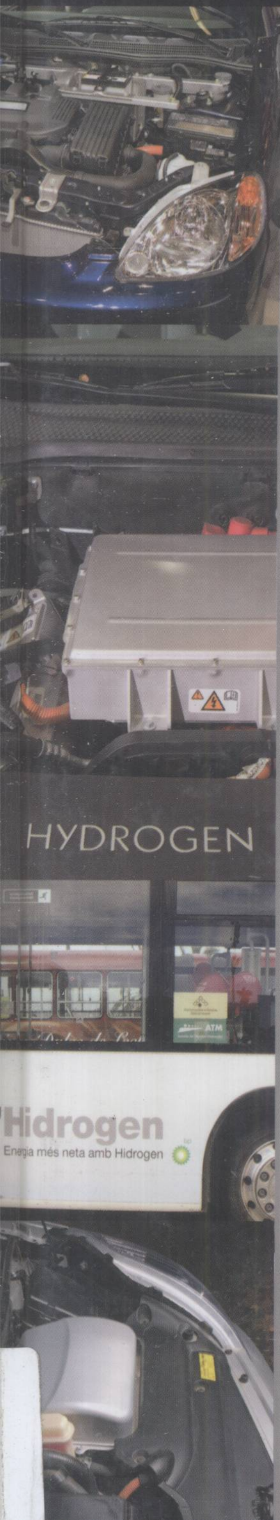
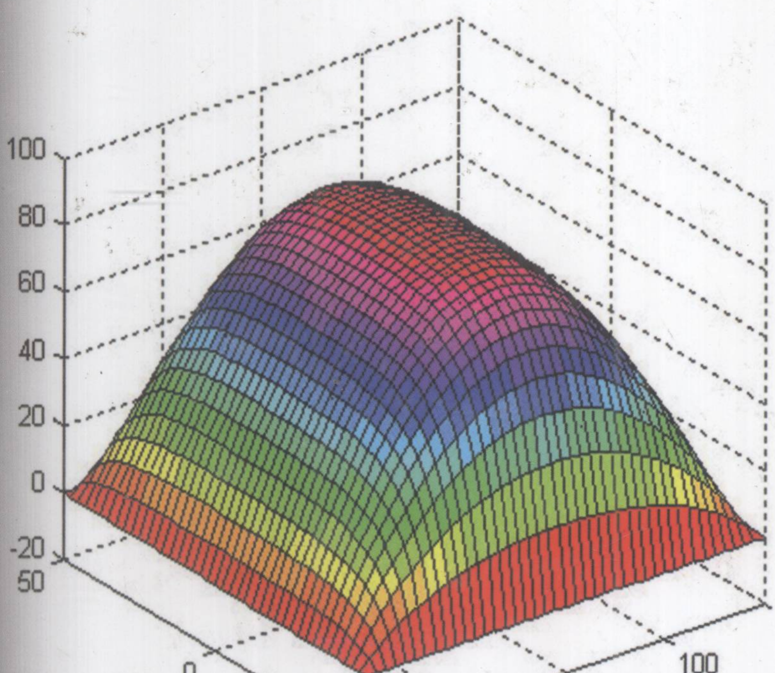
PEM Fuel Cell

Modeling and Simulation Using MATLAB®





COLLEEN SPIEGEL

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Colleen Spiegel

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Contents

CHAPTER 1

An Introduction to Fuel Cells

1.1 Introduction

Fuel cells are set to become the power source of the future. The interest in fuel cells has increased during the past decade due to the fact that the use of fossil fuels for power has resulted in many negative consequences. Some of these include severe pollution, extensive mining of the world's resources, and political control and domination of countries that have extensive resources. A new power source is needed that is energy efficient, has low pollutant emissions, and has an unlimited supply of fuel. Fuel cells are now closer to commercialization than ever, and they have the ability to fulfill all of the global power needs while meeting the efficacy and environmental expectations.

