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NUMERICAL SIMULATION FOR HYDROGEN PRODUCTION FROM THE STEAM REFORMING OF TOLUENE IN A FIXED BED MEMBRANE REACTOR

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Abstract. *Nowadays, studies on renewable energy sources are increasingly in focus. Hydrogen is considered an attractive option because it allows getting energy of a clean way. One way to produce hydrogen is biomass gasification. However, within this process, there is the formation of tar, which is a severe impediment among the impurities present in the syngas produced. The steam reforming is a widely known technique for the removal of the tar, avoiding equipment damage, and produce* H_2*. In this sense, this paper presents a numerical simulation of hydrogen production from the steam reforming of toluene in a fixed bed membrane reactor. To carry out a dynamical analysis of the behavior of this reactor, the study of a mathematical model was developed to investigate the dynamic evolution of the temperatures and chemical species present in the reactions of reforming. This model is described by a system of Partial Differential Equations (PDEs) was solved by Coupled Integral Equation Approach (CIEA). The use of a fixed bed configuration makes it possible to obtain an energetically efficient process, capable of separating the main product with no further supporting process or even expensive units, providing a cost-effective approach to produce hydrogen.*

Keywords: *Membrane, Hydrogen, Toluene, Mathematical Model*

1. INTRODUCTION

Energy, Environment, and Economy (E.E.E) are fundamental factors for the development of a society that can be delineated according to the availability of power in the market, the environmental impact of this energy, and its availability to society. However, with the high consumption of fossil fuels, the environmental effects of greenhouse gases and the high oil prices, studies on forms of producing renewable energy gains more and more prominence. Among the areas of research in renewable energy and alternative fuels, hydrogen has great potential because it does not emit CO_2 during combustion and has a higher energy density than any other fuel (Anjos et al. 2018).

Hydrogen can be produced by electrolysis, pyrolysis, redox reaction, biological processes, steam reforming, and others. Currently, hydrocarbon steam reforming is the most widely used process for hydrogen production and useful in syngas production (Anjos et al. 2018). Methane and toluene are examples of hydrocarbons for the reforming reaction. In particular, toluene is a promising option because can be used as tar model compound. Tar is a compound produced in the biomass gasification, which damages the equipment, resulting in various operational and financial losses. In this way, the steam reforming of toluene is quite interesting because it will transform the tar (problem) into a feasible solution for the population (Oliveira and Silva, 2013).

The steam reforming of toluene occurs in a Fixed Bed Reactor (FBR). The FBR is defined by the fluid flow characteristic in the downward co-current direction across the fixed bed of the particles in the continuous phase. This reactor has been extensively used in hydrotreating, hydrodesulfurization in petroleum refining, petrochemical hydrogenation, the oxidation process, and the methods of biochemical and detoxification of industrial waste (Anjos et al. 2017). However, to improve this reactor, the coupling with membrane technology is highlighted in several papers.

The method of membrane reactors has been widely researched, due to the ease of production and the concept of process intensification, that is, production and separation in the same equipment through selective membranes (Carvalho et al. 2018).

Most of the researches have been experimentally and numerically investigated to produce H_2 at a high temperature exceeding 700 °C (Cao et al. 2015). The focus of the experimental studies was to develop the robust catalysts which are resistant to carbon deposition (Lao et al. 2017). On the one hand, conventional industrial FBRs have operated between 808 and 3535 kPa and1073-1273 K, but the equilibrium-limited process can reach a conversion of the hydrocarbon of about 93%. Alternatively, applications of Fixed Bed Membrane Reactors (FBMRs) offer a possible form to overcome this limitation through selectively removing hydrogen from a selective membrane system, resulting in higher conversions of methane at lower temperatures. The most commonly used membranes for removing hydrogen are dense palladium membranes or silver-palladium membranes. These membranes offer high selectivity over other gases because of the selective dissolution of hydrogen atoms into the metal matrix (Silva and Abreu, 2016; Cruz and Silva, 2017).

Therefore, the present objective of this work is to perform the mathematical modeling of the Steam Reforming of Toluene (SRT) to produce hydrogen in a FBMR. The mathematical model is composed of partial differential equations (PDEs) of the energy and mass balance. Through of the Coupled Integral Equation Approach (CIEA), these EDP were transformed into ordinary differential equations (ODEs) and with a software in FORTRAN language, was possible to obtain the evolution graphs of the chemical components of the SRT and the evolution of the temperature in the reactor.

