1 Motivation

The use of fossil fuels to cover the energy demand in the future carries key problems to overcome. The environmental and economic concerns regarding the climate change and the decrease in the oil reserves lead the research and industry to the search for alternatives [1]. The increase in the energy demand due to the economic and demographic growth in the world enhances the necessity of these research efforts. The dependency of several developed countries on the fossil fuel economy and political instability for energy supply enforce the search for the alternatives additionally.

The global energy economy is not going to depend on only one single energy source in order to get a secure energy supply. The product range for the energy supply differs from nuclear power to geothermal energy. But renewable energy sources fulfill the requirements as a long term solution. They are getting incrementally more importance for the energy markets due to the depletion of fossil fuels and environmental concerns. The predicted growth in supply of renewable energy sources reaches an average value of 8.1% p.a. until 2035 [2].

The fluctuations in renewable energy production such as solar, wind and hydropower prevent sustainable energy sources to provide a stable solution to the energy problems [3-7]. Storing the energy produced by renewable sources is a key phenomenon in order to remove production instabilities and is focused by research and industry in last decade in order to achieve the global energy goals. The production and storage of renewable energy are significant issues in order to increase the use of renewable energy applications.

Production of hydrogen is considered as an alternative way for storing the electrical energy produced by renewable sources. Production of hydrogen with electrolysis and storing the produced hydrogen in special tanks or underground are actual research efforts and open the gateway to the hydrogen economy. The hydrogen economy is also feasible via producing the hydrogen from fossil fuels by reforming processes but this doesn’t offer a long term solution.

Fuel cell systems represent a potentially viable option with high level of efficiency for re-electrification of hydrogen [8]. Using fuel cells to utilize hydrogen has high efficiency values depending on the type of the fuel cell [9]. The PEM type fuel cells promise several advantages for fuel cell applications due to the low temperature requirements. Hydrogen can also be converted to electrical energy by using a combustion process. However this reduces the overall efficiency [10].

Several PEM fuel cell systems have been demonstrated in the last decade. Besides the hydrogen supply and the costs for the fuel cell systems, the durability of fuel cells plays an important role for the commercial launch. The mechanical stability of fuel cells leads to a higher level of lifespan due to the durability of single fuel cell components like membrane and gas diffusion layers [11, 12]. It is also required to get an optimal mechanical pressure on the fuel cell components in order to get an optimal efficiency from the fuel cell stack.

The overall aim of this work is to enable the explicit analysis of fuel cell stack designs from a mechanical point of view in order to increase the mechanical durability and reach the optimal performance. Understanding the mechanical characteristics of the fuel cell stacks leads to the dimensioning of the stack components and contributes to the optimization procedure during the prototyping process, which assists in the cost reduction of fuel cell stacks. This also enables to make safe and compact fuel cell stack designs depending on the application, which plays an important role for implementation of fuel cells for stationary and transportation applications. The developed design procedure in this study and the analysis for a specific fuel cell stack can also be implemented both for other fuel cell stacks and similar applications.

2 Introduction

A fuel cell is a device, which converts chemical energy directly to the electrical energy in a single electrochemical step with the help of catalyst. In principle a fuel cell operates similar to a battery. A fuel cell does not require recharging in comparison to a battery. It produces energy in the form of electricity and heat as long as fuel is supplied.

Different from Carnot heat engines, the efficiency of the fuel cells reaches to the theoretical values of $\eta = 83.3\%$ owing to the elimination of the mechanical energy conversion process [9]. There are no moving parts in the fuel cells involved in the production process of electricity which contributes to the higher level of efficiency. A single fuel cell consists of two electrodes sandwiched around an electrolyte layer and produce electrical current principally by consuming hydrogen and oxygen.

2.1 Fuel Cell Applications

Fuel cells are used for several stationary, transportation and portable applications. The power range generated by fuel cells can differ from milliwatts to hundreds of kilowatts. Additionally there are several types of fuel cells with different operating temperature levels and properties (see section 2.2.1) leading to an extended area of potential applications. Principally fuel cells can be used for any power generation application. In this section some selected applications are categorized and given in subsections to provide an overview of the wide range of fuel cell applications and required conditions in order to understand the mechanical requirements of fuel cells.

2.1.1 Stationary Applications

The stationary fuel cell applications denote power generation units for homes, buildings and auxiliary power units etc. The power range of stationary fuel cell applications can be between 0-500kW [19]. Some types of fuel cells are commonly used for stationary applications due to their specific properties as handled in section 2.2.1.