Polymer electrolyte membrane (PEM) fuel cells are the most popular type of fuel cell, and traditionally use hydrogen as the fuel. PEM fuel cells also have many other fuel options, which range from hydrogen to ethanol to biomass-derived materials. These fuels can either be directly fed into the fuel cell, or sent to a reformer to extract pure hydrogen, which is then directly fed to the fuel cell.

There are only 30 additional years left of the supply of fossil fuels for energy use. Changing the fuel infrastructure is going to be costly, but steps should be taken now to ensure that the new infrastructure is implemented when needed. Since it is impossible to convert to a new economy overnight, the change must begin slowly and must be motivated by national governments and large corporations. Instead of using fossil fuels directly, they can be used as a "transitional" fuel to provide hydrogen that can be fed directly into the fuel cells. After the transition to the new economy has begun, hydrogen can then be obtained from cleaner sources, such as biomass, nuclear energy, and water. This chapter discusses fuel cell basics and introduces the modeling of fuel cells with the following topics:

- What is a PEM fuel cell?
- Why do we need fuel cells?
- The history of fuel cells
- Mathematical models in the literature
- Creating mathematical models

These introductory fuel cell topics are discussed to help the reader to appreciate the relevance that fuel cell modeling has in addressing the global power needs.

1.2 What Is a Fuel Cell?

A fuel cell consists of a negatively charged electrode (anode), a positively charged electrode (cathode), and an electrolyte membrane. Hydrogen is oxidized on the anode and oxygen is reduced on the cathode. Protons are transported from the anode to the cathode through the electrolyte membrane, and the electrons are carried to the cathode over the external circuit. In nature, molecules cannot stay in an ionic state, therefore they immediately recombine with other molecules in order to return to the neutral state. Hydrogen protons in fuel cells stay in the ionic state by traveling from molecule to molecule through the use of special materials. The protons travel through a polymer membrane made of persulfonic acid groups with a Teflon backbone. The electrons are attracted to conductive materials and travel to the load when needed. On the cathode, oxygen reacts with protons and electrons, forming water and producing heat. Both the anode and cathode contain a catalyst to speed up the electrochemical processes, as shown in Figure 1-1.

A typical PEM fuel cell (proton exchange membrane fuel cell) has the following reactions:

Anode: $H_2\ (g) \rightarrow 2H^+\ (aq) + 2e^-$

Cathode: $\frac{1}{2}O_2\ (g) + 2H^+\ (aq) + 2e^- \rightarrow H_2O\ (l)$

Overall: $H_2\ (g) + \frac{1}{2}O_2\ (g) \rightarrow H_2O\ (l)$ + electric energy + waste heat

Reactants are transported by diffusion and/or convection to the catalyzed electrode surfaces where the electrochemical reactions take place. The water and waste heat generated by the fuel cell must be continuously removed and may present critical issues for PEM fuel cells.

The basic PEM fuel cell stack consists of a proton exchange membrane (PEM), catalyst and gas diffusion layers, flow field plates, gaskets and end plates as shown in Table 1-1: The actual fuel cell layers are the PEM, gas diffusion and catalyst layers. These layers are "sandwiched" together using various processes, and are called the membrane electrode assembly (MEA). A stack with many cells has MEAs "Sandwiched" between bipolar flow field plates and only one set of end plates.

