What is a fuel cell environmental sciences essay

Abstract

In present literature review presented the technology of fuel cells. The types of fuel cells, their main components, their advantages and applications are discussed. Moreover, the necessity of modeling fuel cells, their advantages and their approaches are explained followed by some examples of modeling. In the last part of the literature review presented previous models of DEFCs

Introduction

The pollution produced from the use of fossil fuels is continually increasing. The use of fossil fuels affects the environment in many ways. First of all the carbon dioxide diffused in the atmosphere while burning fossil fuels to produce electricity and/or heat remains one of the most major sources of environment infection (air pollution and greenhouse gas problems)[1, 2] Secondly the heavy use of fossil fuels lead to heavy concentrations of pollutants in air and water. Moreover, it is clear that in the near future the " traditional" power sources such as oil, constantly reducing. The gap between power demand and power supply shall be filled by other kind of sources. The increasing pollution in addition to the increasing/fluctuating prices of fossil fuels led to the effort of finding alternative sources to produce energy. More specifically, this effort focusing on renewable or alternative energy sources such as wind, solar, tidal energy, energy produced from fuel cells and other kind of sources. This literature review is focusing on fuel cells; their fundamentals and more specifically direct ethanol fuel cells, which are a clean, environmental friendly source, which does not pollute the atmosphere with greenhouse gasses. Moreover, and will be developed a model for a direct ethanol fuel cell in order to find these parameters that effect the efficiency of this kind of fuel cell.

What is a fuel cell

During last decades, fuel cells attracted significant attention from the scientific community. This is happening because of fuel cells are counted as a good replacement of other energy storages like batteries [3, 4]. The operation of a fuel cell is common to the operation of a battery as it converts chemical energy into electrical energy. The basic difference between them is that a fuel cell will produce electricity as last as long as a fuel (hydrogen, methanol, ethanol, etc) and an oxidant (oxygen) is provided [5] In contrast, a battery produce electrical power through chemical reactions between the materials that already are in it. So a battery can be discharged when these materials depleted. In other words, fuel cell is a device that converts chemical energy into electrical energy by using a fuel. Furthermore, producing electrical energy from chemical energy is different between a fuel cell process and the electricity generation from fuels. The typical process to produce energy from fuel is the following [6] : Chemical energy is converted to heat through the combustion of fuelHeat is boiling water to generate steamThermal energy is converted to mechanical energy through the use of a turbineMechanical energy with the help of a generator is producing electricityA fuel cell has the same result (converts chemical energy into electrical) in only one step.

Components of a fuel cell

A fuel cell basically composed from an anode electrode, a cathode electrode, a proton exchange membrane, a diffusion layer and a catalyst layer. Fuel is provided in the anode and then the moles of hydrogen are diffused to electrolyte where split into protons and electrons with the help of a catalyst. Protons and electrons transfer from the anode to the cathode following different ways. Electrons travel to cathode through an external circuit while protons travel through the membrane. The membrane has this unique capability to allow protons to pass through it but does not allow gasses [6]. At the cathode, where oxygen is provided, protons and electrons with the help of the catalyst react with oxygen producing water, which has to be removed out of the fuel cell. The diffusion layer is from electrically conductive material and it has porous in order to allow electrons produced in anode to travel to cathode. All the above can be summarized to figure 1 where a hydrogen fuel cell and a direct ethanol fuel cell are presented.

Figure 1. Hydrogen Fuel Cell [7]

Types of Fuel Cell

Fuel cells continue to develop for many years. This in turn led to the development of different types of fuel cells. The basic differences between these different kinds of fuel cells are the material of the chosen electrolyte and the temperature that they operate. Due to the different electrolyte, there are differences to the ions that are being produced. The nature of produced ions and the choice of the fuel determine the chemical reactions of anode and cathode. Basically, fuel cells taking the name of the electrolyte that they use.

