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A three-dimensional simulation of a mid-and-low temperature solar receiver/reactor for hydrogen production

Yanjuan Wang [a,b,c], Qibin Liu [b,c,*], Jing Lei [a], Hongguang Jin [b,c]

[a] School of Energy, Power and Mechanical Engineering, North China Electric Power University, Changping District, Beijing 102206, China
[b] Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing 100190, China
[c] University of Chinese Academy of Sciences, Beijing 100049, China

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ABSTRACT

The solar receiver/reactor is a key component that influences the conversion efficiency in the solar thermochemical process. A thermochemical solar reactor/receiver consisting of a porous Cu/ZnO/Al_2O_3 catalyst bed is studied in this paper. A three-dimensional thermochemical coupling model that incorporates the fluid flowing through the porous catalyst bed and energy conservation equations coupling the radiation/convection/conduction heat transfer with the reaction kinetics is proposed to investigate the performances of the receiver/reactor. The factors of influencing the hydrogen production and the temperature distribution, including the mole ratio of water/methanol, the solar radiation and the inlet temperature, are numerically investigated. Numerical simulation results indicate that the deactivation of the catalyst may appear near the receiver/reactor tube wall. The methanol conversion decreases with the increase of the methanol feeding rate, and the low inlet methanol feeding rate should be avoided for the protection of the catalyst bed. A new solar receiver/reactor is proposed by changing the aperture width along the flow direction to make the concentrated solar energy level match the chemical reaction. Compared with traditional solar receivers/reactors, the thermochemical efficiency can be increased by 3% points. The research findings will pave the way for the future development of the mid-and-low temperature solar receiver/reactor.

1. Introduction

Solar energy is considered to be a promising energy in the 21th century due to its infinite reserves and cleanness nature. It may be one of most effective routes to solve the energy problems caused by the exploitation and utilization of the fossil fuels. Among the three main solar thermal technologies, i.e., the parabolic trough, the central receiver and the parabolic dish, the parabolic trough solar technology is the most proven and cost-effective, large-scale solar power technology available today (Price et al., 2002; Xu et al., 2015).

Hydrogen, as a fuel, likely becomes one of most promising energy carriers in the near future for environmentally benign and sustainable development. The major benefit of using hydrogen as an energy carrier is that it only produces water and liberates large amounts of energy per unit weight as be combusted. With the increasing demand of hydrogen, it is anticipated that the role of hydrogen will become more significant (Abuiadala and Dincer, 2012; Gadalla et al., 2010; Muradov and Veziroglu, 2008).

Recently, hydrogen production by solar energy has received increasing attentions. Many potential methods have been exploited. Chueh et al. proposed a simple and scalable reactor using the porous ceria directly exposed to the concentrated solar radiation, and thus the high-temperature heat can be transformed to the reaction sites. They studied the feasibility of a solar-driven thermochemical cycle for the dissociation of H_2O and CO_2 using the nonstoichiometric ceria (Chueh et al., 2010). The thermochemical hydrogen production from a two-step solar-driven water-splitting cycle based on cerium oxides and solar hydrogen production from the thermal splitting of methane in a high temperature solar chemical reactor were studied by Stephane Abanades (Abanades and Flamant, 2006a,b). Zamfirescu and Dincer (2014) developed a novel integrated system that converts solar radiation into hydrogen by combining photocatalytic reactor, photovoltaics, thermal engine and chemical energy storage for solar energy harvesting. It was shown that the annual average factor of the light absorption of the novel system is increased by 9% points. Furthermore, the overall exergy efficiency of the hydrogen production is

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* Corresponding author at: Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing 100190, China.

E-mail address: qibinliu@mail.etp.ac.cn (Q. Liu).

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Nomenclature

d_p	equivalent diameter (m)
D_i^T	the generalized thermal diffusion coefficient (kg/(m s))
D_{ij}	the *ij* component of the multi-component diffusivity coefficient (m^2/s)
M	molar mass of species
n_{CH_3OH}	mole feeding rate of methanol
n_{un,CH_3OH}	non-reacted methanol
p	pressure (Pa)
Q	heat source (W/m^3)
Q_{so-ch}	he solar thermal energy converted into the chemical energy
r	reaction rate (mol/(m^3 s))
R	universal gas constant
T	temperature (K)
u	velocity (m/s)
x_{CH_3OH}	methanol conversion
$\Delta_r H$	enthalpy of reaction (J/mol)