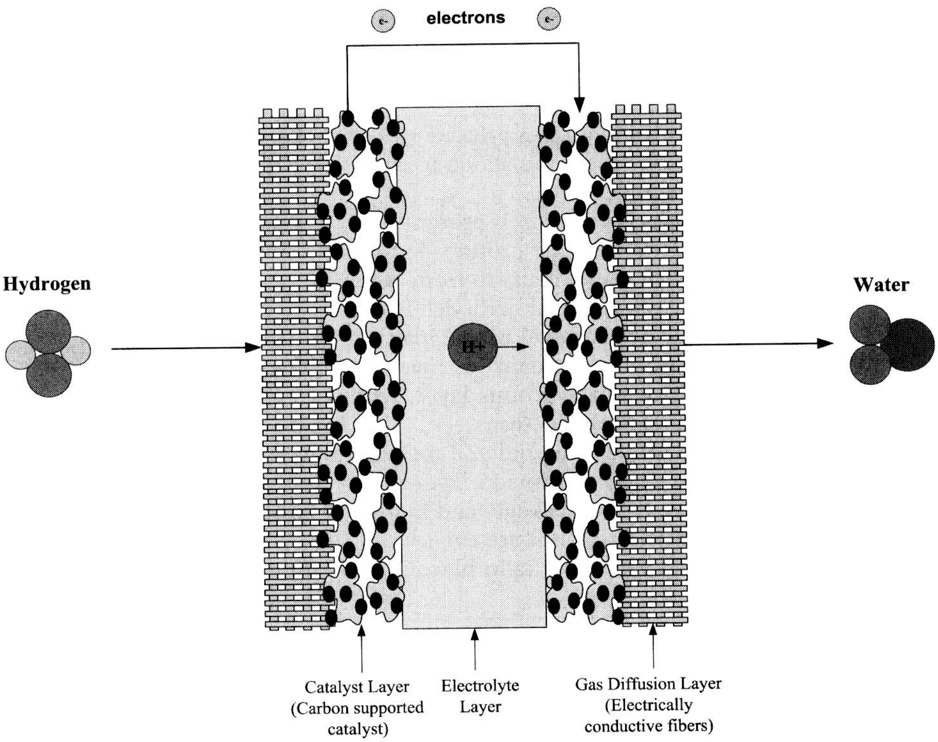

FIGURE 1-1. A single PEM fuel cell configuration.

Some advantages of fuel cell systems are as follows:

- Fuel cells have the potential for a high operating efficiency.
- There are many types of fuel sources, and methods of supplying fuel to a fuel cell.
- Fuel cells have a highly scalable design.
- Fuel cells produce no pollutants.
- Fuel cells are low maintenance because they have no moving parts.
- Fuel cells do not need to be recharged, and they provide power instantly when supplied with fuel.

Some limitations common to all fuel cell systems include the following:

- Fuel cells are currently costly due to the need for materials with specific properties. There is an issue with finding low-cost replacements. This includes the need for platinum and Nafion material.

TABLE 1-1
Basic PEM Fuel Cell Components

Component	*Description*	*Common Types*
Proton exchange membrane	Enables hydrogen protons to travel from the anode to the cathode.	Persulfonic acid membrane (Nafion 112, 115, 117)
Catalyst layers	Breaks the fuel into protons and electrons. The protons combine with the oxidant to form water at the fuel cell cathode. The electrons travel to the load.	Platinum/carbon catalyst
Gas diffusion layers	Allows fuel/oxidant to travel through the porous layer, while collecting electrons	Carbon cloth or Toray paper
Flow field plates	Distributes the fuel and oxidant to the gas diffusion layer	Graphite, stainless steel
Gaskets	Prevent fuel leakage, and helps to distribute pressure evenly	Silicon, Teflon
End plates	Holds stack layers in place	Stainless steel, graphite, polyethylene, PVC

- Fuel reformation technology can be costly and heavy and needs power in order to run.
- If another fuel besides hydrogen is fed into the fuel cell, the performance gradually decreases over time due to catalyst degradation and electrolyte poisoning.

1.3 Why Do We Need Fuel Cells?

Power traditionally relies upon fossil fuels, which have several limitations: (1) they produce large amounts of pollutants, (2) they are of limited supply, and (3) they cause global conflict between regions. Fuel cells can power anything from a house to a car to a cellular phone. They are especially advantageous for applications that are energy-limited. For example, power for portable devices is limited, therefore, constant recharging is necessary to keep a device working.

Table 1-2 compares the weight, energy, and volume of batteries to a typical PEM fuel cell. As shown in the Table 1-1, the fuel cell system can provide a similar energy output to batteries with a much smaller system weight and volume. This is especially advantageous for portable power system. Future markets for fuel cells include the portable, transportation and stationary sectors (basically every sector!). Each market needs fuel cells for varying reasons, as described in sections 1.3.1 to 1.3.3.

