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Use of Synthesis Gas as Fuel for a Solid Oxide Fuel Cell

Jesus A. Alvarez-Cedillo[1*], Teodoro Alvarez-Sanchez[2], Raul J. Sandoval-Gomez[1], Alexis Gonzalez-Vasquez[1], Teresa Sarabia-Alonso[4]

[1] Instituto Politécnico Nacional, UPIICSA, CDMX, Av. Té 650 sn, Col. Granjas México, 08400, México

[2] Instituto Politécnico Nacional, CITEDI, Instituto Politécnico Nacional 1310, 22430 Tijuana, B.C., México

[3] Instituto Tecnológico Superior del Oriente del Estado de Hidalgo, Carretera Apan-Tepeapulco, Las Peñitas, 43900 Apan, Hgo., México

[*] Corresponding author's email: jaalvarez@ipn.mx

ABSTRACT

There is a real need to use various efficient energy supply systems that are not aggressive towards the global environment. Hydrogen has been seen in different research papers presented in the literature as an essential fuel to generate energy in various energy storage systems. As it is well-known, it is possible to generate renewable electricity using electrolysis. The hydrogen produced can be sold as fuel for various systems, most notably its use in solid oxide fuel cells and a host of modern applications today. Current low-temperature fuel cells are ideal for hydrogen operation, but are not suitable for hydrogen mixtures. In this article, a mathematical analysis was carried out to generate electrical energy in a fuel cell, fed with synthesis gas from the residual biomass gasification process; the primary interest was the generation of electrical energy, solid oxide fuel cell (SOFC), which operate at the temperature of the gas at the outlet of the gasifier were analyzed. The practical efficiency obtained and the theoretical results of the SOFC operation were shown.

Keywords: anode, cathode; electrolyte, biomass, syngas, solid oxide fuel cell, mathematical model, steady state.

INTRODUCTION

The growth of the world population brings a problem of energy consumption; electric power has presented an increase in its demand in recent years due to the increase in the devices connected to the internet and the rise of smart devices. The need to meet this demand has led researchers to seek alternative ways and energy sources to the conventional ones. Fossil resources are not present on earth, and their exploitation generates such effects as acid rain, photochemical smoking, and global warming from the release of gases (Haile 2003). New energy production alternatives should be less aggressive towards the environment. Solid oxide fuel cells experience a rise in popularity and constitute a new opportunity to use alternative sources to the conventional ones published in the literature (Zhu and Deevi 2003), (Evans et al. 2009), (Mahmud, Muchtar, and Somalu 2017).

Solid oxide fuel cells (SOFC) are devices used to transform renewable energy sources such as biomass into electrical energy (Ivers-Tiffée, Weber, and Herbstritt 2001). SOFCs have a theoretical efficiency of 100% that favors their operation and application; it commonly works with hydrogen as fuel (Buonomano et al. 2015). In this article, the synthesis gas obtained from the uncooled biomass gasification process is used as fuel, because high temperature is required for its feeding; the authors' proposal avoids the increase in operating costs, and focuses on the analysis of a mathematical model for the design of a fuel cell (SOFC).

It was studied how the production of electrical energy was favored by the composition, the operating temperature, and the reactions that take place inside the anode flow channel to produce hydrogen, resulting from the Nernst equation that allows calculating the reduction potential of the

electrodes, which were compared with the results obtained with literature; the convenience of its implementation was shown (Schlichting, Padture, and Klemens 2001).

MATERIALS AND METHODS

The materials that are part of the presented design comprise the following components: anode, cathode, and electrolyte. The electrolyte can be made of different ceramic materials. In the literature, the material used in non-porous solid electrolytes is combinations of oxides, the most widely used material being yttria-stabilized zirconia (YSZ) (Hayashi et al. 2005), which is commercially available and inexpensive. Studies have been carried out with other combinations of oxides, such as samarium-doped cerium oxide (SCD), bismuth yttrium oxide (BYO), or lanthanum gallate ceramic (LSGM) which have better ionic conduction than YSZ and they work best at the temperature threshold used (Zhang 2014), as shown in Figure 1.