Alkaline Fuel Cells (AFC)

Alkaline fuel cells were one of the first types that developed. NASA used them into the Apollo program in 1960. As electrolyte in AFCs is used aqueous potassium hydroxide (KOH) while as catalysts can be used some noble metals [8]. The temperature to operate a AFC is between 50 oC and 250 oC. The newer generation of AFCs operating from 23 oC to 80 oC. At higher operation temperatures (250 oC) the concentration of KOH is 85 wt% while in lower temperatures (below 120 oC) the concentration of KOH 30-50 wt% [6, 9]. The chemical reaction that taken part in an AFC are the following: At the anode (oxidation): At the Cathode (reduction): Overall reaction equation: In figure 3 the above reaction are being explain graphically. Macintosh HD: Users: billtrias: Downloads: AFC schematic diagram. jpgFigure 2: Schematic diagram of an Alkaline Fuel Cell [10]

Phosphoric Acid Fuel Cells (PAFC)

As indicated by the name the electrolyte is phosphoric acid in highly concentrated form. Furthermore, the electrodes are made by carbon, which has a small quantity of platinum. The operating temperature of PAFCs ranges from 175 oC to 200oC. This type of fuel cells is usually used for stationary application although it might use in big vehicles such as buses. The main reason is that these fuel cells are heavy and big constructions. Moreover, they are more resistant to CO than Proton Exchange Membrane but they have less current density. The electrochemical reactions occurring in PAFCs are: At the anode: At the cathode: The overall cell reaction is: Macintosh HD: Users: billtrias: Downloads: Phosphoric acid fuel cell (PAFC)—principle of operation . gifFigure 3: Phosphoric acid fuel cell (PAFC)—principle of operation [11]

Molten Carbonate Fuel Cell (MCFC)

This type of fuel cell is operating in high temperature (620 oC- 660oC), and can use as fuel carbon. Because of the high operating temperature give the advantage to use of cheaper catalysts. On the other side, high temperature affecting the cells lifetime due to the accelerated corrosion of fuel cell components. A MCFC produces current density 0. 16 A/cm2 and voltage 0. 75V. The electrodes are made from nickel while the electrolyte is made from a molten carbonate salt mixture an electrolyte composed of suspended in a porous, chemically inert ceramic matrix (LiAlO2). The chemical reactions of the electrodes are: At the anode: At the cathode: Overall reaction: Macintosh HD: Users: billtrias: Downloads: MCFC. jpgFigure 4: Operating principles of a MCFC [12]

Solid Oxide Fuel Cells (SOFC)

This type is a high temperature fuel cell, which use a different type of electrolyte than the other fuel cells. Instead of a liquid electrolyte, in SOFC is using yttrium-stabilized zirconia because of its toughness. Moreover, operating at 1000 oC means it is not needed a metal catalyst. Solid oxides form hydrogen ions, which react with carbon monoxide and hydrogen, releasing electrons. The reactions taking place in a SOFC are: Anode reaction: Cathode reaction: Overall reaction: Macintosh HD: Users: billtrias: Downloads: SOFC single structure. . jpgFigure 5: Planar SOFC single structure [13]

Proton Exchange Membrane Fuel Cells (PEMFC)

Two electrodes and a membrane compose PEM fuel cells. The key in the operation in this kind of fuel cells is the membrane, which is made from perfluorosulfonic acid also known as Nafion. Platinum and a porous carbon electrode coat both sides of the membrane. In this way the gas diffusion is allowed. To allow ions to flow the membrane has to be hydrated at all times, which in turn means that PEMFCs has to operate in less 90 oC. This capability of PEMFCs makes them a very good choice for transport applications instead of the previous mentioned types of fuel cell. Although, operating in lower temperature affecting the efficiency of the fuel cell. Moreover, the operational principals of PEMFCs remain the same, a fuel is feeding to the anode where protons and electrons split and travel to the cathode through different ways. Electrons go to cathode through an external circuit while protons through the membrane. At the cathode oxygen reacts with the protons and electrons to form water. The advantages of this fuel cell technology are: Operates in low temperatuesThey do not produces polluting substances during their operationTheir efficiency is 35-40%Because it is missing movable parts does not produce noiseA PEMFC has a high power density. On the other side, the cost PEMFCs remain high due to the use of platinum which is an expensive and hard to acquire material. Macintosh HD: Users: billtrias: Downloads: Schematic design of the PEM fuel cell. jpgFigure 6: Schematic design of the PEM fuel cell [14]Figure 7 shows a summary of the types of fuel cells in addition to the advantages and disadvantages of each type. Figure 7: Table for different fuel cells with their characteristics [15]

Limitations of fuel cells

Besides the benefits that the technology of fuel cells provides there are still some barriers to overcome to be ready for commercial use. First of all the cost of fuel cells remains high due to the material being used in catalyst. Moreover, when the fuel is not in hydrogen in pure form then it is needed to taken into account the reform of the fuel. In addition to this, the use of non pure hydrogen affect the catalyst which in turn means that the overall performance of the fuel cell is decreasing.

