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MATHEMATICAL MODELLING TO THERMAL PERFORMANCE ANALYSIS OF A SOLAR THERMOCHEMICAL REACTOR

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Abstract. *The distribution of concentrated solar irradiation has a significant impact on temperature distribution in solar reactors. In this way, the objective of this paper is to analyze the thermal performance of a fixed-bed solar thermochemical reactor through a mathematical model. Partial differential equations formed this model and were transformed into ordinary differential equations by the finite difference method. In addition, a code in the Mathematica software with NDSolve was used to obtain the results. Furthermore, to carry out the investigation of the thermic behavior of radiation and temperature distribution, the Rosseland approximation was used. Thus, the typical influences of the radiation heat flux, porosity, emissivity, and temperature distribution were investigated.*

Keywords: *Thermal, Finite Difference, Thermochemical Reactor*

1. INTRODUCTION

Nowadays, due to population growth and increased energy consumption, which lead to the gradual depletion of conventional fossil fuels, studies about new ways of energy production are of interests of several researchers (Lougou et al., 2017). The solar energy, which is clean and renewable, is abundant and widespread to meet the demand for fuels in an environmentally friendly and sustainable way (Wang et al., 2018). A method to use this solar energy is the conversion of solar radiation into energy for obtaining chemical fuels, like hydrogen, which is an alternative fuel and can be produced by solar radiation in a solar thermochemical reactor. However, the reactor design and its thermal performance are the relevant factors that have a significant impact on production efficiency and need to be investigated.

There are several studies about the importance of heat transfer in a solar thermochemical reactor. Wang et al. (2013) studied that the distribution of concentrated solar irradiation has a significant impact on the temperature distribution of the porous media receiver. They investigated the thermal performance by combining the Monte Carlo Ray Tracing method and secure software with user-defined functions, in this way typical influences of the heat flux boundary condition, radiation heat loss, porosity, emissivity, flow mass and the average particle diameter on the temperature distributions were investigated. Paal et al. (1997) have developed a heat transfer performance analytical approach for volumetric porous media receiver, which has taken into the consideration of three-dimensional irradiation distribution and its influence on fluid flow. The numerical results show that temperature distributions of volumetric porous media receiver are strongly influenced by solar radiation distribution. Zhang et al. (2018) studied 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. The results indicate that the local thermal non-equilibrium model and radiative transfer model are proved to be indispensable for the thermal performance analysis of high working temperature thermochemical reacting system. However, the calculation of solar radiation can be calculated by different methods, and there are many doubts about the best way to simulate the radiation and how to analyze the effect of temperature in a solar thermochemical reactor.

The mathematical model and the numerical simulation are used to gain a better overall understanding of the Solar Thermochemical Reactor (STR) through consideration of turbulence, heat and mass transfers, chemical reactions as well as the phenomenology of the reactor. Mathematical models are useful to investigate the effects of primary operating conditions, optimization, and scale-up in the STR. The performance of the absorber systems can be investigated beyond the range of parameters and should not study experimentally due to limitations imposed by economic and safety considerations (Anjos et al., 2017; Anjos et al., 2019). Physical and chemical parameters should be simultaneous of the coupled way from the mathematical model, such as fluid-solid mass transfer, fluid-solid heat transfer, adsorption and desorption, and chemical reactions (Anjos et al., 2018).

Therefore, in order to study thermal performance analysis of a solar thermochemical reactor, the present work carried out the numerical modeling of the heat transfer in a solar thermochemical reactor with the radiation solar calculated by Rosseland approximation. Thus, based on the heat transfer, the partial differential equation (PDE) was formulated for describing governing equations of the energy balance. In addition, applying the methodology of the Finite Difference (FD) it was possible to transform the PDE into Ordinary Differential Equations (ODE), and with the *NDSolve* command in *Mathematica* software, were obtained the graphs of the temperatures, sensibility analysis of parameters, and value of solar radiation.

2. PROBLEM FORMULATION

In the last two decades, researches have proven the efficient use of solar thermal energy for driving highly endothermic reforming reactions. For this purpose, a schematic setup (see Fig. 1) was employed to study the heat transfer. Fig. 1 shows the simplified schematic of a solar thermochemical reactor that is used as the computational domain geometry for the numerical simulation. It is possible to notice from the figure that the heat transfer that will occur in the reactor will be influenced by the concentrated solar irradiation that will act directly in the porous region.