2. PROBLEM FORMULATION

A fixed-bed membrane reactor with the continuous flow was studied. A schematic configuration of the proposed system used in the development of the mathematical model is shown in Fig. 1. The system consists of two concentric tubes, where the external tube is constructed in steel, and the internal tube constitutes the thin Pd-based membrane. The catalyst is placed in the center of the internal tube, forming the fixed bed (internal reaction zone). During the operation, the reaction zone (fixed bed) is continuously fed with a gas mixture (H_2O/ C_7H_8 = 1.71) inlet, while a pressure reduction is applied inside the external tube (external permeation zone) through of an inert carrier gas flow to further the transport of hydrogen flux as from the membrane until at the permeation zone outlet.

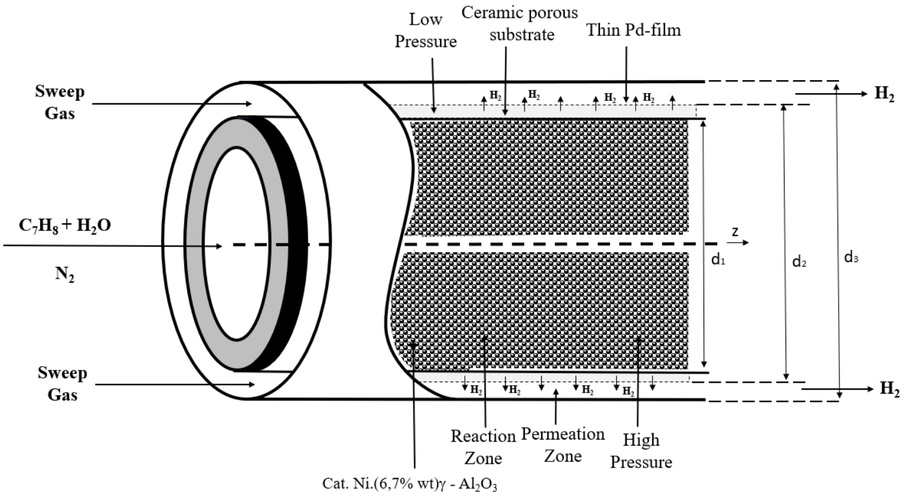

Figure 1. Schematic diagram of a FBMR.

2.1 General equations for the reaction zone

To perform the mathematical modeling proposed in this work, a detailed one-dimensional model is formulated through mass and energy balance equations for a fixed bed membrane reactor. Some considerations are essential to be able to represent the proposed models. In the energy balance, the assumptions considered are: (i) temperature gradients in the axial direction of the FBMR, (ii) temperature gradients in the radial direction of the particle, (iii) in the proposed model, only thermal effects were considered in both phases, (iv) the wall temperature of the FBMR was deemed to be constant and (v) the particle size is uniform. The mass balance equations of the model are based on the following assumptions, (i) the term of accumulation, (ii) convection and (iii) dispersion of the chemical species were considered in the process to have been considered (iv) the rates of the component templates of the reactions. Based on these assumptions, a simplified mathematical model for FBMR is formulated by the simplified mass and energy balance equations that describe the dynamic behavior.

- The energy balance of the gas phase, Eq. (1):

$$\phi_{g\ell}\frac{\partial T_{g,shell}(z,t)}{\partial t}+\vartheta_{g\ell}\frac{\partial T_{g,shell}(z,t)}{\partial z}=\mu_{g\ell}\frac{\partial^2 T_{g,shell}(z,t)}{\partial z^2}-h_{fp}\frac{3}{r_p}(1-\varepsilon_b)\left[T_{g,shell}(z,t)-\mathrm{T}_{\mathrm{s,shell}}(r,t)|_{r=R}\right] \tag{1}$$

Where, $\varphi_{g\ell}$ (Kj/m^{3}K) is the coefficient of the term of thermal accumulation, $T_{gl,\,shell}$ (K) is the fluid temperature, $T_{s,\,shell}$ (K) is the solid temperature ,$\vartheta_{g\ell}$ (kJ/m^{3}K h) is the coefficient of the term of thermal convection, t (h) is the time, z (m) é a coordinate in the axial direction respectively, $\mu_{g\ell}$ (kJ/m^{3}K h) is the coefficient of the term of thermal dispersion, and ε_s (-) is the void fraction of bed.