The low dynamic response requirement is the basic characteristic property of stationary applications. Another common property of stationary applications is the usage of natural gas due to the utilization of existing natural gas infrastructure. Two selected examples of different sized stationary applications are given in Figure 2.1 and Figure 2.2. The size, operating conditions and application areas of stationary fuel cells are various, which contributes to diverse mechanical requirements.

Figure 2.1 CalTech, Bloom Energy (Image Courtesy Bloom Energy)

Figure 2.2 Vaillant CHP System (Image Courtesy Vaillant GmbH & Co.KG)

2.1.2 Portable and Transportation Applications

Batteries don't promise sufficient fast recharging time and energy density for long-term operations both of which are key properties for portable and transportation applications. Fuel cells assure a viable option for battery applications in small power range between 0-100W [19]. The implementation of fuel cells in transportation is one of the foremost fuel cell applications. Dynamic response requirements are the main characteristic property of portable and transportation applications. Volume and weight play also an important role as design parameters. Two selected examples from portable and transportation applications are given in Figure 2.3 and Figure 2.4. The product range differs from small sized fuel cells for the recharging of mobile phones to bigger sized fuel cells for power train in automotive applications. The mechanical requirements of these fuel cell applications depend on the type of the fuel cell, size of the fuel cell stack and application based specifications, which can be varied distinctively.

Figure 2.3 Portable fuel cell application (Image Courtesy PowerTrekk)

Figure 2.4 Fuel cell car (Image Courtesy Honda Motors)

2.2 Theoretical Background

Basic theory and structure of fuel cells regarding the issues of this work are handled in this section. For further details it is referred to literature [9, 10, 18-21].

2.2.1 Type of Fuel Cells

Fuel cells can be classified as given in Table 2.1 based on working principle and operating temperature.

Table 2.1 Type of Fuel Cells and Their Properties

Type of Fuel Cell	Electrolyte	Operating temperature	Power level and electrical efficiency	Fuel Transferring ion	Application areas
AFC Alkaline fuel cell	Potassium hydroxide (KOH)	50-200°C	10-100kW 60-70%	Hydrogen OH^-	Space, power generation, military
PEM Polymer electrolyte membrane fuel cell	Sulphonic acid incorporated into a solid membrane	50-90°C	0.01-1000kW 50-68%	Hydrogen H^+	Transport, power supplies CHP, space, military
DMFC Direct methanol fuel cell	Sulphonic acid incorporated into a solid membrane, or Sulphuric acid solution (Nafion, Dow)	50-110°C	0.001-100kW 20-30%	Methanol H^+	Portable electronic systems, mobile consumer electronics
PAFC Phosphoric acid fuel cell	Phosphoric acid (H_3PO_4)	190-210°C	100-5000kW 55%	Hydrogen H^+	CHP, power generation
MCFC Molten carbonate fuel cell	Molten lithium carbonate (Li_2CO_3,K_2CO_3)	630-650°C	1-100MW 65%	Hydrogen CO_3^{2-}	Large stationary power
SOFC Solid oxide fuel cell	Ceramic, solidoxide, zironia (ZrO_2/YO_3)	800-1000°C	0.1-100MW 60-65%	Hydrogen O^{2-}	CHP power generation, transport

There are various fuel cell types mainly categorized with respect to electrolyte, which bases on different transferring ion types. Each of them has distinct advantages and disadvantages upon other ones such as starting time, operating temperature, efficiency and sensitivity to the fuel purity. This leads to different application areas as seen in Table 2.1.

PEM fuel cells have low operating temperature, which makes this type of fuel cells appropriate for a wide range of applications as it can be seen in Table 2.1. Therefore, PEM fuel cells have been widely focused on by researchers because of its high power density and short starting time due to the low temperature requirements. These make PEM fuel cells remarkable also for transportation applications.

2.2.2 Thermodynamics of PEM Fuel Cells

Basically fuel cells are working in a reverse principle of electrolysis. They consume oxygen and hydrogen and produce water and energy in terms of heat and electricity. The basic reactions of a PEM fuel cell can be seen in Eq. 2.1-3. The reactions in Eq. 2.1 and Eq. 2.2 take place at the anode (-) side and cathode (+) side respectively [9, 10].

$$H_2 \Rightarrow 2H^+ + 2e^- \qquad \text{Eq. 2.1}$$

$$\frac{1}{2}O_2 + 2H^+ + 2e^- \Rightarrow H_2O \qquad \text{Eq. 2.2}$$

The overall reaction at cathode side is the sum of both reactions (see Eq. 2.1 and Eq. 2.2) and can be seen in Eq. 2.3.

