

# **Fuel Cell Modeling And Simulation (Renewable Energy)**

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ISLAMIC UNIVERSITY OF TECHNOLOGY (IUT)

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Department of Electrical and Electronic Engineering (EEE)  
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A Thesis Presented to  
The Academic Faculty

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# **Declaration**

This is to certify that the project entitled “Fuel Cell Modeling and Simulation (Renewable Energy)” is supervised by Ashik Ahmed. This Project work has not been Submitted anywhere for a degree.

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# Abstract

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This paper presents a linearized dynamic model of a Solid Oxide Fuel Cell (SOFC) and its performance test under DC operation conditions. The model based on electrochemical, Nernst voltage equations and all voltage losses. The output voltage response of a stand-alone fuel-cell plant to a step load change, a fuel flow step change, and fast load variations are simulated to illustrate the dynamic behavior of SOFC for fast and slow perturbations. However, the partial pressure of the species (fuel, air, and water) in the distributed model is assumed to vary through the length of the fuel cell. After developing a linearized model, we check the stability of our system.

SOFC model is developed on MATLAB environment. The performance of this model is compared with a detailed distributed model and experimental results. A method for interfacing the proposed fuel-cell models to a power system stability package is developed.

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# Chapter 1

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## Introduction

### 1.1 Current Situation and Challenges

The world's primary energy consumption has been increasing steadily since the beginning of the industrial revolution around 1850. Most of today's energy supply is based on fossil resources. Oil has been the most important source of energy since the 1960s. At present, natural gas is the energy source with strongest growth in use, and it may possibly continue this trend and gradually displace the oil in the current and next decade.

Fossil energy sources are finite. First of all this means that they will be depleted one day. Today, many experts and also government representatives are convinced that the global peak in oil production is imminent and will appear during the next five to fifteen years [ASPO 2005]. Already today, the steadily increasing oil price levels indicate that production cannot fully satisfy the world's oil thirst.

Yet another problem bound to the use of fossil fuels is the greenhouse effect. Even though not properly provable, most scientists approve that anthropogenic emissions contribute to global warming, and there is high chronological correlation between CO<sub>2</sub> concentration and global average temperature. An argument of the opponents of greenhouse theory is that anthropogenic greenhouse gas emissions only make a few percent of the natural emissions. However, this can be enough to displace the earth's energy equilibrium. The importance of the magnitude of one percent may become apparent when considering that on a Kelvin temperature scale, one percent temperature increase would already yield app. 3°C. The direct effect of a higher temperature may be a higher frequency of natural disasters such as floods and storms.

Concluding, the challenge the energy sector faces today is to move towards more sustainability and security of supply to avoid the worst scenarios. There are many ways towards this goal. Hence there is not yet a reason to despair, but to hit the road.

## 1.2 Tasks and Trends of the Energy Sector

The means to approximate the goal of a sustainable and secure energy economy may be classified into three groups:

1. Decrease consumer energy demand
2. Increase efficiency of energy conversion
3. Transition to primary energy sources with less carbon content and higher/infinite availability

**The first group** is generally called “energy saving” and is rather socio-political. The main task is to create a consumer’s conscience for rational use of useful energy. This does not necessarily involve a decrease in standard of living, as the possibilities to save energy without even noticing are manifold: Turning off the light and turning down the heating while being away from home is only one example. According to the European Commission's data, total energy end-use consumption in the European Union could be reduced by around 20% without reducing comfort or standards of living [Rothe 2005], and the European Parliament has recently decided a directive for the reduction of consumer energy demand by 11.5% between 2006 and 2015 [EP 2005]. Energy saving behaviour can be and is being effectuated mainly by educational campaigns.

**The second group** attacks at a higher step in the energy supply chain which is only partially the end user’s responsibility, namely the methods of conversion from primary to useful energy. There are several ways for energy conversion; for example electricity from oil can be produced in a gas turbine plant with app. 30% efficiency, or in a combined cycle plant with up to 60%. Furthermore, cogeneration of heat and power concepts improve the energy efficiency as they allow for utilization of the waste heat which is inevitable in thermal power cycles. This is especially facilitated by distributed generation plants situated close to heat and power consumers. An example for conversion from secondary to useful energy is electric heating by either a standard electric oven or a heat pump which provides the same heat at app. 50% less power consumption.

The latter conversion step is usually the end user’s responsibility and can be influenced through governmental stimulation programs, as for example grants on the purchase of innovative technology. Conversion from primary to secondary energy is usually performed in industrial scale and can be influenced through economic measures such as regulation of primary energy prices or the newly introduced emission trading system.

**The third group** is finally the shift of the primary energy carriers. Since the industrial revolution, “decarburization” of primary energy has been advancing by the gradual shift from coal to oil and now from oil to gas. Following this trend, future energy carriers would thus involve even less or no fossil carbon at all, which at the same time is mitigating greenhouse gas emissions. Carbon-free primary energy sources at our disposal are

renewable and nuclear energy. Even though the latter is CO<sub>2</sub>-free, its sustainability is strongly questionable due to nuclear waste and the risk connected to it.

For the transition phase, a further possibility can be to make conventional fuels CO<sub>2</sub>-neutral by capturing and storing the CO<sub>2</sub>. Secondary CO<sub>2</sub>-neutral energy carriers are based on electricity, hydrogen and biofuels.

The task to move towards a CO<sub>2</sub>-neutral energy economy is a long-term and expensive process, but also the only possible path which leads all the way to the final goal of a sustainable and secure energy economy. Hence, it is necessary today to develop and demonstrate the technology and construct the political and socioeconomically road maps towards this goal. At the same time, the previously mentioned methods are required to decrease the total amount of primary energy in need of replacement and therewith the costs.