Applications of fuel cells

Fuel cells have the capability to produce power in a range of 1 Watt to hundred of KiloWatts. Due to the high efficiency of fuel cells and the clean energy they produce, they can be used in in a big variety of applications. The most common of these applications are:

Automobiles

Most of car manufactures already have produced prototype cars based on fuel cells and they are planning to produce more in the future [16]. Back in 1994, Ballard and Daimler-Benz built cars powered by PEMFC. The first models were using as fuel pure hydrogen until 1997 where Daimler-Benz introduce a methanol fuel car. Moreover, it is expected that by 2015 more and more manufactures will sell fuel cell powered cars for commercial use. Although, they are needed some hydrogen fuel infrastructures in order to happen this [6, 17].

Portable Applications

Due to high power density that fuel cells can provide they have great potential in portable applications [18]. They can be used to supply with electricity portable devices such as laptops, mobile phones, MP3s and many more. Moreover, they can be used in military applications like portable soldier power, skid mounted fuel cell generators etc [19]. In this category usually used PEMFCs and DMFCs because of their small size in combination with their energy density. For instance, USA army requires power sources, which provide efficiency and reliability for portable power electronic devices that used in battlefield. Moreover, a fuel cell would be able to reduce the burden that a soldier has to carry [18, 20]Macintosh HD: Users: billtrias: Downloads: Fuel cell stack with four cells and 55 W maximum power connected with a dc-converter to deliver 3. 5–15 V. jpgFigure 7: Fuel cell stack with four cells and 55 W maximum power connected with a dc-converter to deliver 3. 5–15V [21]

Stationary applications

In this category belong the back up power supplies (UPS), the Distributed power generators and generally devices that they are not easy to move once they are installed. UPSs are necessary in technologies that uninterrupted power is needed, such as telecommunication and radio towers. A device based on fuel cell technology it could substitute power generators due to the lower start up time that it can provide. In 2000, Ballard with the collaboration of Coleman did the first attempt to construct 1a backup power supply of 1kW [22]. On the other hand, when a distributed power generators applied to a house, they can provide electricity and heat as well if are combined with a boiler [6, 22]. Constructions like this they could be also used in industries, hospitals, companies and institutes to provide uninterrupted electricity. Although, these constructions require the development of a low cost, reliable and efficient inverter and an interconnection system with the electrical network[9]. Stationary units can be used to replace the grid in areas with no grid infrastructure [23]. Figure 8 it is shown the categories of basic applications that fuel cells can be used. Macintosh HD: Users: billtrias: Downloads: Fuel Cell Applications. jpgFigure 8: Applications of fuel cells [22]

Modeling a fuel cell

A mathematical model describes a system or a process using mathematical language or mathematical equations. It makes the system easy to understand and helps in predicting the behaviour. All the laws of physics can be seen as a mathematical model predicting or explaining a particular property of the physical world. A mathematical model describes a system by a set of variables which are related together by set of equations. However a trade-off exist between simplicity and accuracy. If the model is highly accurate, it would be complex and vice versa. They help in the actual design of the system. Also the outputs can be predicted without doing any experiment.

Advantages of modeling a fuel cell

It is easily to understand that a model provides a lot of benefits in the field of fuel cells. Firstly, it can lower the cost and save time due to the avoidance of using inappropriate materials and designs before the physical testing. In addition to this, a model can pinpoint the points that a researcher can focus during his research. Analyzing the results of a model can provide useful information before the design decision. Moreover, it provides an insight view of the fuel cell that otherwise it cannot be studied experimentally such as the losses of the fuel cell. In this way the development of a fuel cell is accelerated and can provide quick results in less time than experiments. Besides the benefits that a model can provide is not a standalone tool or a replacement of experiments. Experimental data is needed to confirm the validity of the model. This paper is going to review some of the modeling of fuel cells.