- The energy balance of the solid phase, Eq. (2):

$$\rho_s\, C_{p,s}\frac{\partial T_{s,shell}(r,t)}{\partial t}=\frac{\lambda_s}{R^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial T_{s,shell}(r,t)}{\partial r}\right]+\rho_S\,(\Delta H_R)\,R_{tol} \tag{2}$$

Where, ρ_s (kg/m^3) is the density of the solid phase, $C_{p,s}$ (kJ/kg·K) is the heat capacity of the solid phase, respectively; λ_s (kJ/m K h) is the thermal conductivity for the solid phase, R (m) is the superficial radius of the solid phase, r (m) is the particle radius, R_{tol} is the global rate of toluene and is detailed in Silva and Abreu, (2016).

- The mass balance of components, Eq. (3):

$$\varepsilon_g\frac{\partial C_i(z,t)}{\partial t}+\varepsilon_g\frac{4Q_g}{\pi d_{shell}^2}\frac{\partial C_i(z,t)}{\partial z}=\varepsilon_g\, D_i\frac{\partial^2 C_i(z,t)}{\partial z^2}+(1-\varepsilon_s)\, r_i \tag{3}$$

Where, i = toluene (C_7H_8), water (H_2O), carbon monoxide (CO), methane (CH_4) and carbon dioxide (CO_2), ε_g (-) is the void fraction of the gas phase, C_i (kg m^{-3}) is the concentration of components, Q_g (m^3/h) is the gas flow rate, d_{shell}(m) is the catalytic reactor diameter, D_i (m^2/h) is the diffusion coefficient of the components and r_i (kg m^{-3} h) is the rate of liquid for each element and detailed too in Silva and Abreu (2016).

- The mass balance of hydrogen, Eq. (4):

$$\varepsilon_g\frac{\partial C_{H_2}(z,t)}{\partial t}+\varepsilon_g\frac{4Q_g}{\pi d_{shell}^2}\frac{\partial C_{H_2}(z,t)}{\partial z}=\varepsilon_g\, D_i\frac{\partial^2 C_{H_2}(z,t)}{\partial z^2}+(1-\varepsilon_s)\, r_{H_2}-\pi d^2{}_{shell}\, J_{H_2}^s \tag{4}$$

Where, J_{H2} is the molar flow of hydrogen in the reaction zone towards the permeation zone.

- The initial and boundary conditions for the mass and energy balance:

$$\left.\frac{\partial T_s}{\partial r}\right|_{r=0}=\left.\frac{\partial C_i}{\partial z}\right|_{z=L}=\left.\frac{\partial T_{g\ell}}{\partial z}\right|_{z=L}=\left.\frac{\partial C_{H_2}}{\partial z}\right|_{z=L}=0 \tag{5}$$

$$\left.\frac{\partial T_{g\ell}}{\partial z}\right|_{z=0^+}=\frac{\vartheta_{g\ell}}{\mu_{g\ell}}\left[T_{g\ell}\big|_{z=0^+}-T_{g\ell}\right];\ \left.\frac{\partial T_s}{\partial r}\right|_{r=R}=\frac{h_{sc}}{\lambda_s}\left[T_{g\ell}-T_s\big|_{r=R}\right];\ \left.\frac{\partial C_i}{\partial z}\right|_{z=0^+}=\frac{4Q_g}{\pi d_c^2 D_i}\left[C_i\big|_{z=0^+}-C_i\right] \tag{6}$$

2.2 General equations for the permeation zone

Hydrogen permeation through a palladium membrane can occur through different forms, depending on the type of membrane. Two assumptions made have been made: the membrane is dense, and hydrogen transport occurs through the solution-diffusion mechanism. In addition to membrane properties, the amount of hydrogen permeating through the membrane also depends on the driving force generated by the pressure differential between the two sides of the membrane.

The recovery of the hydrogen in the permeation zone can be described through the mass and energy balances shown in Eq. (7) and (11), respectively:

$$\frac{dY_{H_2,per.}}{dz} = \frac{2\pi R_m L_z}{\delta_m {F^{in}}_{CH_4}} Q_0\, exp\left(-\frac{E_{H_2}}{RT_{av.}}\right)\left(P^{0.5}_{H_2,per.} - P^{0.5}_{H_2,shell}\right) \tag{7}$$

Eq. (7) has the following boundary conditions:

