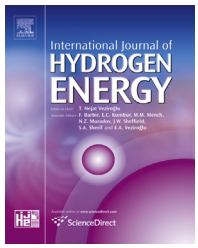
Available online at www.sciencedirect.com

ScienceDirect

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



A transient heat transfer model for high temperature solar thermochemical reactors

Like Li [a,*], *Chen Chen* [a], *Abhishek Singh* [a], *Nima Rahmatian* [a], *Nick AuYeung* [b], *Kelvin Randhir* [a], *Renwei Mei* [a,**], *James F. Klausner* [a,***], *David W. Hahn* [a], *Jörg Petrasch* [c]

[a] *Department of Mechanical and Aerospace Engineering, University of Florida, Gainesville, FL 32611, USA*
[b] *School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvalis, OR 97331, USA*
[c] *Energy Research Center, Vorarlberg University of Applied Sciences, 6850 Dornbirn, Austria*

ARTICLE INFO

Article history:
Received 18 September 2015
Received in revised form
10 November 2015
Accepted 17 November 2015
Available online 28 December 2015

Keywords:
Solar reactor
Thermochemical fuel production
Heat transfer
Monte-Carlo ray tracing
Lattice Boltzmann

ABSTRACT

We present a heat transfer model for energy transport in a solar thermochemical reactor for CO_2 and/or H_2O splitting to produce chemical fuels CO and/or H_2. The reactor is comprised of a horizontal cavity-receiver packed with several insulation layers, an array of tubular absorbers in which the reactive metal oxide is loaded, and a windowless aperture that allows the incident concentrated solar energy to enter the receiver. A framework for modeling the complex multimode thermal transport within the reactor system is developed. The concentrated solar radiation from a high flux solar simulator to the cavity-receiver is simulated using a Monte-Carlo ray tracing model. Heat transfer within the tubular absorbers, including conduction, convection, radiation, and chemical reactions, is simulated using a lattice Boltzmann (LB) model. These two models are coupled by taking into account the temperature-dependent radiative emission from the absorber surfaces. Two particular techniques are employed to improve the numerical accuracy and stability: appropriate rescaling of the relaxation coefficients in the LB method and implicit treatment of the heat source/sink terms due to chemical reactions. The numerical method is validated with two test cases for which analytical solutions are available. Simulation results for the heating process and one thermal reduction step under near-vacuum pressures are presented. The predicted solar-to-fuel energy conversion efficiency varies from 5% to 10% and is determined based on the simulated O_2 release during the reduction step. The model is able to provide insight into the optimum operating conditions, the reactor design and the scale-up. The results suggest that high temperatures for both reduction and oxidation steps and near-vacuum pressure ($\sim 10^{-4}$ atm) for thermal reduction are critical for improved solar-to-fuel conversion efficiency with the ceria-based reactive material.

* *Corresponding author.*
** *Corresponding author.*
*** *Corresponding author.*
E-mail addresses: likelichina@ufl.edu (L. Li), rwmei@ufl.edu (R. Mei), klaus@ufl.edu (J.F. Klausner).

http://dx.doi.org/10.1016/j.ijhydene.2015.11.079

Introduction

Solar energy, especially concentrated solar thermal energy, has vast potential to contribute towards a more sustainable and clean energy portfolio. Storing solar thermal energy chemically as a fuel is of enormous interest. In the last decade, metal oxide reduction-oxidation (redox) cycles have been intensively studied as chemical loops for fuel production. Two-step CO_2 and H_2O splitting redox processes can be generally represented as

$$\text{Thermal reduction}: \ MO_x \rightarrow MO_{x-y} + \frac{y}{2} O_2, \tag{1}$$

$$CO_2 \text{ splitting oxidation}: \ MO_{x-y} + yCO_2 \rightarrow MO_x + yCO \tag{2a}$$

and

$$H_2O \text{ splitting oxidation}: \ MO_{x-y} + yH_2O \rightarrow MO_x + yH_2, \tag{2b}$$

where the metal oxide is thermally reduced at high temperatures to a lower oxidation state (Reaction (1)), then oxidized using CO_2 and/or H_2O to form CO and/or H_2 (Reactions (2a, 2b)). CO and H_2 in tandem, also known as syngas, can be a precursor to synthetic liquid fuels such as jet fuel, gasoline, or diesel [1]. Though very attractive, economic viability will require well-designed energy conversion devices to maximize the overall conversion efficiency. This will in turn minimize costs associated with the concentrating solar radiation and the reactor hardware necessary per unit of fuel [2].