### **1.3 Role of Fuel Cells**

Fuel cells are electrochemical energy converters and do not underlie the Carnot efficiency law in practice. They offer high electric efficiency (a typical value is 50%, based on LHV) as well as low noise and emission levels and are arbitrarily scalable.

The main benefits of fuel cells here are increased efficiency, especially in part-load operation which is predominant in vehicle propulsion, as well as reduction of emissions and noise. In stationary power production, fuel cells have the advantage that they are saleable and achieve high efficiencies and low emissions even at very small scale. If high temperature fuel cells are applied, carbon containing fuel may be utilized directly or in combination with reformers.

Disadvantages are the high system costs, low fuel flexibility (premium fuel is hydrogen) and sensitivity to impurities. Power generation sectors where an impact of the different types of fuel cells is expected, are portable (electronic devices, small power supplies), mobile (transportation) and stationary (power generation). In the portable sector, fuel cells compete with batteries, and their main benefit is quick refueling and the potential of achieving high energy density. For mobile applications, they compete with internal combustion engines.

Application possibilities of these fuel cells range from heat and power supply for private houses to medium-scale power generation. From a scale of app. 100 kW, they further facilitate the combination with a bottoming thermal power cycle in a so-called hybrid cycle. With up to 70% based on LHV, this method promises higher electric efficiencies than any other electricity generation process at present.

## 1.4 Types of Fuel Cells

There are many fuel cell types, but the principal ones include the Alkaline Fuel Cell (AFC), Proton Exchange Membrane (PEM) fuel cell, Direct Methanol Fuel Cell (DMFC), Molten Carbonate Fuel Cell (MCFC), Phosphoric Acid Fuel Cell (PAFC), and Solid Oxide Fuel Cell (SOFC).

Each fuel cell type has its own unique chemistry, such as different operating temperatures, catalysts, and electrolytes. A fuel cell's operating characteristics help define its application – for example, lower temperature PEM and DMFC fuel cells are used to power passenger vehicles and forklifts, while larger, higher temperature MCFC and PAFC fuel cells are used for stationary power generation.

- **Proton Exchange Membrane Fuel Cell (PEM)**  
Electrolyte: Solid polymer membrane  
Catalyst: Platinum is the most active catalyst for low-temperature fuel cells  
Operating Temperature: 50-100°C  
Electrical Efficiency: 40-60 percent
- **Direct Methanol Fuel Cell (DMFC)**  
Electrolyte: Solid polymer membrane  
Catalyst: Platinum is the most common  
Operating Temperature: 90-120°C  
Electrical Efficiency: Up to 40 percent
- **Alkaline Fuel Cell (AFC)**  
Electrolyte: Potassium hydroxide solution in water  
Catalyst: Can use a variety of non-precious metal catalysts  
Operating Temperature: 90-100°C  
Electrical Efficiency: 60-70 percent
- **Phosphoric Acid Fuel Cell (PAFC)**  
Electrolyte: Liquid phosphoric acid ceramic in a lithium aluminum oxide matrix  
Catalyst: Carbon-supported platinum catalyst  
Operating Temperature: 150-200°C  
Electrical Efficiency: 36-42 percent

- **Molten Carbonate Fuel Cell (MCFC)**

Electrolyte: Typically consists of alkali (Na & K) carbonates retained in a ceramic matrix of LiHO<sub>2</sub>

Catalyst: High MCFC operating temperature permits the use of lower-cost, non-platinum group catalysts

Operating Temperature: 600-700°C

Electrical Efficiency: 50-60 percent

- **Solid Oxide Fuel Cells (SOFC)**

Electrolyte: A solid ceramic, typically yttria-stabilized zirconia (YSZ)

Catalyst: High SOFC operating temperature permits the use of lower-cost, non-platinum group catalysts

Operating Temperature: 700-1000°C

Electrical Efficiency: 50-60 percent

## Other Fuel Cell Types

- ❖ Regenerative Fuel Cells (RFCs)
- ❖ Zinc Air Fuel Cells (ZAFCs)
- ❖ Microbial Fuel Cells (MFCs)

## 1.5 Thesis Description

### 1.5.1 Rationale

This thesis is targeted at the investigation of Solid Oxide Fuel Cells (SOFC).

Because SOFC-

- Operates at a higher temperature, eliminating the need for precious metals.
- Operates on a number of different hydrocarbon fuels, chiefly natural gas.
- Better suited for continuous operation.
- Produces the highest electrical efficiency (up to 60%).
- Can use heat recovery technologies for a total system efficiency of up to 85 per cent.
- Near zero emissions and quiet operation, with low maintenance requirements compared to existing generation technologies.

**More importantly,**

Ceramic Fuel Cells' products deliver the most efficient source of electricity for small scale co-generation applications with a focus on maximizing electrical output.

With SOFC powered co-generation units, the heat generated from the fuel cells can be integrated with heat exchangers to preheat water and maximize the overall system efficiency.

Because Ceramic Fuel Cells' products can be connected to a regular natural gas network, the fuel cells do not need a separate hydrogen infrastructure for operation. This includes equipment to create hydrogen gas and deliver this pure hydrogen to the customer.

### **1.5.2 Objectives**

- Develop a computational model for the simulation of the mentioned system able to predict load characteristics as well as transient behaviour.
- Gain knowledge on part-load performance, load-varying characteristics of the mentioned system.
- Development of Linearized model of the system
- Checking the stability of the model

# Chapter 2

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## Solid Oxide Fuel Cell(SOFC)

The following chapter briefly introduces the components of SOFC systems. Focus is on working principles, design options and operational characteristics and issues connected to the specific components.