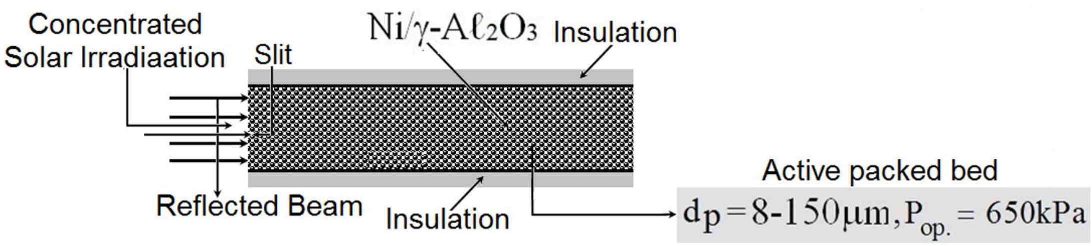

Figure 1. Simplified Model of a Solar Thermochemical Reactor.

2.1 Mathematical model

The primary purpose of this section is the development of a precise mathematical model that will be able to simulate the behavior of the heat transfer in the STR. To evaluate the key variables of the developed mathematical modelling, the following assumptions were adopted: (i) ideal gas phase, (ii) axial dispersion inside from STR, (iii) no diffusion phenomena of chemical components at the catalyst surface and inside the catalyst occur, (iv) constant STR pressure (no pressure drop in the STR) and constant superficial velocity, (v) STR operates under stationary regime, (v)) porosity in the axial direction from STR was considered constant, (vi) constant physical properties (density, catalyst weight, uniform particle sizes) over the range of operating conditions from STR, respectively. Based on the above assumptions, the energy equation (inside from STR) is formulated as follows.

- Energy balance in the gas phase;

$$v\frac{\partial T_g}{\partial z}+V_{sg}\frac{\partial T_g}{\partial x}=\frac{\lambda_{eff}}{\rho C_p}\frac{\partial^2 T_g}{\partial x^2}+\frac{(1-\varepsilon_b)}{\varepsilon_b}\frac{3}{R_p}\frac{h_{gs}}{\rho C_p}\left(T_g-T_s\big|_{r=R_p}\right) \tag{1}$$

In the Eq.1, ρ (kg/m^3) is the density of the gaseous mixture, T_g (K) is the temperature of the gaseous phase, C_p (kJ/kg K) is the molar heat capacity at constant pressure of the gaseous mixture, h_{gs} (W/m^2 K) volumetric convection heat transfer coefficient between the fluid phase and the solid phase, ε_b (m^3 gas/m^3 reactor) is the void fraction of bed, r_p (m) is the particle radius, T_s (K) is the temperature of the solid phase, respectively.

$$\lambda_{eff}=\left(\lambda_g+\frac{16\,n^2\sigma T_\infty^3}{3k_R}\right) \tag{2}$$

Where, λ_g (W/m K) is the gas thermal conductivity, n (-) is the refractive index, σ (W/m^2 T^4) is the Stefan-Boltzmann constant, T_∞ (K) is the ambient temperature, k_R (m^{-1}) is the Rosseland extinction coefficient in porous medium respectively, The symbol h_{gs} is the volumetric convection heat transfer coefficient between the fluid phase and the solid phase. The empirical correlation proposed by Wu et al. (2011) is used:

$$h_{gs} = \lambda_f (32.504\varepsilon_b{}^{0.38} - 109.94\varepsilon_b{}^{1.38} + 166.65\varepsilon_b{}^{2.38} - 86.598\varepsilon_b{}^{3.38})\frac{Re^{0.438}}{d_c^2} \tag{3}$$

This correlation is valid for 0.66< ε_b < 0.93 and 70 < Re < 800

The suitable initial and boundary conditions from Eq. (1) are given as follows

$$\lambda_g \frac{\partial T_g}{\partial z_j}\bigg|_{z=0^+} = \frac{DNI}{T_{g,0}} \tag{4}$$

