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Numerical investigation of the thermophysical characteristics of the mid-and-low temperature solar receiver/reactor for hydrogen production

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ABSTRACT

With the considerations of the complex kinetic mechanisms of the methanol steam reforming using Cu/ZnO/Al_2O_3 catalyst, in this paper a multiphysics coupling model that integrates the mass, momentum and energy conservation governing equations is proposed to investigate the thermophysical performances of the mid-and-low temperature solar receiver/reactor for hydrogen production. The factors influencing the hydrogen production and temperature distributions of the catalyst bed, including the diameter of the receiver/reactor, the non-uniform distribution of the solar flux and the porosity of the catalyst bed, are numerically studied. The temperature distributions, mole fractions of the components and reaction rates are obtained. The influence rules of the diameter of the receiver/reactor tube on the performances of the receiver/reactor are revealed. The non-uniform distribution of the solar flux has a significant influence on the cross-sectional temperature difference of the receiver/reactor tube, the catalyst bed and the temperature rise of the catalyst bed, while has a slight impact on the methanol conversion and the collector efficiency. The effect mechanisms of the porosity on the performances of the receiver/reactor are revealed. The research findings provide a fundamental reference for the development of the mid-and-low temperature solar receiver/reactor.

1. Introduction

The use of the renewable and clean energy sources, such as solar, wind, hydrogen, may be a promising solution of the problems related to the continuous rising of energy demand and serious environmental pollutions caused by the utilization of fossil fuels. Hydrogen has been recognized as one of the most important energy carriers in the future for environmentally benign and sustainable development [1]. 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. The technologies are available and being tested for the hydrogen production, including steam methane reforming, water electrolysis, coal gasification, thermochemical water-splitting cycles, etc.

Recently, the solar hydrogen production has attracted increasing attentions. It is possible to obtain the high temperatures necessary for the hydrogen production processes by concentrating the sunlight and with the help of suitable reactors [2–4]. Solar thermochemical processes to produce hydrogen takes place in solar reactors. The design concept of a solar reactor plays a significant role in better absorption of the incident solar radiation and the higher thermochemical efficiency. Therefore, numerous studies on solar reactors have been implemented. For example, 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 [5]. A two-zone solar reactor for the steam-based gasification of biomass particles using concentrating solar energy has been developed and experimentally evaluated with particles of sugarcane bagasse at a 1.5 kW solar input scale. The results indicate that the lower heating value of the syngas produced by the two-zone reactor was around 15.9 MJ/kg, which is substantially higher than typically obtained in conventional autothermal bagasse gasification. The maximum energy conversion efficiency can reach 21%

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Nomenclature

T	temperature [K]
C_p	specific heat [J/(kg·K)]
c	mole fraction
Q	heat source [W/m^3]
p	pressure [Pa]
u	velocity [m/s]
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
$\Delta_r H$	enthalpy of reaction [J/mol]
r	reaction rate [mol/(m^3·s)]

Subscripts

f	gaseous phases
s	catalyst bed
g	gas mixture

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

[6]. 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 [7,8], whereas other successful examples of solar reactors can be found elsewhere for other hydrogen production techniques [9,10].

The above-mentioned hydrogen production methods are often in a high working temperature, i.e., over 800 K, which will require the high resistance materials and bring a higher radiation thermal loss. The technology discussed in this paper focuses on the development of a mid-and-low temperature solar receiver/reactor, in which the concentrated solar heat at around 423–573 K is utilized to drive the methanol steam reforming reaction proposed by Jin and his group, and a clean hydrogen-rich gas stream is generated with multistage processes (fuel vaporization, steam reforming, carbon monoxide reduction) within the solar chemical receiver/reactor [11–14]. For this process, methanol was selected as the hydrogen source due to its high ratio of hydrogen to carbon and readiness of being activated at relatively low temperature. Liquid methanol can readily be produced from biomass, unlike gasoline or diesel fuel [1]. Many studies were carried out to provide insights into the thermal performances and the heat transfer in a steam methanol reforming reactor. Lots of kinetics models for the steam methanol reforming had been reported. Suh et al. [15] analyzed the methanol-steam reformer, with the considerations of the two-dimensional variation of the transport and thermal properties of the gas mixture. They obtained the correlation, i.e., the conversion efficiency of methanol is a function of the operating temperature, and a dimensionless time parameter. Karim et al. [16] studied the kinetics of methanol steam reforming on a commercial CuO/ZnO/Al_2O_3 catalyst. They assessed the impact of deviations from isothermality in a packed bed reactor on the rates of methanol steam reforming. Numerical studies on the performances of a plate methanol steam micro reformer were carried out by Hsueh et al. [17]. The effects of the flow configurations, the Reynolds number and various geometric parameters on the performances of the micro reformer were investigated numerically. It was found that the methanol conversion for the counter-current flow could be improved by 10%. Jin et al. [11] developed an original mid-and-low temperature solar receiver/reactor prototype, and identified the basic principles of the mid-and-low temperature solar reactor. Many benefits were achieved in the process, including ease implementation, accurate tracking of solar concentrators and low cost. The mid-and-low temperature solar receiver/reactor is a crucial component in the solar thermochemical process. Liu et al. [12] 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. [13] developed a procedure to analyze the performances of the non-isothermal solar reactors for the methanol decomposition. However, the influence mechanisms of the non-uniform distribution of the solar energy flux are omitted, and three-dimensional numerical simulations on the hydrogen production are absent.

In this paper, naturally, the performances of the mid-and-low temperature solar receiver/reactor for the hydrogen production are numerically studied, and the main contributions can be summarized as follows:

(1) A three-dimensional mathematical model incorporating the mass conservation, the fluid flow through a porous catalyst bed, the energy conservation and the complex kinetic behaviors of the methanol steam reforming is proposed to model the complicated thermophysical and chemical processes of the mid-and-low temperature solar receiver/reactor, and the thermal, fluid and chemical reaction characteristics of the receiver/reactor are numerically investigated.
(2) The effect laws of the key operating parameters on performances of the mid-and-low temperature solar receiver/reactor, including the porosity of the catalyst bed, the diameter of the receiver/reactor tube and the width of the aperture, are revealed.
(3) The influence mechanisms of the non-uniform distribution on performances of the mid-and-low temperature solar receiver/reactor with different diameters of the receiver/reactor tube are revealed.
(4) The research findings will provide a reference for the design of the mid-and-low temperature solar receiver/reactor.

The rest of this paper is structured as follows. In Section 2, we introduce the mid-and-low temperature solar receiver/reactor model. The numerical results and detailed discussions are given 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 temperature range of 473–573 K, which can be supplied by the