In the literature found for the electrical conductivity of YSZ (Guazzato et al. 2004), its relationship with the size of the grain was investigated. It was concluded that the grain sizes of the electrolyte equal to 0.1–0.4, 0.3–1.5, 1–5, and 8–15 μm could be used in the SOFC when the cell operating temperature is high (850°C, 1000°C), as the conductivity does not differ between grain sizes. The temperature of 1250°C, it is appropriate to use a grade size between 8–15 μm. The electrolyte properties, especially that of the intergranular region, affect the general conductivity of this significantly; in some cases, when the electrolyte presents poor conductivity, it is due to the low conductivity of the intergranular region (Ud Din and Zainal 2016), (Doherty, Reynolds, and Kennedy 2010).

The conductivity of the interior of the grain is usually two or three times greater than that of the grain limit, due to two factors initially, the first the formation of impurity phases near the grain limit, which have a more intricate appearance when the SOFC operates at low temperature and second, the conduction of oxygen ions is less at the grain boundary due to the decrease in the oxygen vacancy concentration in that same place. The intergranular region thickness decreases along with the grain size YSZ decreases.

Cathode materials

The material used was strontium-doped lanthanum magnetite (LSM). The SOFC operates at high temperatures; for this reason, the only materials used for the cathode are noble metals or conductive oxide. Noble metals are expensive and do not have long-term stability; for this reason, they do not have a practical application in the cell. Heterometallic oxides are the only options. However, it is possible to find several options, such as lanthanum magnetite doped with strontium (LSM), perovskite-type lanthanum strontium manganite, and lanthanum calcium manganite (LCM). Lastly, maintain an excellent thermal expansion in its

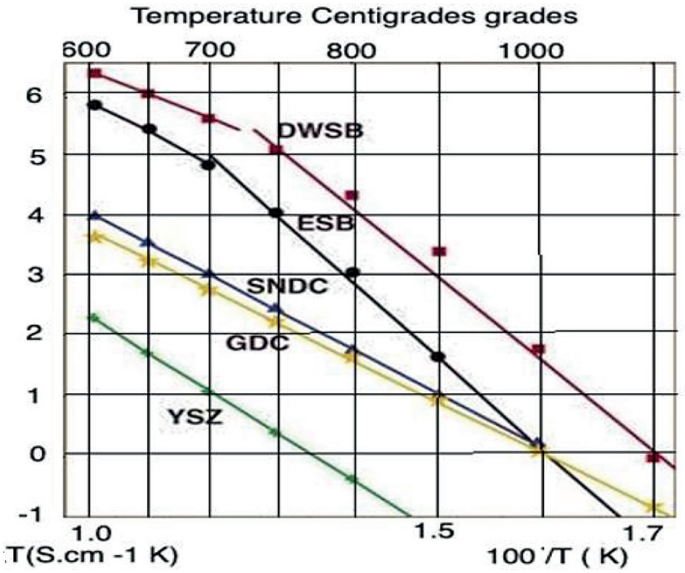

Figure 1. Ionic conductivity of electrolytic materials as a function of temperature.

properties when it is used as a zirconia electrolyte and presents good performance when operated at temperatures higher than 800°C in the ANODE (Fryda, Panopoulos, and Kakaras 2008).

Materials

The material used was Ni-ZrO_2 (Cermet); the anode material is a metal and should not be oxidized due to the fuel composition change during the cell. The anode material is composed of electrolytic material (YSZ, GDC, or SDC) and nickel oxide (NiO), reduced to metallic nickel, which currently inhibits metallic particles, providing a coefficient of thermal expansion similar to that of the other cell materials. When using YSZ as the electrolyte material, NiO/YSZ is the suitable material for the anode , but if the electrolyte material is based on ceria, the anode materials are NiO/SCD and NiO/GDC.