Background of modeling fuel cells

G. Napoli at al. in [24] developed a data driven model of a PEMFC stack using neural networks (NN). This neural network based model helps on the investigation of the variables for different operating conditions. These kinds of models have as basic privilege the computational characteristics of their elements and their training rules. In addition to this, this approach is usually faster and cheaper than other approaches. Although, data driving models introduce an uncertainty to the prediction, especially for a small number of input and inappropriate data. A different approach of modeling PEMFC developed from Gwang-Soo Kim et al. in [25]. A 2+1D model developed to compare the results from a 3D CFD model. The comparison of these two models shows that the coupling between mass, heat and charge transport is important. A 3D CFD model can be time consuming when it is extensive, despite the computational power of computers these days. Hajimolana S. A. et al in [15] developed a model for the SOFC by taking into account the electrochemical model, diffusion through porous media, mass, energy and momentum conservation balances. For the First principles modelling the SOFC was divided into several subsections. Subsections for the tubular SOFC are: Subsystem 1: Air inside injection tube. Subsystem 2: Injection tube. Subsystem 3: Air inside space between cell and injection tube. Subsystem 4: Cell tubeSubsystem 5: Fuel mixture over the anode side of cell tube. These subsystems are then individually modelled based on electrochemical reactions, diffusions, mass, energy and momentum transfer balances. An analytical model for DMFC proposed by Kulikovsky in [26]. This model takes into account non-Tafel's equation of methanol oxidation. Although in his model is not studied the effect of two phases flow and transport in electrode zones. In Casalegno et al. [27] model, analysed the methanol cross-over and the effect on DMFC performance. As a result is found that the cross-over is constant to diffusion transport and affect the overall cell's performance. Taking this into account, Esmaili in[28] proposed a two dimensional model (1D+1D) , where the cell split in more elements, in order to achieve high accurate data and to examine the effects of the concentration of the reactants and the operating temperature of the DMFC.

Direct Ethanol Fuel Cell Modeling

Direct ethanol fuel cell belongs to PEMFC category that analyzed previously. Instead of pure hydrogen as a fuel is used ethanol . Ethanol is taking a lot of attention as a fuel because of the following reasons: It is non toxicIt is renewableIt is easy to produce in high quantitiesIt has high theoretical mass energy density (8. 00 KWh-1) [29]A schematic design of a DEFC is shown in figure 9. Macintosh HD: Users: billtrias: Downloads: Schematic of a single DE-PEMFC with the operational principles depicted. jpgFigure 9: Design of a DEFC [30]The reactions for a DEFC are as followAnode Reaction: Cathode Reaction: Overall Reaction: A graphical representation of the above reactions can also be seen in the next figureMacintosh HD: Users: billtrias: Downloads: Reaction of DEFC. pngFigure 10: Reaction of ethanol in a fuel cell [31]In [32] Sarris et al. developed a CFD a three dimensional (3D) CFD model for a DEFC, in order to examine the anode flow field. Besides the benefit of low cost that CFD models have, they can easily analyse the flow field in a fuel cell. Furthermore, to achieve insight view of the flow in anode electrode the velocity and streamline distributions were needed. Andreadis et al. [33] developed an one-dimension, steady-state model in order to describe a direct ethanol fuel cell with a Nafion 115 membrane and more specifically the mass transport of ethanol. They used the FORTRAN language to calculate the parameters that affecting the fuel cell performance such as the temperature and the fuel concentration. To validate the results a simulation of the model for a range of temperature taken part (30-90 0C). Figure 11: (exchange current) and (anode charge transfer coefficient) values calculated from the experimental results[33]Finally, they concluded that for temperatures below 75 0C the results between simulations and experiments are almost the same, while at 90 0C there was a deflection. Although this may be due to the one phase model that used. The basic issues of a DEFC are the anode's kinetics and the fuel cross-over. There are studies that instead of Pt catalyst there were used a mixture of Pt-Sn or Pt-Pd alloy. These had as a result anode's oxidation at lower potentials. Suresh et al. in [34] developed a model, which include these parameters. The polarization behavior is shown in figure 11 where the results compared with the experimental results of Song et al. in [35]Macintosh HD: Users: billtrias: Downloads: Cell polarization behavior predicted by the present model (solid lines) and experimental data (markers) for various ethanol feed concentrations and flow rate of 1 ml min−1 at 75 °C and at an air feed cathode pressure of 2 bara. jpgFigure 11: Cell polarization behavior predicted by Shuresh model [34]Ethanol is present in large quantities in sugar rich biomass. Thus is a better choice than methanol in terms of quantity. It is also less volatile and non-toxic. However, to achieve a complete electrooxidation at low temperature, it is needed to beak the C-C bonds in ethanol, which is very difficult. The high anodic over potential is one of the problems in the field of DEFC hampering its growth. Pramanik et al. [36] developed a model considering the over potentials. Activation over potential was modelled by considering electrooxidation mechanism as well as Butler-Volmer equation. Ohmic overpotential is modeled considering the proton conduction by the Nafion membrane and the losses at electrodes, current collectors and electrodes interfaces. The concentration over potential is modeled using Fick’s law, Butler-Volmer equation and transport from electrodes to electrolyte. The predicted value by the model was verified from the experimental data and had minimum variation.

