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Analysis of thermal transport and fluid flow in high-temperature porous media solar thermochemical reactor

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ABSTRACT

As a key technical indicator of porous media solar thermochemical reactor, thermal transport and fluid flow characteristics have significant impacts on hydrogen production efficiency. These issues could be achieved more efficiently and at a lower cost by applying computational fluid dynamics (CFD). However, the choice of different thermal transport models might cause the variation of results. In this study, the thermal transport and fluid flow characteristics in high-temperature porous media solar thermochemical reactor were investigated with different thermophysical models using FLUENT software user-defined functions (UDFs). The results indicate that the local thermal non-equilibrium model (LTNE) and radiative transfer model are proved to be indispensable for the thermal performance analysis of high working temperature thermochemical reacting system. Besides, Wu model of momentum source is more suitable for pressure simulation, while Wu model and Vafai model of heat transfer show little difference in temperature distribution.

1. Introduction

Nowadays, a high-temperature concentrated solar-driven thermochemical reacting system for hydrogen and syngas production has been an effective alternative to fossil fuels to tackle energy problems and climate change (Steinfeld, 2005; Agrafiotis et al., 2014). The research and development of concentrated solar radiation utilization as a heat source to induce high-temperature raw materials conversion into fuels accessible has attracted tremendous interests worldwide (Yadav and Banerjee, 2016; Marxer et al., 2017; Villasmil and Steinfeld, 2010; Agrafiotis et al., 2015). Integrating porous media in the solar reactor has become the focus in recent years (Zhao, 2012; Torabi et al., 2017) for the thermal performance enhancement of solar thermochemical reacting system (Mahmoudi and Maerefat, 2011; Zhao and Cheng, 2010).

Many researchers have investigated the numerical simulation of thermal transport and fluid flow performance of porous media reactor. Pitz Paal et al. (1997) developed a numerical approach for volumetric porous media reactor with the aim to describe the realistic three-dimensional irradiance distribution and its influence on fluid flow. The results indicate that the temperature distribution in volumetric porous media is strongly dependent on solar irradiation distribution. Alazmi and Vafai (2000) analyzed four major categories of porous media in order to compare the variants within different porous media transport models. They reported that the variances have more influence on the velocity field than the temperature field and Nusselt number distribution. Wu et al. (2010) have numerically studied the pressure drop characteristics and flow field characteristics in the ceramic foams and proposed a generalized model for predicting pressure drop. Soon afterward, in 2011, Wu et al. (2011) have investigated the effect of solid phase thermal conductivity on the temperature fields by considering the pressure drop and interfacial heat transfer between the flowing fluid and solid in ceramic foams. Moreover, Villafán-Vidales et al. (2011) developed a numerical model coupling the heat and mass transfer, fluid flow, and the chemical reactions to predict the thermal performance inside the volumetric porous receiver. A numerical model MCRT method (Li et al., 2018a, 2018b) combined to FLUENT software with UDFs has been developed by Wang et al. (2013) to obtain the heat flux distribution on the surface of porous media receiver. Cheng et al. (2013) and Huang et al. (2015) investigated an axisymmetric numerical model of pressurized volumetric receiver using MCRT-FVM method to study the complex coupled heat transfer performance of porous media receiver. Different transport and thermophysical models were investigated by Wang et al. (2014a, 2014b) for the thermal and physical

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performance of porous media receiver by adopting a simple cylindrical cavity structure without further optimization. A numerical model coupling solar radiation transport and internal heat transfer with P1 approximation and LTNE model were developed by Chen et al. (2016) to investigate the thermal performance of solar porous media receiver. Recently, Du et al. (2017) presented a fully coupled heat transfer model at pore-scale with the aim to obtain the pore-scale heat transfer characteristics of volumetric solar receiver. Besides, many efforts have been developed on the solar thermochemical reactor. The structural properties of the reactor have been constantly changed and optimized by many researchers with a deeper investigation of thermal transport and fluid flow characteristics. The Computational Fluid Dynamics (CFD) simulation offers the possibility to investigate operating conditions of the solar thermochemical reactor (Meier et al., 1996). Moller and Palumbo (2001) developed a one-dimensional unsteady and steady-state heat transfer model for a solar reactor of simple construction to analyze the thermal decomposition of ZnO within the temperature of 1950–2400 K. Soon afterwards, Möller and Palumbo (2001) have designed a cylindrical solar chemical reactor taking advantage of inert gas to keep the reactor's window clean of Zn and ZnO. A MCRT method coupled with optical properties was developed by Yong et al. (2011) to predict radiative properties of solar reactor with quartz window. Costandy et al. (2012) developed different struts of spherical and cylindrical solar reactor to investigate the effect of reactor geometry on the temperature distribution and heat loss inside the reactors. Thomey et al. (2012) have developed a multi-chamber solar porous media reactor design for the decomposition of sulphuric acid. Since the metal oxide is being regenerated during the process, Konstandopoulos and Agrofiotis (2006) have designed a two-reactor 'Conti-reactor' chamber to solve the intermittent problem relative to hydrogen production. Moreover, a modified solar reactor for a two-step solar-driven thermochemical production was developed by Chueh et al. (2010). On these basis; Bachirou Guene et al. (2016), Guene Lougou et al. (2017a, 2017b) have optimized the partial structure of solar thermochemical reactor and completed many numerical simulations for heat transfer performance and optimal operating conditions analysis. According to the literature review, the transport and thermophysical models play an important role in the thermophysical analysis of porous media solar thermochemical reactor. Many numerical models have been put forward to predict the heat transfer and flow characteristics of the reactor. However, few literatures have evaluated the effect of various transport and thermophysical models on the simulation results of porous media solar thermochemical reactor, especially for the optimized reactor structure of references (Chueh et al., 2010; Bachirou Guene et al., 2016).

