information, local thermal non-equilibrium (LTNE) model coupled with P1 approximation is established to investigate the thermal performance of porous medium solar thermochemical reaction. Effects of radiative heat loss and thermal conductivity of porous matrix on temperature distribution and thermochemical reaction for solar driven steam methane reforming process are numerically studied. Besides, the relationship between hydrogen production and thermal conductivity of porous matrix are analyzed. The results illustrate that hydrogen production shows a 3 order polynomial relation with thermal conductivity of porous matrix.

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1. Introduction

Hydrogen is an important energy carrier, ultimately clean fuel and raw materials of chemical industries, which can be produced by various feedstocks, such as fossil fuel, biomass, or water [1–3]. Nowadays, main sources of hydrogen production are steam methane reforming (SMR) and CO_2 methane reforming, represented by the following equations:

$$CH_4 + H_2O \Rightarrow 3H_2 + CO \quad \Delta H^0_{298\ K} = +206\ kJ/mol \tag{1}$$

$$CH_4 + CO_2 \Rightarrow 2H_2 + 2CO \quad \Delta H^0_{298\ K} = +247\ kJ/mol \tag{2}$$

As the above reactions are highly endothermic, the caloric values of products-syngas (H_2, CO_2 and CO, etc.) are higher than those of reactants [4]. The methane reforming reactions are performed at high working temperature. In conventional reforming process, the required high working temperature is maintained by combusting additional methane which is up to 20% of total methane consumption [5].

In 1980, the Naval Research Laboratory in USA first put forward the concept of solar driven methane reforming, and this novel concept received great interest during the following decades [6]. The

solar driven methane reforming is based on the utilization of concentrated solar irradiation (CSI) as energy source to maintain high working temperature. Solar energy is converted to syngas energy with the term of "solar fuel" [7]. With the aid of concentrated solar energy, hydrogen is entirely produced from renewable energy [8]. During the last decades, a large amount of work had been performed to develop the technology of solar driven methane reforming at DLR in Germany, ETH/PSI in Switzerland, SNL and NREL in USA, ENEA in Italy, CRIRO in Australia, WIS in Israel, Tokyo Institute of Technology in Japan and the Inha University in Korea, Harbin Institute of Technology in China and other research institutes [9–13].

Generally, the solar reactor for methane reforming can be divided into two categories: indirectly irradiated reactor (IIR) and directly irradiated reactor (DIR). For the IIR, there is an opaque wall to receive the CSI on one side and transfer the heat to heat transfer fluid (HTF) on the other side, for example: tubular receiver/reactor. For the DIR, fluid streams or solid particles are directly exposed to CSI and absorb concentrated solar energy. The HTF flows in the DIR and transports energy within the DIR. Compared to IIR, the DIR can enable the CSI to penetrate deeper and be absorbed within the entire volume of the receiver/reactor [14]. Besides, the surface of DIR can be coated with catalyst layer to perform high-temperature chemical reactions. Therefore, the DIR entails that the CSI absorption, heat extraction as well as chemical reaction take place on the same surface simultaneously [15]. In this

Nomenclature

c_p	specific heat, J/(kg K)
d_s	mean cell size, mm
D_m	mass diffusion coefficient
D_T	thermal diffusion coefficient
E_{sun}	solar irradiance, W/m^2
G	integrated intensity, W/m^2
h_i	partial enthalpy of species i, J
h_v	volumetric heat transfer coefficient, W/(m^3 K)
k_α	absorption coefficient
k_e	extinction coefficient
k_s	scattering coefficient
L	length of receiver, mm
M	mole fraction of gas species
p	pressure, Pa
r	radius, m
R	universal gas constant
S	source term of energy equation
T	temperature, K
T_0	environmental temperature, K
u	velocity in x direction, m/s
v	velocity in y direction, m/s
x, y	coordinates in flow region, m

Greek symbols

ρ	density, kg/m^3
ϕ	porosity
α	absorptivity
μ	dynamic viscosity, kg/(m s)
α_{sf}	surface area per unit volume, 1/m
λ	conductivity, W/(m K)
ε	emissivity
σ	Stefan–Boltzmann constant
Φ	irradiation intensity, W/m^2
ω	albedo coefficient

Subscripts

c	chemical reaction
con	convective heat transfer
e	effective
f	fluid phase
i	the ith species
In	inlet
MC	Monte Carlo
r	irradiative heat transfer
s	solid phase
w	wall

way, absorbed CSI could be stored in chemical energy rather than thermal energy in the fluid flow.