### 2.1 Solid Oxide Fuel Cell

The solid oxide fuel cell is the core technology of the investigated system. In the following, its basic working principle is briefly introduced. Furthermore, materials and manufacturing techniques will be described and an overview over current cell and stack design options is provided

#### 2.1.1 Fundamentals

The fuel cell effect has first been described by the Christian Friedrich Schönbein in 1839. Some years later, Sir William Grove built the first practical fuel cell. The SOFC technology, however, dates from Walther Nernst, who around 1890 discovered that stabilized zirconia is an isolator at room temperature, but turns into an ionic conductor between 600 and 1000 °C and an electronic and ionic conductor around 1500 °C. The first solid oxide fuel cell based on zirconia was introduced by Baur and Preis in 1937. Since then, research on SOFC has been steadily increasing until today. With zirconia remaining the key material, first units have left the lab for prototype and field testing. However, market readiness is still not achieved. The main characteristics of the solid oxide fuel cell are its solid-phase oxygen-ion conducting electrolyte and its high operation temperature.



## 2.1.2 Electrochemistry

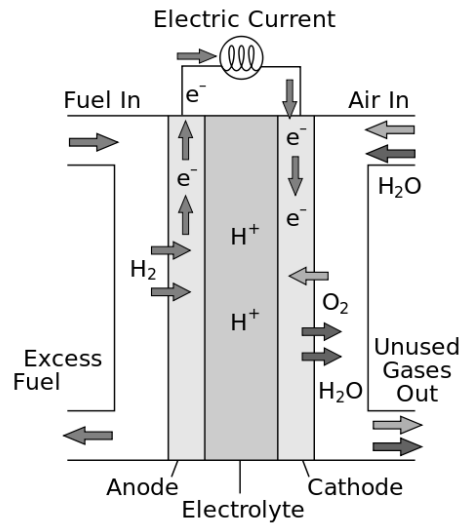
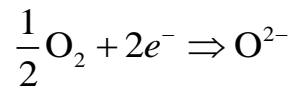
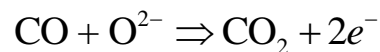
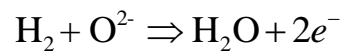


Fig-2.1: Electrochemical principle of the SOFC

The reactions occur at the three phase boundary (TPB) where the gas meets electrode and electrolyte material. The reaction occurring at the cathode TPB is

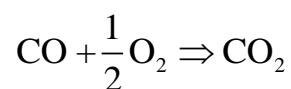
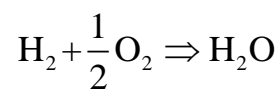


While the following reactions may occur at the anode TPB:



The oxygen ions are conducted through the electrolyte, while the electrons are conducted through an external electric circle.

The overall reactions are



### 2.1.3 Losses

If a current is flowing, the voltage supplied at the electrodes will be different from the reversible potential due to losses. The reversible potential is therefore also called “open circuit voltage” (OCV). The dependency of these losses on temperature, current density and species concentrations mainly determine the characteristics of a fuel cell.

Three main mechanisms of voltage losses exist:

- **Activation or polarization losses:**

At open circuit, no outer current is flowing. However, reactions are still taking place, but at equal rates in both directions. Just regarding the current which flows into one of the directions, we find the “exchange current density”. In order to achieve an outer current higher than this, an extra potential is required to achieve the desired reaction rate, called activation voltage. The voltage drop is increasing fast at low reaction rates and is from a certain level almost constant. Activation is the dominant source of loss for low temperature fuel cells, while their influence is smaller for SOFCs.

- **Ohmic losses:**

Ohmic losses occur due to the resistance along the flow paths of electric and ionic current. At a given temperature and geometry, the voltage loss is proportional to the current.

- **Diffusion or concentration losses:**

Reactants must flow through the porous electrodes to the TPB, and products must flow into the other direction, driven by diffusion. This implies that the concentration of reactants at the TPB is lower and the concentration of products is higher than in the bulk phase. Using TPB instead of the bulk concentrations in Equation 2-4, the calculated potential will be lower and the difference is called diffusion or concentration losses. The voltage drop increases with increasing current against an asymptotic maximum current. At this point, the concentration of one of the reactants at the TPB is zero and no further current increase is possible.

## 2.1.4 Materials and Production

Materials and fabrication methods are the key issue of SOFC research. The following section introduces briefly the state of the art and the trends of SOFC materials and fabrication.

The materials must fulfill different requirements:

- **Electric and mechanical performance:** The ionic conductivity of the electrolyte and the electronic conductivity of the electrodes and the interconnect must be high enough to facilitate efficient operation. At the same time, the electrolyte must have a very low electronic conductivity in order to avoid internal short-circuiting. Furthermore, the electrolytes must possess high permeability for the reaction gases while the electrolyte and interconnect must be impermeable.
- **Chemical stability:** All SOFC components must remain chemically stable across the desired lifetime. Critical phenomena are especially reoxidation of the anode and micro-structural changes in the TPB due to inter diffusion.
- **Mechanical stability:** The high temperature operation in combination with dissimilar thermal expansion coefficients imposes high mechanical stresses on the materials. Due to the brittleness, micro-cracks and delamination are likely to appear where the stresses are highest. These incidents lower the electric performance of the fuel cell and must be minimized by choice of materials, production and operation methods.
- **Inexpensive production and processing:** In order to penetrate the market, it is important that the materials and processing methods are inexpensive and reproducible and may be scaled up from lab to industrial scales.