Subscript

f	gaseous phases
g	gas mixture
s	catalyst bed

Greek symbols

η	dynamic viscosity (kg/(m s))
κ	hydraulic permeability (m^2)
ε	porosity
λ_{sr}	effective thermal conductivity of the catalyst bed (W/(m K))
λ_s	thermal conductivities of catalyst particle (W/(m K))
λ_g	thermal conductivities of gas mixture (W/(m K))
ω_i	mass fraction of the *i*-th gas
f_j	mole fraction of the *j*-th gas
η_{so-ch}	thermochemical efficiency

increased by 40%, as compared with a conventional tower system that runs an electrolyzer. The solar hydrogen production by the thermal decomposition of natural gas using a vortex-flow reactor was proposed by Hirsch (Hirsch and Steinfeld, 2004). Thermal characterizations of a cavity receiver for the hydrogen production by the thermochemical cycles operating at a moderate temperature had been investigated by Lanchi et al. (2013), whereas other successful examples can be found elsewhere for other solar hydrogen production techniques (Steinfeld and Meier, 2004; Steinfeld, 2005; Segal and Epstein, 2003; Dufour et al., 2009).

The above-mentioned hydrogen production methods often need to concentrate the solar thermal energy above 800 K to provide the necessary reaction heat, which leads to technological difficulties on using the solar radiation as a driving energy for reactions. More recently, based on the parabolic trough technology, an effective hydrogen production approach via the integrating utilization of the middle temperature solar thermal energy and methanol was proposed by Jin and his group (Jin et al., 2007; Hong et al., 2005; Liu et al., 2009, 2010). Compared with other hydrocarbons, methanol has certain advantages, such as the relatively low reforming temperature (423–573 K) and easy implementation. Many benefits can be achieved in the process, e.g., ease implementation, accurate tracking of solar concentrators, low-cost investments, etc. Jin et al. (2007) developed an original mid-and-low temperature solar receiver/reactor prototype. The mid-and-low temperature solar receiver/reactor is a key component in the mid-and-low temperature solar thermochemical process, and directly influences the conversion efficiency of solar thermal energy into chemical energy, and thus the investigations of the characteristics of the receiver/reactor are crucial for practical applications. Liu et al. (2010) investigated a novel solar thermochemical receiver/reactor, and developed a non-isothermal model to analyze the performances of the mid-and-low temperature solar receiver/reactor.Hou et al. (2007) developed a procedure to analyze the performances of the non-isothermal solar reactors for the methanol decomposition. However, the considerations of the influences of the non-uniform three-dimensional distribution of the solar flux on the solar hydrogen production are absent.

The understanding of the complicated physical and chemical mechanism of the hydrogen production by the steam methanol reforming method is beneficial for the efficient utilization of mid-and-low temperature solar thermal energy. In this paper, naturally, we employ the numerical simulation approach to investigate the performances of the receiver/reactor under non-uniform distribution of the solar flux, and the influences of the key operating parameters on the thermal, fluid and chemical characteristics of the solar receiver/reactor are revealed. The main contributions are summarized as:

(1) The solar receiver/reactor consists of a porous catalyst bed made of $Cu/ZnO/Al_2O_3$ (see Fig. 1 for more details) where the endothermic methanol steam reforming reaction occurs. A multiphysics coupling model of the receiver/reactor is proposed to model the steam methanol reforming process, which incorporates mass, momentum and energy conservation equations as well as the methanol steam reforming reaction. The solar flux profile is calculated by the solar ray-tracing method. The thermal and chemical characteristics of the mid-and-low temperature solar receiver/reactor are revealed.

(2) The influences of the key operating parameters on the performances of the mid-and-low temperature solar receiver/reactor are investigated, including solar radiation, inlet temperature of reactants, mole flow rate of reactants and mole ratio of water/methanol on the deactivation of the catalyst and hydrogen production.

(3) Due to the characteristics of the chemical reaction of the methanol steam reforming, we find that the required reaction heat is large at the beginning part of the chemical reaction, and becomes very small when the reaction is almost reacted. Thus, a new solar receiver/reactor is proposed by changing the aperture width along the flow direction to well match the concentrated solar energy level with the chemical reaction.

The rest of the paper is structured as follows. The mid-and-low temperature solar receiver/reactor model and the performance simulations of the mid-and-low temperature solar receiver/reactor are implemented in Section 2. The numerical results and detailed discussion on the results are presented in Section 3. Finally, Section 4 summarizes the main conclusions.

2. Mid-and-low temperature solar receiver/reactor model

2.1. Configuration of the solar receiver/reactor

The methanol steam reforming requires energy input with a range of about 473–573 K, which can be supplied by the solar