$$H_2 + \frac{1}{2}O_2 \Rightarrow H_2O + 285.8kj/mol \qquad \text{Eq. 2.3}$$

The overall reaction is an exothermic reaction and releases an amount of energy as it can be seen in Eq. 2.3. The higher heating value of hydrogen $\Delta H_H^o = 285.8\mathrm{kJ/mol}$ is taken into account to calculate the maximum amount of available energy by using liquid water as product [9, 10]. The total amount of available energy cannot be converted to the electrical energy by fuel cell due to the entropies occurring during the reaction. The maximum amount of electrical energy generated in a fuel cell corresponds to the Gibbs free energy ΔG_H^o.

Therefore the overall theoretical fuel cell efficiency can be calculated as in Eq. 2.4 with the help of Gibbs free energy ΔG_H^o.

$$\eta = \frac{\Delta G_H^O}{\Delta H_H^O} = \frac{237.3kJ/mol}{285.8kJ/mol} \times 100 = 83\% \qquad \text{Eq. 2.4}$$

The theoretical potential is calculated as in Eq. 2.5 assuming that all of the Gibbs free energy is converted into electrical energy. n is the number of the participating electrons in the reaction (for $H_2 = 2$). F represents the Faraday's constant ($F = 96{,}485\frac{C}{mol}$), which is a product of the number of molecules per mole (Avogadro's number, $N_A = 6.022 \times 10^{23}$) and charge of 1 electron ($e = 1.602 \times 10^{-19}C$).

$$E = -\frac{\Delta G_H^O}{n \times F} = 1.23V \qquad \text{Eq. 2.5}$$

2.2.3 Operating Principles of PEM Fuel Cells

A single PEM fuel cell has the structure as illustrated in Figure 2.5. The hydrogen consumption side of a fuel cell is negatively charged and called anode. Contrary to anode side, the oxygen consumption side is called cathode and positively charged. A fuel cell consists of numerous components as shown in Figure 2.5. Each of them has significant properties, those affect directly the efficiency of the fuel cell.

The central component of the PEM fuel cell is the membrane, which acts as electrolyte in the fuel cell. The membrane is impermeable to gases and has the capability of transmitting protons. The protons are transferred from the anode to cathode side through the membrane and the electrons are delivered to the cathode side through the external circuit by which it produces electricity as illustrated in Figure 2.5. At the cathode side of fuel cell the protons reunite with oxygen ions to water molecules. The solid state of the membrane at the fuel cell operating conditions assures several advantages e.g. handling and assembling.

The reactions defined in section 2.2.2 take place at the catalyst layers which are located on the surfaces of membrane and consist of platinum particles bonded with carbon nanoparticles.