### 2.1.4.1 Electrolyte

Because of its high ionic conductivity, chemical stability and economic availability, the “standard” electrolyte material today is zirconia ( $ZrO_2$ ) doped with about 8-10 mole percent of yttria ( $Y_2O_3$ ), yielding the so-called yttria stabilized zirconia (YSZ) [Singhal 2003b]. Doping is required to stabilise the desired ionic conducting tetragonal lattice structure, which in pure zirconia is exhibited above  $1170^\circ C$ , for temperatures down to ambient level. Other dopants such as bismuth oxide, promise higher ion conductivity, but also problems like higher electron conductivity and costs [Ishihara 2003]. YSZ requires temperatures above  $800-900^\circ C$  for achieving suitable ion conductivity.

Electronic conductivity increases with decreasing partial pressure of oxygen, although the values are sufficiently low for technically occurring oxygen partial pressures. YSZ is generally chemically stable, but above  $1200^\circ C$  it reacts with cathode material to form insulating layers at the boundary which decrease the electrical performance [Yokohawa 2003].

#### **2.1.4.2 Anode**

The anode's main tasks are to conduct electrons, to permeate gases to the TPB and to provide the catalyst for fuel oxidization and possibly hydrocarbon reforming. The most commonly used material is a cermet<sup>10</sup> of nickel (Ni) and YSZ. Nickel is the catalyst for the reforming reaction and at the same time it facilitates electron conductivity, while YSZ is the support material which is introduced to adjust the thermal expansion coefficient to the electrolyte material. Furthermore, its ionic conductivity expands the electrochemical reaction zone.

#### **2.1.4.3 Cathode**

The cathode must mainly provide electrical conductivity, gas permeability, catalytic activity for oxygen reduction as well as chemical and mechanical compatibility with other SOFC components. Beside platinum which is expensive, perovskites<sup>11</sup> are applicable. Today's standard material is Lanthanum Manganite (LaMnO<sub>3</sub>) doped with Strontium. The mole ratio of Strontium (Sr) and Lanthanum (La) decides the catalytic as well as the mechanical properties of the material. Cathodes are prevalently produced by powder processing. As the cathode performance strongly depends on surface area, porosity and microstructure, the processing method is very important. Except the above mentioned high temperature reactions with the electrolyte, LSM is chemically very stable, as long as no chromia forming metallic interconnects are being used [Yokokawa 2003].

#### **2.1.4.4 Interconnect**

The interconnect must maintain its features of high electronic conductivity, low permeability (in planar design) and chemical stability in both oxidizing and reducing atmosphere. For the usual operating range of 900-1000°C, these features can be provided by perovskite-type oxide ceramics based on rare earth chromites. For lower temperatures, metallic alloys are suitable. LaCrO<sub>3</sub> doped with app. 10 mole percent strontium is the most common configuration today, as it merges high electronic conductivity with a thermal expansion coefficient close to the other components [Anderson 2003].

#### **2.1.4.5 Seals**

Sealing of SOFCs is a very critical task, as the sealing material must be stable in oxidising and reducing atmospheres and be compatible with the SOFC materials. Today, gaskets made of cements, glasses and glass-ceramics are applied. Another type of sealing is to apply mechanical loads to compress the cell components to form a seal, even though at the risk of leakage by uneven surfaces and high mechanical stress [Kendall 2003].

#### **2.1.4.6 Cell Fabrication**

The suitable cell fabrication method is strongly depending on the cell design. Generally, fabrication methods are based on the particulate approach or the deposition approach for the electrolyte. The particulate approach comprises compaction of ceramic powder into cell components and densification at high temperatures. Examples of the particulate approach are tape casting and tape calendaring. The deposition approach on the other hand comprises formation of the cell components on a support by a chemical or physical process, such as chemical vapor deposition, plasma spraying or spray pyrolysis [Kendall 2003]. All these processes are applied for planar SOFCs. The tubular SOFC of Siemens- Westinghouse is manufactured by extrusion of the cathode tube and electrochemical vapor deposition of electrolyte and anode [Singhal 2000].

### **2.1.5 Cell and Stack Design**

In SOFC design, many degrees of freedom exist in the three levels of the membrane electrode assembly (MEA), the single cell design and the stacking. The following section briefly describes and discusses the most common designs.

#### **2.1.5.1 Membrane Electrolyte Assembly (MEA)**

In general, thin layers are required in the MEA in order to reduce the losses through ionic and electric conduction and gas diffusion. Thicknesses in the magnitude of 10  $\mu\text{m}$  are common. In order to achieve a mechanically stable assembly, however, a thicker support is required. In a self-supporting configuration, one of the layers (anode, electrolyte or cathode) acts as the structural support, while in an external supporting configuration, the thin cell layers are supported by the interconnect or a porous substrate. An electrolyte supported configuration (electrolyte thickness  $>100 \mu\text{m}$ ) requires higher operation temperatures in order to reduce ohmic losses in the electrolyte. On the other hand, if an electrode acts as support, the temperature may be lower, but the electrode mass transport will be slower, leading to higher diffusion losses. Interconnect and porous substrate supports allow for thin cell components, but impose limitations to the flow field design respectively add complexity to the configuration due to addition of new materials.

### 2.1.5.2 Cell Geometry

Many different cell configurations have been studied for the time being. The most important requirements to a cell design are:

- **Electrical performance:** The ohmic losses should be low. Short current paths as well as sufficient contact areas are means to provide this.
- **Electrochemical performance:** High reversible voltage and low activation losses can be achieved through good separation of the gas flows, avoidance of electrical shortcuts and a uniform gas distribution across the cell.
- **Thermal management:** Sufficient cooling and uniform temperature distribution across cell and stack are required. The design must allow for efficient cooling and appropriate gas flow configuration and withstand the expected thermal stresses.