Where, DNI (W/m²) is the Direct Normal Irradiance and $T_{g,0}$ (K) is the initial temperature of the gaseous phase.

$$\frac{\partial T_g}{\partial z}\bigg|_{z=L_z} = 0 \tag{5}$$

2.2 Solar Radiation

Among the thermal phenomena that can occur in a solar thermochemical reactor, the radiation term is considered the most complex when compared to convection and conduction. In this way, your study gets a highlight. Since the porous medium absorbs the solar radiation strongly, presents a medium path of short radiation transport, and is of high optical thickness, the Radiative Transfer Equation (RTE) needs to be resolved to obtain the radiation source term (Wang et al., 2017):

$$\frac{dI(z)}{dz} = -k_e I(z) + k_a I_b(z) + \frac{k_s}{4\pi}\int_{4\pi} I(z,\vec{\Omega}')\Phi(\vec{\Omega}',\vec{\Omega})d\vec{\Omega}' \tag{6}$$

Where the symbol *I* is the local radiation intensity in the porous medium that varies with space (z) and the direction (Ω), the phase function Φ varies with direction. The symbol K_e is the extinction coefficient of the solar receiver of porous media, K_a is the absorption coefficient, and K_s is the dispersion coefficient.

To solve the RTE, the Rosseland Approximation is one of the best options because this method is used for sizeable optical thickness problems, does not consume time due to simplicity and can provide reasonably good predictions compared to experimental measures to study the transfer mechanisms radiative in porous media (Kodoma and Gokon, 2007).

2.3 Rosseland Approximation

Through the Rosseland approximation, the RTE can be simplified as (Magyari and Pantokratoras, 2011):

$$q_r = \frac{4n^2\sigma}{3k_R}\frac{\partial T^4}{\partial z} \tag{7}$$

Was assumed that the temperature differences within the flow are such that the term T^4 may be expressed as a linear function of temperature. This is accomplished by expanding T^4 in a Taylor series about T^1 and neglecting higher order.

$$T^4 \cong 4T_\infty^3 T - 3T_\infty^4 \tag{8}$$

So, the irradiative heat transfer problem reduced to be a simple conduction problem with strongly temperature-dependent conductivity, as follows.

$$q_r = \frac{16\,n^2 \sigma T_\infty^3}{3k_R}\frac{\partial T}{\partial z} \tag{9}$$

The extinction coefficient (k_R) is evaluated as the sum of absorption (k_α) and scattering coefficients (σ_s) as follows

$$k_R = k_\alpha + \sigma_s \tag{10}$$

$$k_\alpha = \frac{3\varepsilon_m(1-\varepsilon_b)}{2d_s} \tag{11}$$

$$\sigma_s = \frac{3(2-\varepsilon_m)(1-\varepsilon_b)}{2d_s} \tag{12}$$

Where, ε_m (m^3 gas/m^3 reactor) is the porosity of the reactor, ε_b (m^3 gas/m^3 reactor) is the porosity of the bed, and d_s (m) is the bed diameter.

3. SOLUTION METHODOLOGY

The Finite Difference Method (FDM) was adopted to solve the proposed equations. FDM is a traditional method of solving differential equations that are based on the approximation of derivatives by finite differences. The approximation formula was obtained from the Taylor series of the derivative function. The definitions below, Eq. (13 – 16), were used with the respective boundary conditions of each element. After the application of the FDM and through software *Mathematica* (with *NDSolve* command) it was possible obtained the results of this work. To illustrate the FDM, Fig. 2 shows a simplified approach to the points of the chosen mesh.

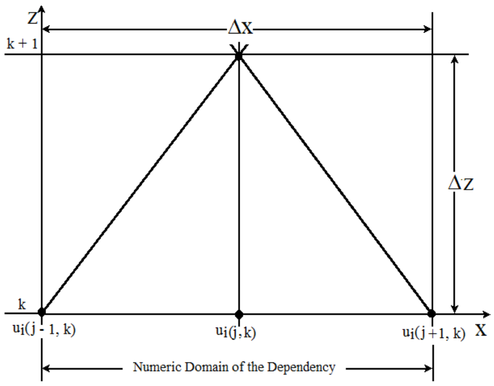

Figure 2. Mesh points for a numerical solution using FDM.