- At the FBMR's inlet (outside the permeation zone, z=0);

$$\left. Y_{H_2,per}\right|_{z=0^+} = 0 \tag{8}$$

- At the FBMR's outlet (outside the permeation zone, z=L$_z$);

$$\left.\frac{dY_{H_2,per}}{dz}\right|_{z=L_z} = 0 \tag{9}$$

The values of hydrogen recovery make possible to obtain the concentration of hydrogen in the permeation zone according to Eq. (10):

$$C_{H_2,per} = \frac{P^{pep}_{op} Y_{H_2,per}}{RT^{per}_{op}} \tag{10}$$

Eq. (11) is the energy balance in the permeation zone,

$$\frac{dT_{per.}}{dz} = \frac{\pi d_{shell}}{Y_{H_2,per.} F_{H_2,0} C^{per.}_{P,H_2}}\left[\frac{Q_0}{\delta_m}\exp\left(-\frac{E_{H_2}}{RT_{av.}}\right)\left(P^{0.5}_{H_2,per.} - P^{0.5}_{H_2,shell}\right)C^{per.}_{P,H_2} + U\frac{d_{per.}}{d_{shell}}\right]\left(T_{g,shell} - T_{per.}\right) \tag{11}$$

Eq. (11) has the following boundary conditions:

- At the FBMR's inlet (outside the permeation zone, z=0);

$$\left. T_{per}\right|_{z=0^+} = T_{per.,0} \tag{12}$$

- At the FBMR's outlet (outside the permeation zone, z=L$_z$);

$$\left.\frac{dT_{per}}{dz}\right|_{z=L_z} = 0 \tag{13}$$

3. NUMERICAL SOLUTIONS

This paper presents a CIEA-based analytical technique for solving Eqs. (1-4). This method aims to simplify the expressions of energy and mass balances equations of the reactor.

The basis for the CIEA is the Hermite approximation of an integral. The Hermite approximation is a technique to approximate an integral through a linear combination of integrand values and their derivatives. It was originally developed by Hermite (1878) and first presented by Menning et al. (1978). This method allows simplifying a complex problem, so that it can be solved with less effort, as well as to make use of the support of analytical methods. The advantage of this technique, compared to other traditional approximation methods is to obtain a smaller error, resulting in a more accurate solution. This method has been used elsewhere as reported by Anjos et al. (2018), Cardoso *et al.* (2014), Knupp et al. (2012), An and Su (2011), Corrêa and Cotta (1998). This technique is represented by the general expression Eq. (14):

$$\int_{x_{i-1}}^{x_i} y(x)dx \cong \sum_{v=0}^{\alpha} C_v(\alpha,\beta)h_i^{v+1}y_{i-1}^{(v)} + \sum_{v=0}^{\beta} C_v(\alpha,\beta)(-1)^v h_i^{v+1}y_i^{(v)} + O(h_i^{\alpha+\beta+3}) \tag{14}$$

Where,

$$h_i = x_i - x_{i-1} \tag{15}$$

$$h_i = x_i - x_{i-1}\ C_v(\alpha,\beta) = \frac{(\alpha+1)!(\alpha+b+1-v)!}{(v+1)!(\alpha-v)!(\alpha+\beta+2)!} \tag{16}$$

Where, y(x) and its derivatives $y^{(v)}(x)$ are defined for all $x \in (x_{i-1}, x_1)$. Furthermore, it is assumed that the numerical values of $y^{(v)}(x_{i1}) \equiv y_{i-1}^{(v)}$ for v = 0,1,2,3...,α and $y^{(v)}(x_i) \equiv y_i^{(v)}$ para v = 0,1,2,3,..., β are available at the end points of the interval.

This integration formula can provide different approximation levels, from the classical lumped system analysis to improve lumped-differential formulations ($H_{0,0}$, $H_{1,1}$, $H_{2,2}$,…). Since approximations of order higher than $H_{1,1}$ involve derivatives of order higher than one, these are avoided for the sake of simplicity of the technique [18]. Hence, only the two different approximations, i.e., Eqs. (17) and (18) are considered:

$$H_{0,0} \rightarrow \int_0^L F(z,t)dz \cong \frac{L}{2}[F(0,t)+F(L,t)] \tag{17}$$

$$H_{1,1} \rightarrow \int_0^L F(z,t)\ dz \cong \frac{L}{2}[F(0,t)+F(L,t)] + \frac{L^2}{12}\left[\left.\frac{\partial F}{\partial z}\right|_{z=0} - \left.\frac{\partial F}{\partial z}\right|_{z=L} \right] \tag{18}$$

Where $H_{0,0}$ and $H_{1,1}$ represent the trapezial and corrected trapezial rules, respectively.