Generally, cell designs can be divided into two groups:

- A.** Planar Cell and
- B.** Tubular Cell

Typically, planar cells have a higher volumetric power density and better electrical performance, while tubular cells have fewer problems with sealing and temperature gradients.

### Planar Cells

The largest planar cells that can be produced today have a size of e.g. 18 x 40 cm [Christiansen 2004]. Air and fuel flow are directed through gas channels in the interconnect. The flow field configuration greatly determines the temperature and reaction rate distribution within the cell. General possibilities are cross-flow, counter-flow and co-flow. In a rectangular cross-flow configuration, fuel and air inlets and outlets are separated from each other, which allows for a simple manifold system.

Therefore it is easy to apply cross-flow in technical systems. Experimental cells are often circular with centre gas inlets and radial co-flow, and also Sulzer Hexis makes use of this configuration. However, counter-flow gives the flattest profiles for temperature and current [Rechenauer 1993]. Mixtures between the flow patterns are for example Z-flow, serpentine flow for rectangular and spiral-flow for circular configurations.

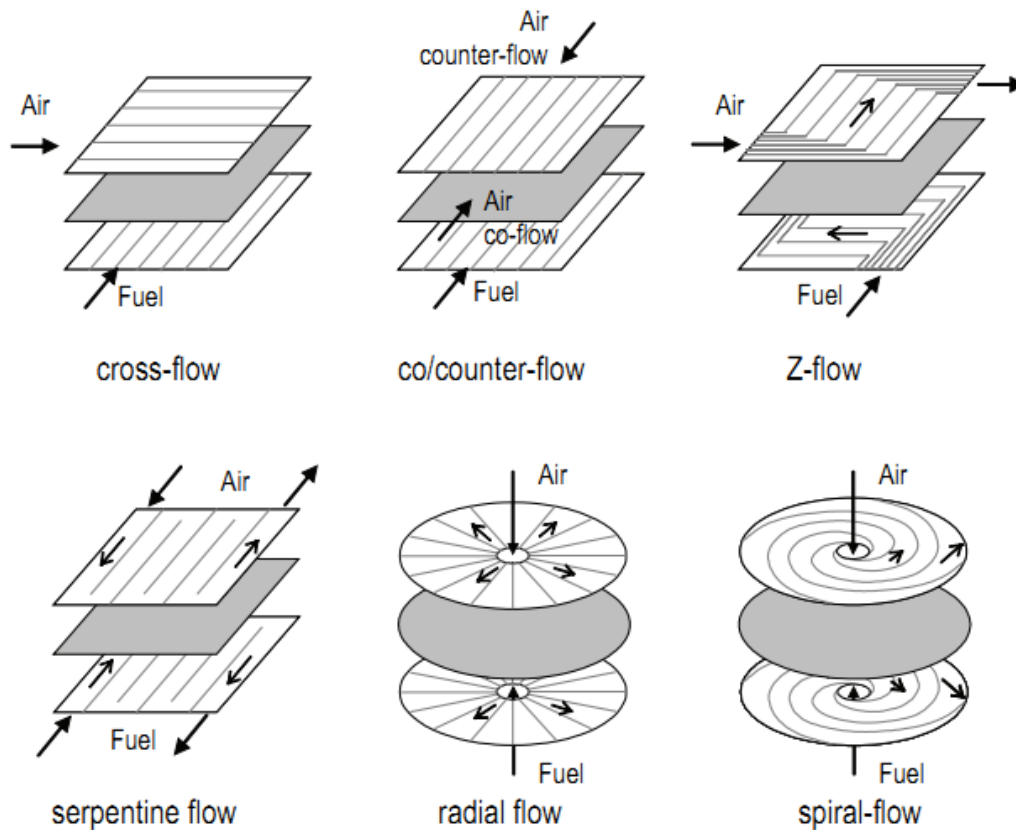


Fig-2.2: Typical flow configurations of planar SOFC

Figure-2.2 shows the most common flow configurations. Planar cells offer principally a high volumetric power density and good electric performance through short current paths. Severe problems are, however, sealing of the cells and mechanical loads due to high thermal gradients.

### Tubular cells

Tubular cells on the other hand offer separation of the gas channels without sealing in the cell itself. A well-known configuration is originating from Siemens-Westinghouse. This design is a cathode-supported, 1.5 m long and 22 mm diameter tube which is closed at one end.

Air enters an inner (injector or air delivery) tube and is being preheated while flowing towards the closed end of the outer tube. There, it turns and flows along the cathode. Fuel is co-currently fed from the outside of the tube. The interconnect is applied at a small segment of the tube, but across its whole length.

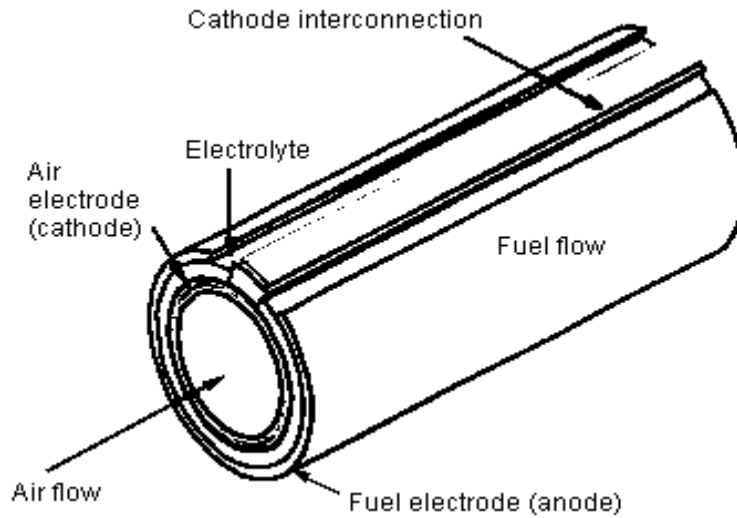


Fig-2.3: A Tubular Cell

The main drawbacks of the tubular cell are the low volumetric power density and the weak electric performance, caused by the long circumferential current paths in the electrodes. In order to increase volumetric power density, Siemens-Westinghouse has recently been focusing on another geometry, which is called the “flattened tubular cell”



Fig-2.4: The Flattened Tubular Cell

### 2.1.5.3 Stacking

The term of stacking is originating from planar cells, which basically are just stacked by connecting electrodes of a cell to the counter-electrode of the adjacent, resulting in a serial electric connection and increased voltage and power. Figure 2-7 shows a circular planar stack with integrated manifolding.