Geometry of the cell

The planar geometric of the Solid Oxide fuel cell is commonly used since its manufacture is not complicated, and it has lower ohmic resistance in the electrolyte, reducing energy losses, and being reflected favorably in the potential of the cell (Buonomano et al. 2015), (Bang-Møller and Rokni 2010), (Bove and Ubertini 2006). Figure 2 shows the typical configuration of a planar SOFC.

Current density

The current density is given owing to the transfer of ions or electrons from one side of the cell to the other concerning the flow; it is the partial density obtained by the fuel cell and is measured by the unit of the area (Panopoulos et al. 2006). See Figure 3.

Table 1 shows the input values of the proposed current density.

Mathematical model

The mathematical model is carried out by considering the balance of matter, energy, momentum, and species using the conditions and the previously-raised parameters. The considerations for the solution of the mathematical model are the following: Steady-state condition; The fuel cell operates at constant pressure and temperature (isothermal); There are no pressure drops in the electrolyte; There is variation in the hydrogen concentration in the anode flux channel and the model; there are no parallel reactions at the limit boundary of the three phases; methane reforming and water displacement reactions are considered; the velocity is constant in the two flow channels; the momentum balance is not considered and the energy balance is not evaluated, because it is an isothermal system (Doherty, Reynolds, and Kennedy 2015). Table 2 shows the values obtained for the solution of the mathematical model.

Two types of continuous models apply to Solid Oxide fuel cells: the quasi-homogeneous, and the heterogeneous. For this mathematical model's solution, a heterogeneous model with a heterogeneous solid phase was chosen, to which simplifications were made to reach the convergence of the method. It was carried out with a Newton Raphson numerical method, control volumes, and finite differences.

When there is a concentration gradient, there is a mass transfer, i.e. the transport phenomenon that occurs between two analyzed points, and the mass transfer can be classified into two phenomena: Convective phenomenon, i.e. the convective mass transfer occurs when the substance that is transported from one point to another is

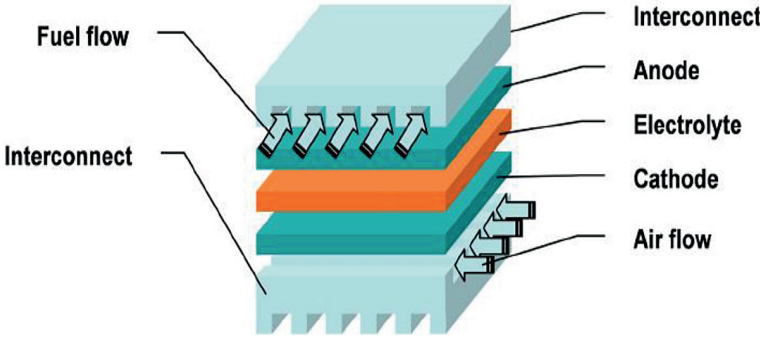

Figure 2. Planar configuration of the SOFC (Buonomano et al. 2015).

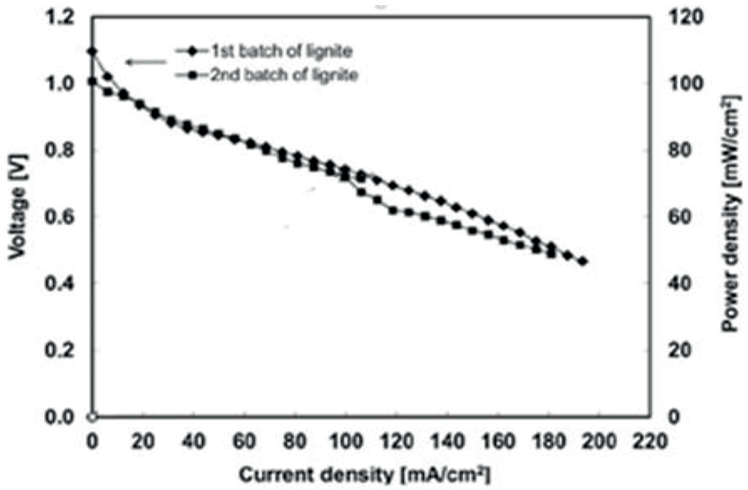

Figure 3. The variation of current density along the axial length of the SOFC at y = 0yz = 0 at a voltage of 0.73V

influenced by the components present in the fluid and the medium in which it diffuses and diffusive phenomenon, i.e. diffusive mass transfer is the step molecule by molecule of a substance neglecting the medium in which it diffuses.