4.1. Transformed Equation

To solve the equations set, *i.e.*, Eqs. (1-4,) using Eqs (23-25), CIEA method was applied. This method is used to transform the PDE into ODE, considering the initial and boundary conditions. The resulting equations are:

- The transformed equation of the energy balance of the gas phase;

$$\frac{d\bar{T}_g(t)}{dt} = \alpha_{9,g}(T_g,0) - \alpha_{10,g}\bar{T}_g(t) + \alpha_{11,g}\left[\bar{T}_g(t) - \bar{T}_s(t)\right] \tag{19}$$

- The transformed equation of the energy balance of the solid phase;

$$\frac{d\bar{T}_s(t)}{dt} = \beta_{9,s}\bar{T}_s(t) + \beta_{12,s}\bar{T}_{g,0} + \beta_{13,s}\bar{T}_g(t) + \beta_{11,s}\ \bar{R}_{tol} \tag{20}$$

- The transformed equation of components i in the mobile gas phase.

$$\frac{d\overline{C_i}(t)}{dt} = \gamma_{9,g}C_{i,0} - \gamma_{10,g}\overline{C_i}(t) + \gamma_{11,g}\ \bar{r}_i \tag{21}$$

- The transformed equation of components H_2 in the mobile gas phase.

$$\frac{d\overline{C_i}(t)}{dt} = \gamma_{9,g}C_{i,0} - \gamma_{10,g}\overline{C_i}(t) + \gamma_{11,g}\ \bar{r}_i - \pi d^2{}_{shell}\,\bar{J}^{s}_{H_2} \tag{22}$$

The parameters ($\alpha_{j,g}$, $\beta_{j,s}$, *and* $\gamma_{j,g}$) are obtained by replacing the boundary conditions in Eqs. (24) and (25) and applying the integral operator (Eq.23) in the general equation Eqs. (1-4).

$$\frac{1}{L}\int_0^1 F_i(z,t)dz = \overline{F_i}(t) \tag{23}$$

$$F_i(L,t) - F_i(0,t) = \frac{L}{2}\left[\left.\frac{\partial F_i(z,t)}{\partial z}\right|_{z=L} + \left.\frac{\partial F_i(z,t)}{\partial z}\right|_{z=0}\right] \tag{24}$$

$$\overline{F}_i(t) = \frac{1}{2}[F_i(L,t) + F_i(0,t)] + \frac{L}{12}\left[\left.\frac{\partial F_i(z,t)}{\partial z}\right|_{z=0^+} - \left.\frac{\partial F_i(z,t)}{\partial z}\right|_{z=L}\right] \tag{25}$$

4. RESULTS

A dynamic mathematical model was developed to analyze the temperature variations ($T_{g,\ shell}$) in the gas phases, and the temperature ($T_{s,\ shell}$) in the solid phase, as well as the chemical concentration of the components, present in the steam reforming of toluene in a FBMR. In addition, the authors solved the set of equations mentioned in this work with the elaborating of a computational code.

Figure 2 shows the dynamic evolution of the reactor temperature. Noticed that over 3 hours the temperatures follow the same behavior and present values very close, reacher 900 K for the solid phase and 860 K for gas phase, this is important to analyze because the reactor has almost the same temperature and become accessible to control and operate the equipment.