The relation below was used in the general equation and in the boundary conditions of the problem, allowing the discretization and obtaining of the EDOs for calculation in *Mathematica* software.

$$\left.\frac{\partial T(x,z)}{\partial x}\right|_{(j,k)} = \frac{1}{\Delta x}\left[(T)_{j+1}^{k} - (T)_{j}^{k}\right] \tag{13}$$

$$\left.\frac{\partial T(x,z)}{\partial x}\right|_{(j,k)} = \frac{1}{\Delta x}\left[(T)_{j}^{k} - (T)_{j-1}^{k}\right] \tag{14}$$

$$\left.\frac{\partial T(x,z)}{\partial x}\right|_{(j,k)} = \frac{1}{2\Delta x}\left[(T)_{j+1}^{k} - (T)_{j-1}^{k}\right] \tag{15}$$

$$\left.\frac{\partial T(x,z)}{\partial x}\right|_{(j,k)} = \frac{1}{\Delta x^2}\left[(T)_{j+1}^{k} - 2(T)_{j}^{k} + (T)_{j-1}^{k}\right] \tag{16}$$

4. RESULTS

A computational algorithm using the *Mathematica* (with *NDSolve* command) was elaborated by the authors to solve the model equations mentioned in this work. Therefore, operating conditions and energy parameters for simulating the STR process variables are presented in Table 1. In this study, the mathematical model was confirmed through the temperature distribution in the STR. Fig. 3 shows the temperature profile obtained by Lougou et al. (2017) and the numerical simulation from the present study. The comparison shows a good fit between the result of this work and the literature, both follow a similar behavior.

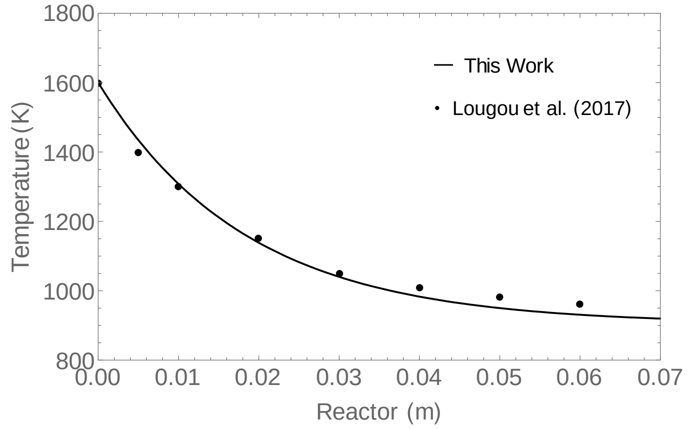

Figure 3. Temperature distribution compared to the literature (Lougou et al. 2017), under 1600 K of operating temperature.

Table 1: Operating conditions, kinetic parameters, and mass parameters.

Categories	Properties	Numerical Values
Operation Conditions	Operating pressure (atm)	1.01
	Operating temperature (K)	1800
	Gas flow rate (m^3/s)	$3.5x10^{-5}$
	Void fraction of bed (-)	0.77
	Void fraction of reactor (-)	0.31
	Emissivity of porous media (-)	0.92
	Reactor diameter (m)	0.032
	Reactor length (m)	0.14
Energy parameters	The density of the gaseous mixture (kg/m^3)	0.693
	The molar heat capacity of the gaseous mixture ((kJ/kg K)	1.079
	STR diameter (mm)	0.32
	Gas thermal conductivity (W/m K)	109.123
	Stefan-Boltzmann constant ($W/m^2 T^4$)	$2.67x10^{-8}$
	Gas-solid heat transfer coefficient	$13.3x10^2$;
	Ambient temperature (T_∞, K)	300
	Rosseland extinction coefficient (m^{-1})	$1.738x10^4$

Figure 4 shows the profile of the temperature distribution of the reactor. As indicated in Fig. 4, the inner cavity of the reactor is heated when the diffuse solar irradiance intensities have been increased from 80 to 100 kW/m². The higher temperature observed in the front region of the reactor is evident due to the higher emitted radiative heat flux because the solar irradiance is diffused directly at this part, Ref. (Lougou et al., 2018). The high-temperature values and the radiation heat flux distribution obtained could respond to the thermal energy required for carrying out the chemical reaction to produce hydrogen or syngas.