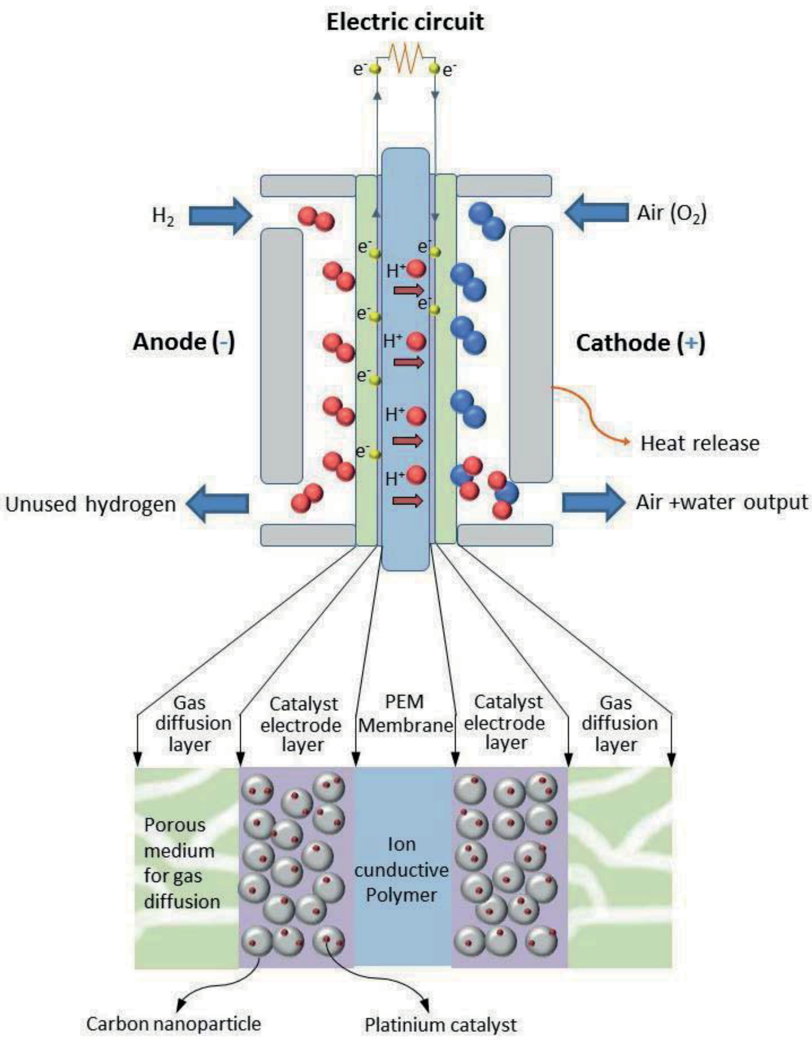

Figure 2.5 The structure and molecular transportation of a PEM fuel cell

The membrane is sandwiched between two porous layers as seen in Figure 2.5, those are electrically and thermally conductive. The porous layers are commonly called GDL (Gas Diffusion Layer) and made from carbon cloth or carbon fiber paper. They are acting as electrodes in fuel cells and have the tasks of gas distribution and transferring the electricity produced in the fuel cell. The porous structure of GDL ensures the uniform distribution of the gases on the entire catalyst surface.

2.2.4 Electrochemistry of Fuel Cells

The basic electrochemical reactions and thermodynamics of a PEM fuel cell are briefly explained before. The polarization curve and electrochemical losses are described in this section to understand the electrochemical characteristics of fuel cells. Further information can be found in literature [9-13, 18, 19].

The polarization curve represents the cell current-voltage relationship and is the most important characteristic property of a fuel cell to evaluate the cell performance. A typical polarization curve is given in Figure 2.6. Mostly the current is also scaled on the membrane active area to get the current density. The current density is a standard comparable quantity for cell evaluation.

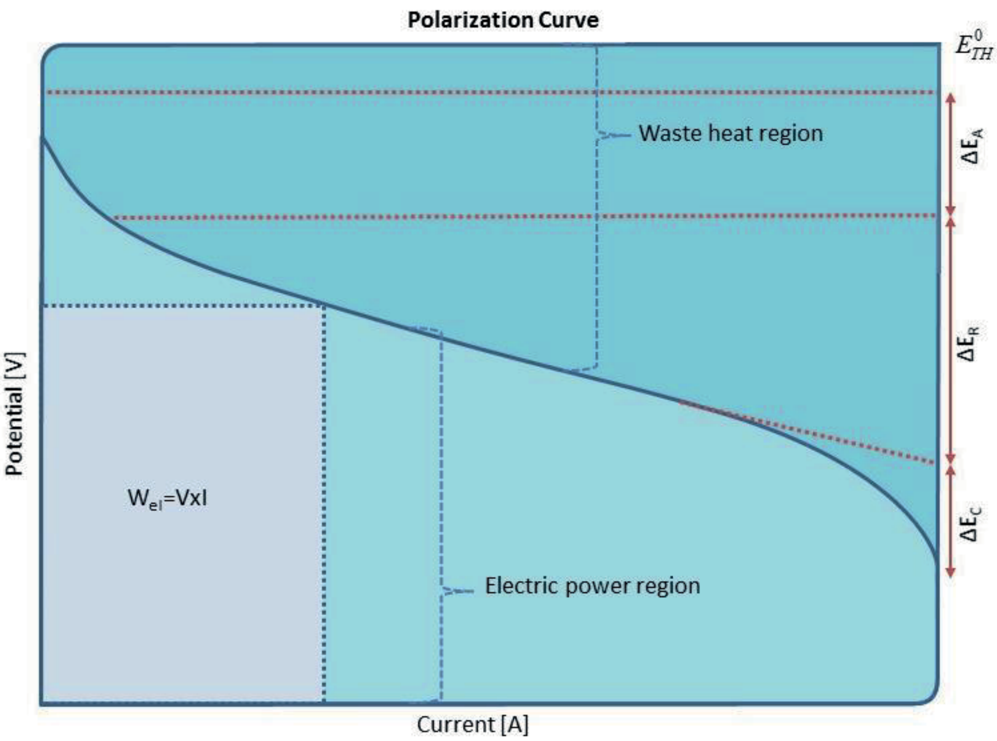

Figure 2.6 Polarization Curve of a fuel cell, schematic diagram

The polarization curve releases essential information for fuel cell analysis. As seen in Figure 2.6, a drop in voltage value is expected as a function of generated current. This occurs due to the irreversible internal losses.