TABLE 1-2
General Fuel Cell Comparison with Other Power Sources

	Weight	*Energy*	*Volume*
Fuel cell	9.5 lb	2190 Whr	4.0 L
Zinc-air cell	18.5 lb	2620 Whr	9.0 L
Other battery types	24 lb	2200 Whr	9.5 L

1.3.1 Portable Sector

One of the major future markets for fuel cells is the portable sector. There are numerous portable devices that would use fuel cells in order to power the device for longer amounts of time. Some of these devices include laptops, cell phones, video recorders, ipods, etc. Fuel cells will power a device as long as there is fuel supplied to it. The current trend in electronics is the convergence of devices, and the limiting factor of these devices is the amount of power required. Therefore, power devices that can supply greater power for a longer period of time will allow the development of new, multifunctional devices. The military also has a need for high-power, long-term devices for soldiers' equipment. Fuel cells can easily be manufactured with greater power and less weight for military applications. Other military advantages include silent operation and low heat signatures.

1.3.2 Transportation Market

The transportation market will benefit from fuel cells because fossil fuels will continue to become scarce, and because of this, there will be inevitable price increases. Legislation is becoming stricter about controlling environmental emissions. There are certain parts of countries that are passing laws to further reduce emissions and to sell a certain number of zero emission vehicles annually. Fuel cell vehicles allow a new range of power use in smaller vehicles and have the ability to be more fuel efficient than vehicles that are powered by other fuels.

1.3.3 Stationary Sector

Large stationary fuel cells can produce enough electricity to power a house or business. These fuel cells may also make enough power to sell back to the grid. This fuel cell type is especially advantageous for businesses and residences where no electricity is available. Fuel cell generators are also more reliable than other generator types. This can benefit companies by saving money when power goes down for a short time.

1.4 History of Fuel Cells

William Grove is credited with inventing the first fuel cell in 1839[1]. Fuel cells were not investigated much during the 1800s and most of the 1900s. Extensive fuel cell research began during the 1960s at NASA. During the past decade, fuel cells have been extensively researched and are finally nearing commercialization.

A summary of fuel cell history is given in Figure 1-2.

The process of using electricity to break water into hydrogen and oxygen (electrolysis) was first described in 1800 by William Nicholson and Anthony Carlisle[2]. William Grove invented the first fuel cell in 1839, using the idea from Nicholson and Carlisle to "recompose water." He accomplished this by combining electrodes in a series circuit, with separate platinum electrodes in oxygen and hydrogen submerged in a dilute sulfuric acid electrolyte solution. The gas battery, or "Grove cell," generated 12 amps of current at about 1.8 volts[3]. Some of the other individuals who contributed to the invention of fuel cells are summarized as follows:

1800	W. Nicholson & A. Carlisle described the process of using electricity to break water.
1836	William Grove fuel cell demonstration.
1889	Separate teams: L. Mond & C. Langer / C. Wright & C. Thompson/ L. Cailleteton & L. Colardeau performed various fuel cell experiments.
1893	F. Ostwald describes roles of fuel cell components.
1896	W. Jacques constructed a carbon battery.
Early 1900's	E. Baur and students conducted experiments on high temperature devices.
1960s	T. Grubb & L. Niedrach invented PEMFC technology at GE.
1990s - Present	Worldwide extensive fuel cell research on all fuel cell types.

FIGURE 1-2. The history of fuel cells.