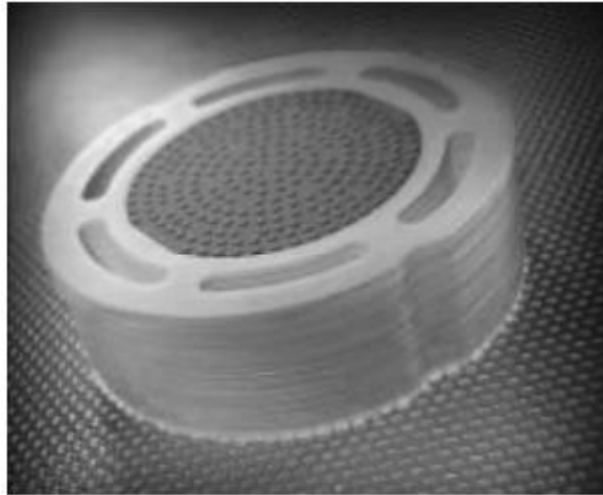


Fig-2.5: Planar SOFC stack with integrated manifolding

It is, however, also common to “stack” tubular cells, even though they are rather bundled. The tubular Siemens-Westinghouse cell is typically arranged vertically in bundles of 3 x 8 tubes. Electrically, three cells each are connected parallel, and eight of these are connected in series, using flexible Nickel felt connectors. A stack contains 48 of these bundles, or 1152 tubes (see Figure 2.6). Indirect internal reformers are arranged between the bundles in order to receive heat by radiation and convection. A certain amount of the anode exhaust gas is recycled in order to supply steam for the reforming reaction. Ejectors are applied to drive this recycling.

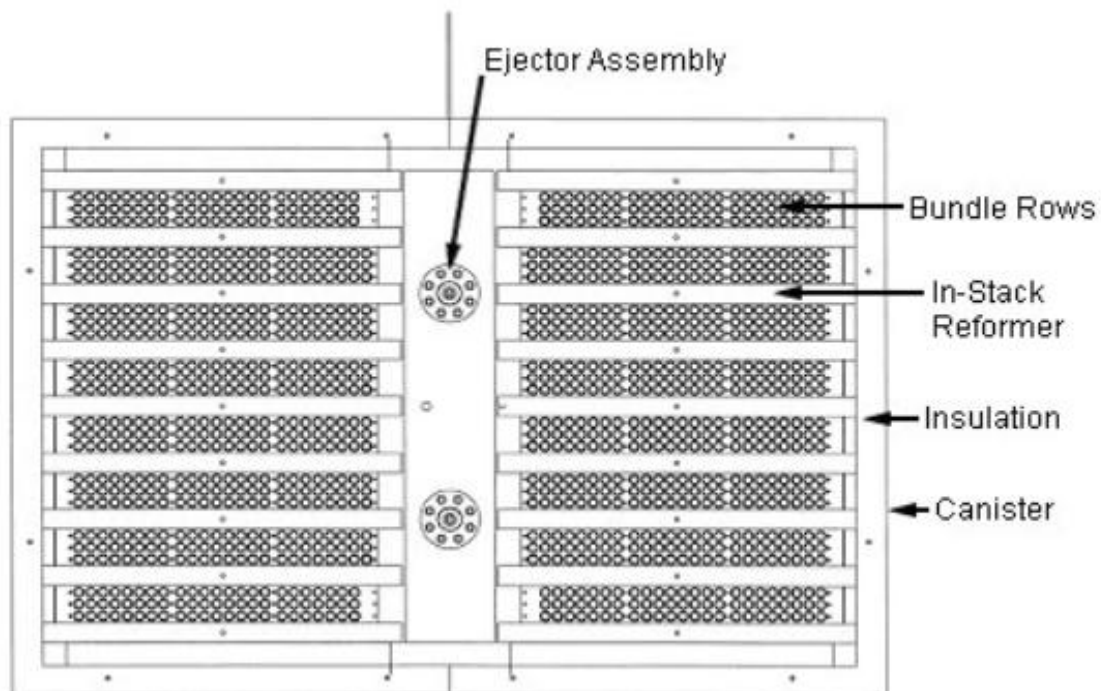


Fig-2.6: Tubular Stack, top view

# Chapter 3

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## SOFC Modeling

This chapter presents an overview of SOFC modeling. Firstly, requirements on process modeling in general are formulated. Next, purposes for modeling of are discussed. Then, the main approaches to SOFC modeling are presented and discussed. Important issues therein are Steady state characteristics, Dynamic Modeling.

### Introduction

The research on solid oxide fuel cells has been steadily increasing since the early 1990s. There still is great uncertainty in the optimum geometrical and system configuration, and experiments with fuel cells are expensive. Thus there is great need for mathematical modeling of fuel cells. There are many different approaches to SOFC and the complexity and accuracy of the models is increasing steadily with computer performance.

