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Numerical analysis of hydrogen production via methane steam reforming in porous media solar thermochemical reactor using concentrated solar irradiation as heat source

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ABSTRACT

The calorific value of syngas can be greatly upgraded during the methane steam reforming process by using concentrated solar energy as heat source. In this study, the Monte Carlo Ray Tracing (MCRT) and Finite Volume Method (FVM) coupling method is developed to investigate the hydrogen production performance via methane steam reforming in porous media solar thermochemical reactor which includes the mass, momentum, energy and irradiative transfer equations as well as chemical reaction kinetics. The local thermal non-equilibrium (LTNE) model is used to provide more temperature information. The modified P1 approximation is adopted for solving the irradiative heat transfer equation. The MCRT method is used to calculate the sunlight concentration and transmission problems. The fluid phase energy equation and transport equations are solved by Fluent software. The solid phase energy equation, irradiative transfer equation and chemical reaction kinetics are programmed by user defined functions (UDFs). The numerical results indicate that concentrated solar irradiation on the fluid entrance surface of solar chemical reactor is highly uneven, and temperature distribution has significant influence on hydrogen production.

1. Introduction

Development and utilization of solar energy can decrease the use of conventional fossil fuels and reduce the burden on environment and carbon emissions [1]. Hydrogen can be used in many applications, such as: fuel cells, electronics, medicine, food, and aerospace [2,3]. The requirements of hydrogen are greatly grown in recent years [4,5]. There are many ways of hydrogen production, such as: fossil fuel reforming, thermal decomposition, and photolysis. Methane reforming with high endothermic process is a mature technology for hydrogen production [6,7]. However, solar energy can reduce the consumption of fossil fuel by providing energy for the endothermic methane reforming process [8].

The utilization of concentrated solar energy for hydrogen production is a sustainable route for future low-carbon energy economy [9]. Hybrid solar and methane reforming process can provide viable and efficient ways for syngas calorific value improving, in which methane is adopted exclusively as the chemical source for hydrogen production and concentrated solar energy is used as the heat source for the endothermic reaction. By providing concentrated solar energy for methane reforming, the calorific value of syngas can be upgraded up to 28%, fossil fuel de-carbonization and CO_2 mitigation can be achieved. In 1991, Böhmer et al. had integrated a 170 kW reformer into the GAST-circuit of the CESA-1 to validate the possibility of hybrid solar and methane reforming process [8]. Levy et al. had studied the feasibility of taking methane reforming as the vehicle for storage and transport of solar energy via a solar chemical heat pipe, and the endothermic reforming reaction was heated by solar furnace [10]. In 2013, Bianchini et al. had set up a hybrid power plant where the solar steam reforming of methane and a gas turbine power plant was integrated, and the experiment results indicated that fossil fuel saving can be reached up to 20% [11].

Due to the advantages of large heat transfer surface, good mass transfer performance and high photo-thermal conversion efficiency [12,13], the utilization of porous medium coated with catalyst layer as solar thermochemical reactor has attracted much attention [14]. In a monolithic dual chamber solar reactor, a quasi-continuous H_2 flow is produced by cyclic operation of the

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Nomenclature

c_p	specific heat, J/(kg K)
CR	concentration ratio
d_s	mean cell size, m
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 reactor, m
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

conv	convective heat transfer
chem	chemical reaction
eff	effective
f	fluid phase
i	the ith species
rad	irradiative heat transfer
s	solid phase
w	wall

two reaction chambers through sequential oxidation and reduction steps at low temperature and high temperature. However, the porous media solar thermochemical reactor can incorporate the heat recuperation between the reduction and oxidation steps [15]. When utilizing porous media solar thermochemical reactor, the endothermic and exothermic processes are conducted in the same thermochemical reactor without interplaying thermochemical reactor [16].

With the aim to receive concentrated solar energy to maintain the operational temperature for methane reforming reaction, porous media solar thermochemical reactor coated with catalyst were manufactured by CNRS-PROMES laboratory [15] and CETRH/CPERI laboratory [17] respectively. Gokon et al. had adopted metallic porous media reactor coated with Ru/g-Al_2O_3 catalyst for solar methane reforming reaction [18]. Sang et al. had experimentally investigated the catalytic solar methane reforming reaction over metal porous media reactors based monolithic catalysts [14].

Numerical analysis of methane reforming in porous media reactor for hydrogen production can be benefit for reactor design and operation improvement. Heat transfer analysis of solar thermochemical reactor fitted with porous medium was conducted under Gaussian heat flux distribution by Villafán-Vidales et al. [15]. A heat and mass transfer model coupled with chemical reaction kinetics was developed by Ni to research the effects of various structural and operating parameters on methane reforming for hydrogen production [19], while the local thermal equilibrium assumption was adopted. Wang et al. had developed a heat and mass transfer model coupled with thermochemical reaction kinetics for the volumetric porous media solar thermochemical reactor, and the LTNE model coupled with modified P1 approximation under Gaussian heat flux distribution was adopted to study the heat transfer performance and hydrogen production performance [20].

Some researchers had developed the MCRT and FVM coupling method for solar applications: Cheng et al. had developed the MCRT and FVM coupling method to investigate the heat transfer and synthetical performance of a pressurized volumetric porous media receiver with local thermal equilibrium assumption [21]. Wang et al. had developed the MCRT and FVM coupling method to study the heat transfer performance of tube receiver for parabolic trough concentrator [22,23]. A detailed temperature distribution of a parabolic trough receiver was simulated by Wu et al. using the MCRT and FVM coupling method [24]. The concentrated solar irradiation distribution had significant effects on the temperature distribution of porous media receiver, the MCRT and FVM coupling method was adopted by Wang et al. to study the heat transfer performance of porous media solar receiver [25,26].

From the literature survey it can be seen that MCRT and FVM coupling method have been adopted widely to investigate the thermal performance of porous media receiver and tube receiver. However, little literatures have been published on solar thermochemical reaction performance analysis by using MCRT and FVM coupling method.

In this study, the temperature distribution and hydrogen production performance in volumetric porous media solar thermochemical reactor under concentrated solar irradiation is numerically investigated by MCRT and FVM coupling method. The methane steam reforming in porous media solar thermochemical reactor includes the irradiative transfer, mass, momentum and energy conservation equations as well as both the reduction and hydrolysis reaction which are solved by MCRT method coupled with Fluent software with UDFs. The LTNE model assumes that the solid phase temperature is different from the fluid phase temperature [27]. Two separate energy equations are adopted to describe the heat transfer within porous media receiver, and each energy equation requires a boundary condition [28,29]. The LTNE model is used to study the solid phase and fluid phase thermal performance to provide more temperature information [25,26].

During the numerical analysis, the fluid phase energy equation and transport equations are solved by Fluent software. The solid phase energy equation, irradiative transfer equation coupled with chemical reaction kinetics is programmed by UDFs. Over the last decades, several methods have been developed to calculate irradiative transfer, for example: P_N, DOM, FEM, MCRT, FVM and Ray Tracing method [30,31]. Since the porous medium strongly absorbing solar irradiation, the porous medium is large optically thickness with a short radiation transport mean free path and the optical thickness is generally larger than five [32]. The P1