- Friedrich Wilhelm Ostwald (1853–1932), one of the founders of physical chemistry, provided a large portion of the theoretical understanding of how fuel cells operate. In 1893, Ostwald experimentally determined the roles of many fuel cell components[4].
- Ludwig Mond (1839–1909) was a chemist who spent most of his career developing soda manufacturing and nickel refining. In 1889, Mond and his assistant Carl Langer performed numerous experiments using a coal-derived gas. They used electrodes made of thin, perforated platinum and had many difficulties with liquid electrolytes. They achieved 6 amps per square foot (the area of the electrode) at 0.73 volt[5].
- Charles R. Alder Wright (1844–1894) and C. Thompson developed a similar fuel cell around the same time. They had difficulties in preventing gases from leaking from one chamber to another. This and other causes prevented the battery from reaching voltages as high as 1 volt. They thought that if they had more funding, they could create a better, robust cell that could provide adequate electricity for many applications[6].
- Louis Paul Cailleteton (1832–1913) and Louis Joseph Colardeau (France) came to a similar conclusion but thought the process was not practical due to needing "precious metals." In addition, many papers were published during this time saying that coal was so inexpensive that a new system with a higher efficiency would not decrease the prices of electricity drastically[7].
- William W. Jacques (1855–1932) constructed a "carbon battery" in 1896. Air was injected into an alkali electrolyte to react with a carbon electrode. He thought he was achieving an efficiency of 82% but actually obtained only an 8% efficiency[8].
- Emil Baur and students (1873–1944) (Switzerland) conducted many experiments on different types of fuel cells during the early 1900s. Their work included high-temperature devices and a unit that used a solid electrolyte of clay and metal oxides[9].
- Thomas Grubb and Leonard Niedrach invented PEM fuel cell technology at General Electric in the early 1960s. GE developed a small fuel cell for the U.S. Navy's Bureau of Ships (Electronics Division) and the U.S. Army Signal Corps. The fuel cell was fueled by hydrogen generated by mixing water and lithium hydride. It was compact, but the platinum catalysts were expensive.

NASA initially researched PEM fuel cell technology for Project *Gemini* in the early U.S. space program. Batteries were used for the preceding Project *Mercury* missions, but Project *Apollo* required a power source that would last a longer amount of time. Unfortunately, the first PEM cells developed had repeated difficulties with the internal cell contamination and leakage of oxygen through the membrane. GE redesigned their fuel cell, and the new model performed adequately for the rest of the *Gemini* flights. The designers of Project *Apollo* and the Space Shuttle ultimately chose to use alkali fuel cells.

GE continued to work on PEM fuel cells in the 1970s, and designed PEM water electrolysis technology, which led to the U.S. Navy Oxygen Generating Plant. The British Royal Navy used PEM fuel cells in the early 1980s for their submarine fleet, and during the past decade, PEM fuel cells have been researched extensively by commercial companies for transportation, stationary, and portable power markets.

Based upon the research, development, and advances made during the past century, technical barriers are being resolved by a world network of scientists. Fuel cells have been used for over 40 years in the space program, and the commercialization of fuel cell technology is rapidly approaching.

1.5 Mathematical Models in the Literature

Fuel cell modeling is helpful for fuel cell developers because it can lead to fuel cell design improvements, as well as cheaper, better, and more efficient fuel cells. The model must be robust and accurate and be able to provide solutions to fuel cell problems quickly. A good model should predict fuel cell performance under a wide range of fuel cell operating conditions. Even a modest fuel cell model will have large predictive power. A few important parameters to include in a fuel cell model are the cell, fuel and oxidant temperatures, the fuel or oxidant pressures, the cell potential, and the weight fraction of each reactant. Some of the parameters that must be solved for in a mathematical model are shown in Figure 1-3.

The necessary improvements for fuel cell performance and operation demand better design, materials, and optimization. These issues can only be addressed if realistic mathematical process models are available. There are many published models for PEM fuel cells in the literature, but it is often a daunting task for a newcomer to the field to begin understanding the complexity of the current models. Table 1-3 shows a summary of equations or characteristics of fuel cell models presented in recent publications.

The first column of Table 1-3 shows the number of dimensions the models have in the literature. Most models in the early 1990s were one dimensional, models in the late 1990s to early 2000s were two dimensional, and more recently there have been a few three dimensional models for certain fuel cell components. The second column specifies that the model can be dynamic or steady-state. Most published models have steady-state voltage characteristics and concentration profiles. The next column of Table 1-3 presents the types of electrode kinetic expressions used. Simple