### 3.1 Requirements on Modeling Approach

A large variety of approaches to modeling a physical-chemical process exist. These variations include the degree of spatial distribution, the levels of detail in modeling the occurring phenomena as well as simplification or neglect of side effects. A main quality indicator of any model is indisputably its degree of accuracy in reproducing the true behaviour of a system. Hence, the acceptability of each simplification must be verified.

Generally speaking, the more detailed model is expectably the more reliable model in terms of accuracy. However, obvious restrictions to the level of detail are the time required for calculation and the stability of the mathematical solver. The purpose of the model and the simulation approach often decides the detailing level. If for example an optimisation using a genetic algorithm (GA) is to be performed, a high number of model evaluations and thus a fast model is required. Likewise, if the controllability of a system is to be investigated, linear or linearized models with a low number of state variables are advantageous.

Another important feature of a model is the flexibility with which the problem may be posed. A classical model has input and output variables. However, for example the point of operation of a fuel cell may be determined by either dictating a voltage or a current as input variable. The free (output) variable is in both cases resulting from the specified one through a non-analytical relationship. For operation, different restrictions on both values exist; hence it is advantageous for most applications if the model is flexible in terms of input and output variables. Using a classical sequential solving approach, this may be realised by adding additional iteration loops for each output variable which is to be changed to an input variable. However, as this boosts simulation time, a better solution is a simultaneous, equation-oriented solving approach.

Summarizing, general requirements on the modeling approach are-

- Accuracy of reproducing the true behaviour of a system
- Quick and stable solving
- Flexibility in input-output structure

### 3.2 SOFC Modeling Purposes

Due to the contradictive nature of the aforementioned requirements, the selection of modeling approach is dependent on the purpose of the model and the way it should be applied. As for other power plant and energy related systems in pre-commercial stages, the main purposes where a model of a SOFC power plant may be applied are:

- **System understanding and analysis:**  
The model shall help to understand phenomena observed in a real system and allow analysis of the system behaviour at different conditions. A model for this purpose must obviously cover the phenomena that should be analysed and those they depend on in a sufficient level of detail. Furthermore, it must be verified that the model and the true system agree. On the other hand, quickness of the solver and model flexibility are of secondary importance. Depending on the nature of the analysed phenomena, the system can be of steady-state or dynamic type.
- **Design calculation and optimisation:**  
Once a system is understood, its components need to be designed in order to achieve an optimum performance. Several objectives may hereby contribute to the optimum; efficiency, specific power output, specific costs and lifetime are only some of them. In an optimisation calculation, typical design values such as physical dimensions and operational parameters are to be optimised and serve as input to the model, while the objectives serve as the output. Several numerical optimisation approaches exist, but they all require a large amount of model evaluations in order

to proceed to the optimum. Therefore, models for design should be quick and stable to solve.

- **Operation calculation and optimisation:**

Having designed the system and fixed a design point, the next step is to investigate and optimise the behaviour of the system at off-design and under dynamic situations. Here, all parameters that are physically constant in a real system (such as dimensions) must also be kept constant in the simulation. Several global input-output structures are possible:

- A reverse structure where the desired power output and operational parameters such as temperatures serve as model input and the system inputs (fuel flow, fuel cell current, etc.) serve as model output. This allows a direct calculation of the input parameters required to achieve the desired output.
- A forward structure where the model and true system inputs and outputs are equal. This is advantageous for mapping valid and invalid operational areas and the stability of the system against malfunction. This structure can be regarded as the numerical equivalent to physical experiments

- **Control modeling:**

A last modeling task is to investigate controllability and to tailor a control design for the developed system. For this task, a dynamic model is required. The input-output structure of model and true system must agree. Conventional methods for analysing system response and controllability require linear input-output models with a limited number of state variables. For a classic feedback control system, the dynamic behaviour of the system is more important than accurate agreement of the steady-state performance. This allows for stronger model simplifications than in the previous cases. As the implementation of the control design adds complexity to the model, it should be provided that the “non-controlled” model is solved quickly and stable.

### 3.3 Model Assumptions [2]

The stack model will be based on the following assumptions.

- ❖ The gases are ideal.
- ❖ The stack is fed with hydrogen and air. If natural gas instead of hydrogen is used as fuel, the dynamics of the fuel processor must be included in the model, upstream of the hydrogen inlet, as a first-order transfer function. The transfer function gain should reflect the changes in composition occurring during the process. The effect of the fuel processor in the model will be tested in the future.



Where,

$I_{fc-ref}$  = reference stack current

$P_{fc-ref}$  = output stack power

$V_{fc}$  = output stack voltage

- To ensure the FC operation within the safe operating area,  $I_{fc-ref}$ , is limited by the following boundaries[5]

$$I_{fc-ref-max} = \frac{U_{max}}{2K_r} q_{H2-in} \quad (3.2)$$

$$I_{fc-ref-min} = \frac{U_{min}}{2K_r} q_{H2-in} \quad (3.3)$$

$$K_r = \frac{N_0}{4F} \quad (3.4)$$

Where,

$U_{max}$  = maximum fuel utilization

$U_{min}$  = minimum fuel utilization

$N_0$  = number of cells in series in FC stack

$q_{H2-in}$  = hydrogen input fuel flow

$F$  = Faraday's constant

- A first order transfer function is used to model the dynamic with the time constant around 0.08 s [5]

$$I_{fc} = \frac{1}{1+T_e s} I_{fc-ref} \quad (3.5)$$

- Fuel processor depicts the dynamic of fuel supply by a first-order transfer function[5]