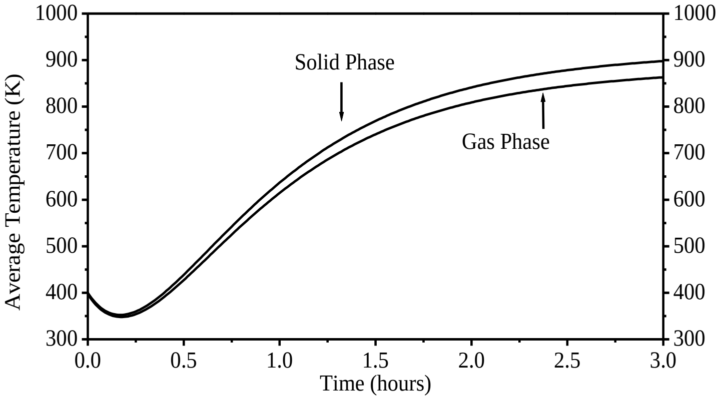

Figure 2. Dynamic evolutions of the reactor temperatures

Figure 3 shows that the dynamic evolutions of the product gas distribution reach stable levels right away the feed is introduced. Usually, it can be seen that about 2 hours of the start of the running of the FBMR initial conditions, all curves describing the product gas distribution achieve to steady-state. During the transient period, it is remarked that as the operation proceeds, methane and toluene are consumed with water available in the inlet gas mixture (steam reforming). Under the prescribed operating conditions, the product gas temperature is about 1128K steady-state, the wet basis products contain about 0.55 kmol/h of H_2, 0.10 kmol/h of CO, 0.45 kmol/h of CO_2, 0.015 kmol/h of CH_4, 0.015 kmol/h of C_7H_8 and 0.17 kmol/ of H_2O.

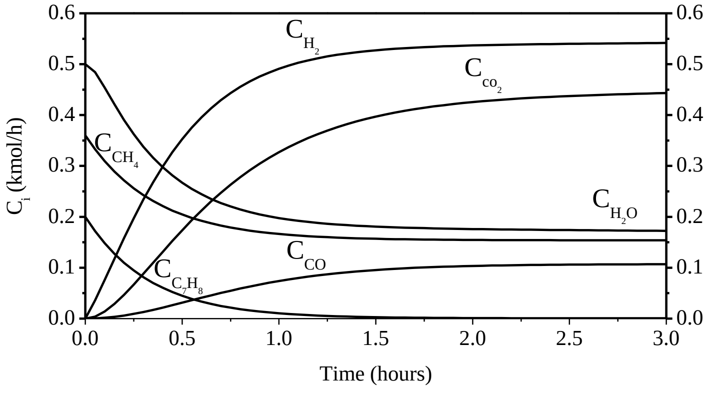

Figure 3. Dynamic behavior of the components of the reaction.

Figure 4 evaluates the effect of different thicknesses for hydrogen production on the permeation side of the FBMR. The hydrogen production increases with the decrease from the thickness of Pd-based membrane. The influence of different Pd-based membrane thicknesses on the FBMR is positive under SRT, and the hydrogen production enhances at low thicknesses. As result mentioned in this figure, thinner film, the hydrogen production increases because of the smaller mass transfer resistance. Another important note is that the effect of thickness is not linear due to mass transfer limitations inside of the FBMR. This result was obtained at 3 hours after the process beginner, the yields of hydrogen reach 3.7, 3.1, 2.6, 2.1 and 1.6 when operating with a thickness from 1.5 μm, 2.5 μm, 3.5 μm, 4.5 μm, and 5.5 μm, respectively.

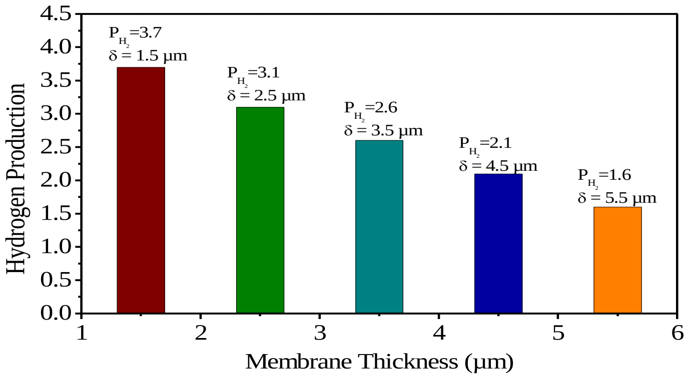

Figure 4. Hydrogen Production for Different Membrane Thicknesses

5. CONCLUSION

This paper reports the study and development of a mathematical model to analyze the hydrogen production process from the steam reforming of toluene using a FBMR. A set of partial differential equations specified the energy and mass balances of the process components, subsequently converted to ordinary differential equations with the CIEA method.

The numerical solution allowed to carry out simulations as well as dynamics analysis of the main behaviors of the variables of this study, resulting in the following observations: (i) After 3 hours, the temperatures follow the same behavior and present values very close, reacher 900 K for the solid phase and 860 K for gas phase, this is important to analyze because the reactor has almost the same temperature and become accessible to control and operate the equipment; (ii) The mathematical model of the steam reforming process for hydrogen production using the FBMR allows determining the optimal toluene conversion throughout operating time; (iii) The study of hydrogen production was performed using different thickness membranes, observing that the hydrogen production increases while the membrane thickness decreases.

6. ACKNOWLEDGMENTS

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