There are several important elements which induce voltage losses during operation of a fuel cell. The three basic ones are ΔE_A, ΔE_R, ΔE_C and illustrated in three different regions in the Figure 2.6. They are also listed in Table 2.2 and analyzed further in the following sections.

Table 2.2 Basic types of voltage losses

ΔE_A	Activation losses
ΔE_R	Resistive losses
ΔE_C	Concentration losses

Understanding the potential losses enables the analysis of the polarization curve structure and the electrochemical behavior of the fuel cell. It is required to conceive the basics of the simulations performed in section 4.3.

The cell potential can be defined as in Eq. 2.6. E_{TH} is the theoretical potential and given as 1.23 [V] in Eq. 2.5.

$$E_{cell} = E_{TH} - \Delta E_A - \Delta E_R - \Delta E_C \quad \text{Eq. 2.6}$$

The area under the polarization curve represents the electric power region. The rest of the available energy is released as heat as depicted in Figure 2.6 and can be calculated by cell voltage value as dealt in section 2.2.5.1.

2.2.4.1 Activation Loss

Under low current operating conditions the activation losses dominate the cell potential as shown in Figure 2.6. The activation loss represents the voltage drop required to initiate the reactions. The activation losses occur at both anode and cathode side of the fuel cell. The cathodic overpotential is significantly higher than the anodic overpotential. Neglecting the anodic overpotential, the activation loss can be defined as in Eq. 2.7 [9, 10].

$$\Delta E_A = \frac{RT}{\alpha F} ln\left(\frac{i}{i_0}\right) \quad \text{Eq. 2.7}$$

R and T represent the gas constant and temperature respectively. α and F are transfer coefficient and Faraday's constant. i and i_0 represent the current density and exchange current density respectively.

2.2.4.2 Resistive Loss

The voltage value drops in a linear behavior at moderate current density region as shown in Figure 2.6. The main contribution is the ohmic resistance of the electrolyte caused by limited proton conductivity. The electrical resistance of the cell components induce an additional voltage drop. The contact between electrical conductive fuel cell components leads to the contact resistance. These result in an overall potential loss which can be calculated using Ohm's law as defined in Eq. 2.8.

$$V = IR_0 \quad \text{Eq. 2.8}$$

The values of electrical and ionic resistance of fuel cell components can be found in section 4.3.2.4.

2.2.4.3 Concentration Loss

The concentration loss denotes the reduction in the reactant concentration on the membrane surfaces due to rapid consumption. The reactant supply on the electrolyte surfaces reaches to its limits to cover the reaction rates at higher level of current densities. This results in a potential drop. Concentration losses dominate the voltage drop at higher current densities and form the tail of the polarization curve as depicted in Figure 2.6.

2.2.5 Operating Conditions of PEM Fuel Cells

Operating conditions of a PEM fuel cell can be specified due to the type of application. Special components and control systems are required to preset the conditions for gas flow, humidifying, cooling etc., mainly for achieving the required power but also the dynamic response characteristics of a fuel cell. The basic operation conditions of a fuel cell are expanded in this section with the interest in understanding of the fuel cell dynamics and simulations made in chapter 4.

2.2.5.1 Operating Temperature

As mentioned before fuel cells release energy in the form of heat and electricity. The amount of available energy which cannot be converted to electrical power is released as heat, which is to be removed from the system to get a stabilized temperature profile in the fuel cell. The heat removal is performed by using a cooling system which depends on the system requirements. Cooling systems of fuel cells are discussed in detail in chapter 2.3.

The optimal operating temperature of a PEM fuel cell can be between 50°-90°C as it can be extracted from Table 2.1. Higher operating temperatures in fuel cells result mainly in higher fuel cell power and efficiency [10, 14, 15]. Nevertheless the highest applicable temperature cannot be inferred due to degradation of the fuel cell [16, 17]. For each fuel cell design and application there is an optimal temperature range. The operating temperature of the standard 50 cm^2 fuel cell design of ZBT is about 70°C.

The generated heat power (Q_{gen}) from the fuel cell can be extracted from Eq. 2.9 [10, 13]. ET_H^0 is the theoretical thermoneutral potential derived from the hydrogen's higher heating value under complete condensation of product water and has a value of 1.482 [V]. V_{cell} and I