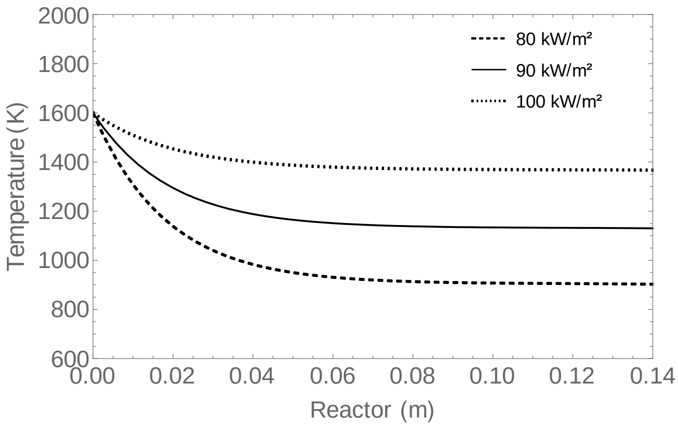

Figure 4. Temperature profile in three values of diffuse solar irradiance intensities.

Figure 5 shows the radiation heat flux along the flow direction of the reactor. The porosity parameter has a robust influence on the extinction coefficient and the heat transfer coefficient of the solar thermochemical reactor. For analyzing this, the effects of porosity on the radiation heat flux distribution were plotted in Fig. 5. Three porosities, 0.7, 0.8, 0.9, were investigated. As can be observed the radiation heat flux increases with the porosity increasing, therefore, has been obtained the maximum temperature with the high porosity value. The Radiation Heat Flux initial with approximately 9100 W/m², 7200 W/m² and 6100 W/m² and with your respective porosity, 0.90, 0.80 and 0.40, stabilizes with 5800 W/m², 4200 W/m² and 3400 W/m². The thickness of thermal non-equilibrium region increases slowly with the porosity increasing, and this phenomenon is also observed in Ref. (Chen et al., 2016).

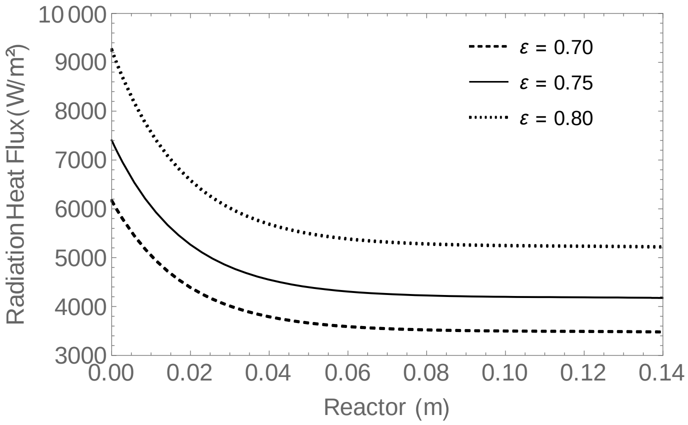

Figure 5. Radiation heat flux profile in different conditions of porosity.

5. CONCLUSION

The thermal performance analysis of a solar thermochemical reactor for syngas production was investigated. This research was carried out numerically through the finite difference method, and *NDSolve* command in the *Mathematica*, the model was validated with the results available in the literature (Lougou et al. 2017). The finite difference method was used to transform the PDEs into ODEs and with *NDSolve* was obtained the temperature profile and the radiation of solar thermochemical reactor. The following conclusions have been drawn:

(i) The radiation heat loss on the fluid inlet surface cannot be neglected during the thermal performance analysis of porous media receiver,

(ii) The maximum radiation heat flux increases with porosity increasing. Its initial values are approximately 9100 W/m², 7200 W/m² and 6100 W/m² and with your respective porosity, 0.90, 0.80 and 0.40, stabilizes with 5800 W/m², 4200 W/m² and 3400 W/m².

(iii) The inner cavity of the reactor is heated when the diffuse solar irradiance has been increased from 80 to 100 kW/m².

6. ACKNOWLEDGMENTS

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8. RESPONSIBILITY NOTICE