A solar thermochemical reactor typically features a cavity-type receiver that captures the concentrated solar energy, and a small open or windowed aperture that allows the sunlight to travel through while minimizing the re-radiation from the receiver. The orientation of the cavity with regard to the incoming concentrated sunlight can be either horizontal or vertical, i.e., the axis of the cavity is either parallel or perpendicular to the centerline of the concentrated sunlight. Active cooling is usually required for a quartz window, and its optical properties such as absorptivity would be affected during multiple cycles as the gases in the cavity may condense on and contaminate the window [3,4]. The reactive materials are in the forms of porous beds such as packed particles or stabilized porous structures that have high surface area for chemical reaction during the extensive cycling process. The reactive beds are either directly exposed to the incident radiation, or packed in tubular absorbers and indirectly irradiated by the solar flux. The engineering design of a reactor requires a functional model to account for heat transfer, species transport, and chemical reaction. Heat transfer in the cavity-reactor system includes radiation, conduction, convection and endothermic/exothermic chemical reactions. Effective modeling of the heat transfer and energy transport in the solar reactor is essential to the reactor design and it also provides valuable insight and guidance for optimizing operating conditions.

A limited number of lab-scale solar reactor prototypes with solar input power in the range of 3–10 kW_{th} for fuel production have been designed, computationally modeled, and experimentally tested worldwide. High flux solar simulators using an array of argon or xenon arc lamps [5,6] have been used to provide a radiant source for those high temperature solar reactors. An even more limited number of solar reactors on the order of 100 kW_{th} to 1 MW_{th} scales have been tested on-sun.

Schunk et al. [4] presented a reactor design with three-dimensional (3D) computational fluid dynamics (CFD) modeling and experimental testing of a 10 kW rotating, windowed, horizontal, directly heated cavity-reactor for thermal dissociation of ZnO. The key design concept of the rotating cavity is that the layer of ZnO particles serves three functions simultaneously: as a radiant absorber, chemical reactants, and a thermal insulator. Müller et al. [7] developed a transient heat transfer model to simulate the coupled radiation, convection, conduction and endothermic reaction in a directly-irradiated solar reactor for thermal dissociation of a ZnO bed. They validated their model by comparing simulated temperature profiles and reaction rates with measured ones. Abanades et al. [8] designed and simulated a windowed, horizontal, directly heated solar chemical reactor for continuous dissociation of metal oxides, which were continuously injected into the cavity through a screw feeder and a rotating driving gear at the backside of the cavity. Kaneko et al. [9] developed and tested a windowed, rotary-type solar reactor for a two-step H_2O-splitting process using reactive ceramics of ceria and Ni, Mn-ferrite ($Ni_{0.5}Mn_{0.5}Fe_2O_4$). A simulation of the rotary-type solar reactor was conducted by Kaneko et al. [9] and the solar reactor was tested with 20 kW input [10]. Diver et al. [11] designed a windowed, vertical-direct counter-rotating-ring receiver/reactor/recuperator (CR5) as a heat engine for solar thermochemical H_2O-splitting. The CR5 uses a stack of counter-rotating rings or disks with fins along the perimeter. The efficacy of the CR5 has been demonstrated by Miller et al. [12] through laboratory and on-sun testing using cobalt ferrite/zirconia mixtures as reactive materials. Ceria-based material was also tested and both CO_2 and H_2O-splitting have been demonstrated using the CR5. Roeb et al. [13] built and tested a quasi-continuously operating horizontal reactor consisting of two separate chambers with fixed honeycomb absorbers for more than 50 cycles. While H_2O splitting was taking place in one chamber, thermal reduction was in progress in the other chamber, so that a continuous production of H_2 is feasible. They also developed a transient 2D numerical model to simulate the heat transfer and H_2 production in the solar reactor using inputs from experimental measurements. Based on their experimental test and simulation results, they also designed a 100 kW_{th} solar pilot plant. Experimental testing of the pilot plant for the two-step H_2O splitting via monolithic honeycomb solar reactors has been operated within a solar tower [14]. Chueh et al. [15] investigated thermochemical dissociation of CO_2 and H_2O using nonstoichiometric ceria. A total of 500 redox cycles in an infrared furnace were conducted, and four consecutive CO_2 and H_2O cycles were performed in a vertical cavity-receiver reactor for which solar-to-fuel efficiencies of 0.7%–0.8% were achieved. They showed that the efficiencies were largely limited by the system scale and design rather than by chemistry. Using a very similar solar reactor but with a reticulated porous ceramic (RPC) foam made of pure ceria, Furler et al. [16] reported an improved average solar-to-fuel efficiency of 1.73% for CO production. The RPC foam had a relatively larger