In this paper, thermal transport and fluid flow in high-temperature porous media solar thermochemical reactor are analyzed with different transport and thermophysical models via FLUENT software user-defined functions (UDFs). The deviation between LTE and LTNE model, the error caused by ignoring the radiation heat transfer between porous media, the effect of porous media, the distinction of adopting different thermal transport models were studied in detail, respectively.

2. Methods

2.1. Physical model

SiC porous media solar thermochemical reactor used for the numerical simulation is shown in Fig. 1. The concentrated solar energy is transmitted into the reactor inner cavity through the transparent quartz glass window installed on the front surface of the reactor. As indicated in Fig. 1, the angle of the front cavity wall is designed to 45° to the axis in order to effectively collect incident solar energy. The reactant gas led into the reactor inner cavity by two opposite inlets in the (y) direction. The quartz window is swept and kept clean from solid deposition due to the effect of carrier gas flow. The water-cooled device is installed at the exit of the reactor in order to lower the temperature of exhaust gas. Moreover, the whole reactor is wrapped with good thermal insulation for protecting the reactor and reducing heat loss during the progress of thermochemical reactions.

2.2. Mathematical model

2.2.1. Continuity equation

$$\nabla\cdot(\rho_f \vec{u}) = 0 \tag{1}$$

where ρ_f is the fluid density, and $\vec{u}$ is the superficial velocity.

2.2.2. Momentum equation

By considering the pressure drop caused by non-Darcy flow effect, an additional momentum source term S_p should be considered in the momentum equation for the numerical simulation of porous media (Wu et al., 2010, 2011). This term consists of two parts: the first one denotes the viscous resistance term, and the second one denotes the inertial resistance term.

$$\nabla\cdot(\rho\vec{u}\,\vec{u}) = \nabla\cdot(\mu\nabla\vec{u}) - \nabla p + S_p \tag{2}$$

where p is the fluid pressure, μ is the dynamic viscosity, and S_p is the source term associated to the pressure drop caused by porous media.

The source term can be calculated by FLUENT software UDFs according to the following two models in Table 1. The first one is Darcy-Forchheimer extended model (DF model), which adopts two key parameters, permeability and inertia resistance factor to express the pressure drop. The second one was proposed by Wu et al. (2010, 2011) based on the experimental and numerical results, which mainly depends on the value of porosity ϕ and mean cell size d_p of porous media. Note that Wu model has its application range of $0.66 < \phi < 0.93$, and a Reynolds number in the range of $10 < Re < 400$.

2.2.3. Energy equation

The local thermal equilibrium model (LTE) is widely adopted to the simulations of porous media heat transfer at low temperatures, which assumes that the temperature of porous solid frame is equal to the fluid parts. However, for the simulation in high-temperature environments, the significant local temperature difference must be considered to provide more heat transfer information and avoid large calculation deviation (Wang et al., 2014). Therefore, the fluid phase and solid phase energy equations should be described based on the LTNE assumption as follows.

$$\nabla\cdot(\rho_f c_{p,f} u T_f) = \nabla\cdot(\lambda_{f,e}\nabla T_f) + S_f \tag{6}$$

$$\nabla\cdot(\rho_s c_{p,s} u T_s) = \nabla\cdot(\lambda_{s,e}\nabla T_s) + S_s \tag{7}$$

where $\lambda_{f,e}$ and $\lambda_{s,e}$ are the effective thermal conductivity of the fluid phase and solid phase, respectively.

The effective thermal conductivity of the fluid phase and solid phase can be calculated via the Schuetz-Glicksman empirical formula (Schuetz and Glicksman, 1984).

$$\lambda_{f,e} = \phi\lambda_f \tag{8}$$

$$\lambda_{s,e} = \frac{\lambda_s}{3}(1-\phi) \tag{9}$$

S_f and S_s are the heat source term of the fluid phase and solid phase, respectively.

The heat source term of the fluid phase and solid phase can be obtained by the following equations.

$$S_f = S_{con,f} \tag{10}$$

$$S_s = S_{con,s} + S_{rad} \tag{11}$$

where S_{rad} is the radiative heat transfer term between the porous media cells, $S_{con,f}$ and $S_{con,s}$ are the convective heat transfer term between the

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