Porous medium is an ideal DIR which enables to absorb highly CSI and provide large heat transfer surface with high thermal shock resistance (caused by cyclic weather and rapid heating–cooling cycles) [16]. The first examples of porous medium solar reactor were demonstrated in the "Catalytically Enhanced Solar Absorption Receiver" experiment for solar driven CO_2 methane reforming conducted by SNL, DLR between 1987 and 1990 [17]. Their prevalence over porous medium reactors for solar driven methane reforming was sought to higher porosity to allow CSI to penetrate deeper in the volume of porous medium. During the following decades, ETH [18], CNRS-PROMES laboratory [19] and CETRH/CPERI laboratory [20] had manufactured many types of porous medium solar thermochemical reactors coated with catalyst to absorb CSI to maintain the operational temperature for methane reforming reaction. Gokon et al. had adopted metallic porous media reactor coated with Ru/g-Al$_2$O$_3$ catalyst for solar methane reforming reaction [21]. Sang et al. had experimentally investigated the catalytic solar driven methane reforming reaction over metal porous media reactors based monolithic catalysts [22].

Numerous numerical studies of methane reforming in porous media reactor had been conducted which could be benefit for reactor design and operation improvement. Villafán-Vidales et al. [19] had established a heat transfer analysis model for porous medium solar thermochemical reactor with Gaussian heat flux distribution as concentrated solar energy distribution. Ni [23] had developed a heat and mass transfer model coupled with chemical reaction kinetics to investigate the effects of structural variables on hydrogen production during methane reforming, while the local thermal equilibrium assumption was adopted. A heat and mass transfer model coupled with thermochemical reaction kinetics for porous medium solar thermochemical reactor was developed by Wang et al. to study the heat transfer and hydrogen production performance during the solar driven SMR process, while the LTNE model coupled with P1 approximation was adopted [15,24].

Generally, porous medium solar thermochemical reactor is impregnated with the catalyst (i.e., Ni/α-Al$_2$O$_3$) and deposited as coated layer. During numerical analysis, the thermophysical properties of porous medium solar thermochemical reactor correspond to those of porous matrix [19,24]. Though researches on the effect of thermal conductivity of porous matrix on temperature distribution were widely investigated for solar receiver [25], little studies were conducted to investigate the influences of thermal conductivity of porous matrix on thermochemical reaction. Besides, effects of radiative heat loss on temperature distribution and thermochemical reaction also need to be investigated.

In order to study the heat transfer and hydrogen production performance during the solar driven SMR process, MCRT and FVM combined method is adopted to establish the heat and mass transfer model coupled with thermochemical reaction kinetics for the porous medium solar thermochemical reactor. The LTNE model with P1 approximation is used to investigate the temperature distributions which can provide more temperature information [26–29]. The influences of radiative heat loss and thermal conductivity of porous matrix on temperature distribution and thermochemical reaction are numerically studied. Besides, a computational formula is put forward to illustrate the relationship between hydrogen production and thermal conductivity of porous matrix.

2. Description of porous medium solar thermochemical reactor

Fig. 1 presents the schematic diagram of porous medium solar thermochemical reactor with parabolic dish collector system [15]. Honeycomb porous coated with catalyst layer (i.e., Ni/α-Al$_2$O$_3$) is wrapped with insulations and assembled within an absorber. The porous medium solar thermochemical reactor is placed vertically in the focal plane of a parabolic dish collector with double-axis sun automatic tracking system (focal length: 3.25 m, aperture radius: 1.4 m), and directly irradiated by CSI. The length of reactor is 0.44 m, and the aperture radius of reactor is 0.0175 m. The reactants (Mole fraction [19]: $CH_4 = 25\%, H_2O = 75\%, T_{f,in} = 300$ K) flows through the honeycomb porous and produces syngas (H_2, CO_2 and CO) removed from the back of reactor.