Solid Oxide fuel cells as a whole can be modeled by the diffusive phenomenon by the cell configuration, although the convective phenomenon can be used in the cell for mass transfer of the flow channel and the diffusive one for the porous medium electrodes.

RESULTS AND DISCUSSION

The following shows the results obtained in the behavior of the synthesis gas concentration profiles at the anode and interface, and the air at the cathode. The synthesis gas concentration profile calculation was performed using Fick's Law for binary diffusion, considering the considerations established above for the cell's section corresponding to the synthesis gas. The material balance was carried out for the syngas flow channel and the anode, based on diffusive, and convective phenomena. The cell sections concentration profiles were calculated; the nodal analysis makes it possible to solve the hydrogen concentration profiles through the length of the electrode. Figure 4 shows the three concentration profiles of nodes 1, 6, and 11, where the behavior of fuel during its journey through the cell can be seen.

The hydrogen composition that enters the anode flow channel is 0.2037; this amount of hydrogen is fed to node 1, where a part of it diffuses, and then another goes to the next node. The diffused hydrogen leads to the electrolytic reaction at the interface, and the methane reforming reaction and water shift (toilet gas shift) are generated in the anode flow channel. The change in

Table 1. The behavior of the input values throughout the study is shown. Source: Our elaboration.

Input	Value
Output temperature	850.2 °C cell
Pressure	1 bar
Active surface area	100 cm^2
Anode current density exchange	0.78 A/cm^2
Density change cathode current	0.12 A/cm^2
Anode gaseous diffusivity	0.2 cm^2/s
Cathode gaseous diffusivity	0.05 cm^2/s
The temperature difference between outlet and inlet	120 °C
Anode	500 µm
Thickness electrolyte	10 µm
Thickness cathode thickness	50 µm

Table 2. Parameters for the mathematical model solution

Parameters	Value
Operating temperature	850.2 – 1000 °C
Current density	850 to 3200 A/m^2
Pressure	1 atm
Flow	104 cm^3/h
Volumetric anode material	N_i/ ZrO_2-Y_2O_3
Electrolyte material	0.2 cm^2/s
Cathode material	0.05 cm^2/s
The temperature difference between outlet and inlet	120 °C
Anode	500 µm
Thickness electrolyte	10 µm
Thickness cathode thickness	50 µm