A brief mathematical model of DEFC

There are 3 different losses, known as activation losses, ohmic loses and concentration losses. All the above can be summarized in the following equation: Where:

Thermodynamics laws

As mentioned above, the ideal voltage of a fuel cell can be predicted using the thermodynamics laws. It is supposed that the fuel cell working under ideal conditions and temperature and pressure are constants, and then the Gibbs free energy is:(1)WhereConsidering the first thermodynamic law:(2)And the second thermodynamic law:(3)Combining equations (2) and (3) and replacing them in equation (1) give as a result:

Thermodynamic Voltage

As mentioned above, the reaction of a DEFC needs two stages to be completed. Using the formulaFor each of three reactions give as a result the estimated voltage. Anode Reaction: (Eanode= 0. 084 V vs SHE)Cathode Reaction: (Ecathode= 1. 229 V vs SHE)Overall Reaction: (Ecell= 0. 084V vs SHE)

Activation losses

A fuel cell in order to begin to operate needs energy, for this reason there are losses that called activation losses. These losses can be modeled by the Butler-Volmer equation as shown below: Where: As it shown from the above equations activation losses at the anode and the cathode of the fuel cells have to be calculated separatelyMore specifically, for direct ethanol fuel cells, the activation losses in anode are:(4)Due to the large amount of H_2O, it is assumed that its activity in equation (4) is oneWhile cathode's activation losses are:

Ohmic Losses

In a fuel cell there are ohmic losses in the diffusion layer, in catalyst layer and finally ohmic losses from the membrane. These losses can be modeled using Ohm's law

Anode Ohmic losses

Electrons produced from the oxidation of ethanol on anode catalyst layer will travel to cathode through the gas diffusion layer. On the other hand, protons will flow to cathode through the membrane. So, anode ohmic losses can be split on ohmic losses on diffusion layer and on catalyst layer. Diffusion Layer (only electronic charge transport occurs)Catalyst Layer (Both electronic and ionic transport occurs)

Cathode Ohmic Losses

Electrons will reach cathode catalyst layer through the external circuit and gas diffusion layer, while protons will travel to cathode through the membrane to the catalyst layer. Diffusion layer ohmic losses: Ohmic losses in Catalyst Layer: Membrane Ohmic losses (Only ionic transport occurs)So the total Ohmic losses in a fuel cell are:

Concentration Losses

In a fuel cell the fuel is fed to the anode constantly, an amount of this fuel is diffused at the diffusion layer in order to reach anode's catalyst. So to calculate the activation losses in anode and cathode it is needed to calculate the concentration of the reactants in these electrodes. The equation for the reduction losses at the cathode is:(4)Where: is the catalyst layer volumeis the oxygen concentration at the inlet of the electrolyteis the diffusive boundary layer thicknessis the Electrochemical Surface Areais the oxygen concentration at the GDLis the geometrical surface area of the cathodeis oxygen's diffusion coefficient in (m2/s)At steady state conditions the concentration of oxygen is zero, which in turn means the equation (4) can be written: orUsing the same methodology it is defined that anode concentration of ethanol is: In further research a more detailed model for DEFCs will be presented and implemented in Matlab to simulate different designs and operating variables. In addition to this, the data from the simulation will be used for developing a neural network to predict the performance of a DEFC under different variables.[1]B. Gou, W. K. Na, and B.

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