INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 39 (2014) 718–730

Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he

Thermal and chemical reaction performance analyses of steam methane reforming in porous media solar thermochemical reactor

Fuqiang Wang [a,*], Yong Shuai [b,**], Zhiqiang Wang [c], Yu Leng [a], Heping Tan [b]

[a] Collage of Pipeline and Civil Engineering, China University of Petroleum (Huadong), 66, West Changjiang Street, Qingdao 266580, PR China
[b] School of Energy Science and Engineering, Harbin Institute of Technology, 92, West Dazhi Street, Harbin 150001, PR China
[c] National Engineering Laboratory for Coal-fired Pollutants Emission Reduction, Shandong University, 17923, Jingshi Street, Jinan 250061, PR China

ARTICLE INFO

Article history:
Received 10 September 2013
Received in revised form
12 October 2013
Accepted 24 October 2013
Available online 23 November 2013

Keywords:
Hydrogen
Solar receiver
Reactor
Steam reforming
Methane
Porous media

ABSTRACT

In order to investigate the thermochemical reaction performance of steam methane reforming (SMR), the steady heat and mass transfer model coupled with thermochemical reaction kinetics is developed for the volumetric porous media solar thermochemical reactor. The local non-thermal equilibrium (LNTE) model with modified P1 approximation is adopted to investigate the temperature distributions of the solid phase and fluid phase. For the solid phase energy equation, the irradiative heat transfer coupled with chemical reaction kinetics is programmed via User Defined Functions (UDFs). The concentrated solar irradiation is not only considered as the boundary condition at the reactor front surface, but also as the irradiative heat source in the whole volume of reactor. The parametric studies are conducted to investigate the thermal and hydrogen production performances as a function of operational parameters. The numerical results indicate that SMR reaction has big effects on temperature distribution. The generated H_2 mole fraction decreases sharply with the increasing of fluid inlet velocity, porosity and mean cell size. The generated H_2 mole fraction increases significantly with the increasing of incident solar irradiance.

1. Introduction

With solar energy being transduced to chemical energy, the utilization of solar fuel can upgrade the calorific value of fossil fuel, and the greenhouse emission can be dramatically decreased [1]. Take methane reforming as an example, the life cycle analyses indicate that the CO_2 equivalent emission can be reduced to 41% and the calorific value of the product of synthesis gas can upgrade to 28% when the process heat is supplied by concentrated solar irradiation [2].

* Corresponding author. Tel./fax: +86 532 8698 1767.
** Corresponding author.
E-mail addresses: Aaronwang544@gmail.com (F. Wang), Shuaiyong@hit.edu.cn (Y. Shuai).

http://dx.doi.org/10.1016/j.ijhydene.2013.10.132

Nomenclature

c_p	specific heat, J/(kg K)
C_R	concentration ratio
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
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

During the hybrid solar and fossil endothermic process, conventional fossil fuels (i.e. natural gas, coal, or petroleum coke) are adopted as the chemical source for H_2 production, and concentrated solar irradiation is used as the energy source to provide high working temperature [3,4]. Compared to solar thermal power generation, the energy conversion efficiency is greatly improved for solar fuel as the hybrid solar and fossil endothermic process is not limited by Carnot efficiency.

Steam reforming of hydrocarbon fuels is a promising way for hydrogen production compared to water electrolytic hydrogen production which needs expensive catalyst, i.e. Pt [5]. The SMR process comprises two steps, methane steam reforming (MSR) and water gas shift reaction (WGSR) [6,7]. In the MSR process (as shown in Eq. (1)), hydrogen and carbon monoxide can be obtained from the reaction of methane with water in the catalyst layer of reactor, which is a highly endothermic process. Meanwhile, water reacts with carbon monoxide which is called WGSR process and proceeds to generate additional hydrogen and carbon dioxide, which is a slightly exothermic process (as shown in Eq. (2)).

MSR:

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2 \tag{1}$$

WGSR:

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \tag{2}$$

The required heat for MSR process is much higher than the generated heat by WGSR process. Therefore, the whole process for hydrogen production by SMR is an endothermic process [8]. The additional heat for hydrogen production can be provided by combustion or concentrated solar energy [9]. The SMR process driven by concentrated solar energy is called "Solar SMR". Bianchini et al. had built a hybrid power plant where the "Solar SMR" and a gas turbine power plant were integrated for solar syngas production and utilization. The experiments indicated that the natural gas saving can be reached up to 20% when the gas turbine was fed only by solar syngas [9].

Numerical analyses of SMR for hydrogen production can be benefit for reactor design and operation improvement. Ni had developed a 2D heat and mass transfer model coupled with chemical reaction kinetics to research the effects of various structural and operating parameters on reaction rate of hydrogen production by SMR [10,11], while the local thermal equilibrium (LTE) assumption was adopted in the study. A 3D calculation model combined with chemical reactions and gas permeation to/from the porous catalyst reforming layer was developed by Yuan et al. to investigate the effects of design and operating parameters on the SMR performances, the numerical results indicated that characteristic ratios had significant effects on the MSR and WGSR conversion rate [12]. Hou and Hughes had conducted experiments in an integral reactor using Ni/α–Al_2O_3 as catalyst to investigate the kinetics of MSR and WGSR processes, and intrinsic reaction rate equations were derived based on the experimental data [13]. One dimensional model with the consideration of thermal effects was developed by Yu et al. to illustrate the performances of porous ceramic membrane reactor for SMR, the numerical results indicated that using steam as the sweep gas had better performance of methane conversion and hydrogen recovery [14]. A CFD model was developed by Zhai et al. to examine the elementary reaction kinetics for the process of SMR in a micro reactor, and the numerical results illustrated the significance of heat conduction ability and interplay between the exothermic and endothermic reactions [15,16]. The