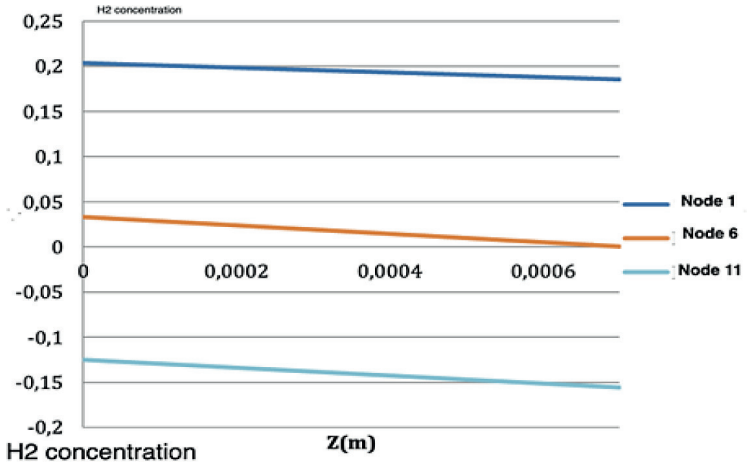

Figure 4. Concentration profiles of nodes 1, 6, and 11

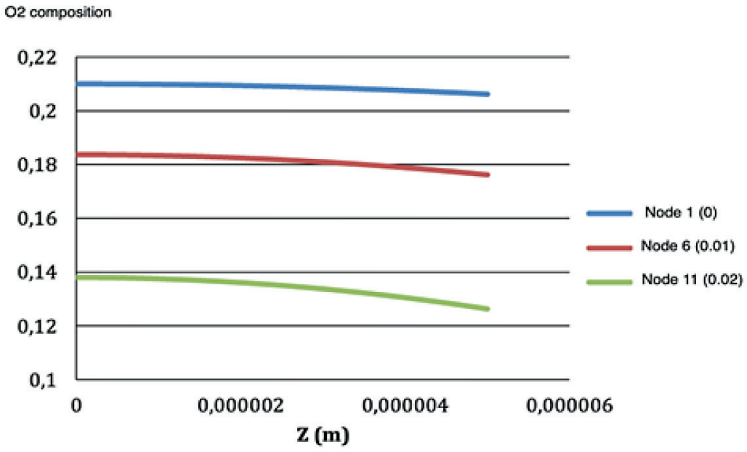

Figure 5. Nodal composition of oxygen

hydrogen composition at the beginning, middle, and end of the cell concerning the thickness of the anode (0.0007m) is demonstrated, where at the end of (node 6), negative composition values begin to be obtained, that is, the hydrogen was wholly consumed before reaching node 7.

This result is attributed to several factors; The first is the Knudsen diffusivity, which makes the amount of hydrogen diffused by each node is more significant, and therefore the concentration at the entrance of the following nodes is drastically reduced; the second is that the reaction by the two secondary reactions does not represent a change that was considered significant.

The current density applied in a cell is lower (1000–3000 A/m^2) than a Solid Oxide fuel cell (it can reach 11000 A/m^2). The air that enters the cathode flow channel has a composition of 0.21 for oxygen and 0.79 for nitrogen; as previously said, nitrogen acts as inert in this reaction, so it is not considered. Figure 5 illustrates the behavior of the composition profile at the cathode.

In Figure 5, it is shown that the behavior of oxygen during the entire length was 0.02m in the cell, and these decreases; for the concentration profile of the cathode, no negative values are obtained, oxygen is not consumed. It is possible to observe that in the last node, the final oxygen composition is close to 0.12. The composition of oxygen has an adequate decrease due to the constant diffusivity, because a binary mixture is not present, the oxygen is pure, and there are no reactions yet.

In this work, little significant changes were obtained in the composition of hydrogen, but an increase in the cell potential (1.12 V) is observed, compared to some works shown in the literature (Lim et al. 2008; Burt et al. 2004), which was 0.52 V. From the mathematical model solution, it was possible to analyze the behavior of synthesis gas and oxygen, with the diffusive phenomenon in porous media (electrodes) using Fick's Law, where the initial composition of hydrogen in the synthesis gas is 0.2037 (node 0). When reaching

node one at an exact length of 0.000362 m, the hydro-gen has a composition equal to zero; that is, it was completely consumed.

CONCLUSIONS

The above happened due to the previous general considerations shown for the solution of this mathematical model. However, the model obtained differs from the reality, because the proposed model was evaluated in a steady-state, which is one of the main reasons why the cell does not present a possible result for the initiation of tests at the laboratory level, and the cell operates continuously. The current density ranges (700 to 3000) established for this model's solution are a parameter that affects the result obtained, since the amount of energy generated by the cell depends on this. In the comparison between the potential generated by a fuel cell under the established conditions and when using a gasifier engine, the power of the 64-cell cell was equal to 3762.6 W, and that of the engine is 15000 W. This is why the battery is 12.24 times more expensive than the motor. The efficiency of the cell with an internal combustion engine is found in the literature, where the efficiency of the cell is 65%, and that of the engine did not exceed 32%; however, the results of the obtained model do not make the SOFC. A viable device in economic terms, this is due to the considerations that were made in this mathematical model, since the energy balance is not assumed. The cell operates continuously, but for this model, it was assumed stationary.

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