$$q_{h2-in} = \frac{2K_r}{U_{opt}} \frac{1}{1+T_f s} I_{fc-ref} \quad (3.6)$$

Where,

$U_{opt}$  = optimal fuel utilization

$T_f$  = time constant of dynamic of fuel supply

- Blocks of ‘conversion constants’ and ‘chemical reaction’ in figure-2.7 represent the chemical process of fuel reaction inside the FC stack. Its dynamic is described by three first order transfer functions for hydrogen, oxygen and water, respectively. [5]

$$q_{O2-in} = \frac{1}{r_{ho}} q_{H2-in} \quad (3.7)$$

$$P_{H2} = \frac{1}{K_{H2}} \frac{1}{1+T_{H2}s} (q_{H2-in} - 2K_r I_{fc}) \quad (3.8)$$

$$P_{O2} = \frac{1}{K_{O2}} \frac{1}{1+T_{O2}s} (q_{O2-in} - K_r I_{fc}) \quad (3.9)$$

$$P_{H2O} = \frac{1}{K_{H2O}} \frac{1}{1+T_{H2O}s} 2K_r I_{fc} \quad (3.10)$$

Where,

$r_{ho}$  = ratio of hydrogen to oxygen flow rate

$K_{H_2}$  = molar constant for hydrogen

$K_{O_2}$  = molar constant for oxygen

$K_{H_2O}$  = molar constant for water

$T_{H_2}$  = time constant for hydrogen flow

$T_{O_2}$  = time constant for oxygen flow

$T_{H_2O}$  = time constant for water flow

$P_{H_2}$  = partial pressure of hydrogen

$P_{O_2}$  = partial pressure of oxygen

$P_{H_2O}$  = partial pressure of water

$q_{O_2-in}$  = oxygen flow rate

- The FC stack voltage is given by the following equation [1] [5]

$$V_{fc} = N_0 \left[ E_0 + \frac{RT}{2F} \ln \left( \frac{P_{H_2} * P_{O_2}^{1/2}}{P_{H_2O}} \right) \right] - rI_{fc} \quad (3.11)$$

Where,

$E_0$  = ideal standard potential

$R$  = universal gas constant

$T$  = absolute temperature

$r$  = ohmic loss



### 3.5 The Non-linear Equations

The non-linear differential equations of the FC model used in this study are-

$$\dot{I}_{fc} = [I_{fc-ref} - I_{fc}] \frac{1}{T_e} \quad (3.12)$$

$$\dot{q}_{H2-in} = [2K_r I_{fc} - q_{H2-in} U_{opt}] \frac{1}{T_f U_{opt}} \quad (3.13)$$

$$\dot{P}_{H2} = [q_{H2-in} - 2K_r I_{fc} - P_{H2} K_{H2}] \frac{1}{T_{H2} K_{H2}} \quad (3.14)$$

$$\dot{P}_{O2} = [q_{O2-in} - K_r I_{fc} - P_{O2} K_{O2}] \frac{1}{T_{O2} K_{O2}} \quad (3.15)$$

$$\dot{P}_{H2O} = [2K_r I_{fc} - P_{H2O} K_{H2O}] \frac{1}{K_{H2O} T_{H2O}} \quad (3.16)$$

### 3.6 Initial Conditions

In order to solve the non-linear equations using Euler's method, we need the initial conditions to be defined. The following equations have been used to determine the initial values-

$$I_{fc(0)} = I_{fc-ref} \quad (3.17)$$

$$q_{H2-in(0)} = \frac{2K_r I_{fc(0)}}{U_{opt}} \quad (3.18)$$

$$P_{H2(0)} = \frac{q_{H2-in(0)} - 2K_r I_{fc(0)}}{K_{H2}} \quad (3.19)$$

$$P_{O2(0)} = \frac{q_{O2-in(0)} - K_r I_{fc(0)}}{K_{O2}} \quad (3.20)$$

$$P_{H2O(0)} = \frac{2K_r I_{fc(0)}}{K_{H2O}} \quad (3.21)$$

Where, '0' indicates the initial values of the system

# Chapter 4

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## Stability Analysis

### 4.1 Stability

Stability properties of a physical system refers to how the system responds to some perturbation; whether the system can recover on its own after being perturbed or whether it goes haywire. Stability analysis helps us to understand what happens when we perturb a system.

Stability analysis of systems allows us to determine whether or not a system is stable or will be stable if perturbed. This is important in a wide range of applications since many behaviours observed in the real world can be described using differential equations.

### 4.2 Eigenvalues and Stability

Eigenvalues are a special set of scalars associated with a linear system of equations (matrix equation) that are sometimes also known as characteristic roots, characteristic values.

Eigenvalues tell us the exponential part of the solution of the differential equation system

Three possible values for an eigenvalue

1. **Positive value:** system will increase exponentially
2. **Negative value:** system will decay exponentially
3. **Imaginary value:** system will oscillate

### 4.3 Linearization

In the study of dynamical systems, linearization is a method for assessing the local stability of an equilibrium point of a system of nonlinear differential equations or discrete dynamic systems.

### 4.4 Purpose of Linearization

- ✓ Linearization makes it possible to use tools for studying linear systems to analyze the behavior of a nonlinear function near a given point.
- ✓ It allows to design controller using the knowledge of 'linear control'.
- ✓ In stability analysis of autonomous systems, one can use the eigenvalues of the Jacobian matrix evaluated from the linearized model at a hyperbolic equilibrium point to determine the nature of that equilibrium.

### 4.5 Linearized Model

Linearizing the set of equations using Taylor Series Expansion around an operating condition of the FC stack, we get the following new set of equations-

$$\Delta \dot{I}_{fc} = -\frac{P_{fc-ref}}{(V_{fc_0})^2} \left[ C_1 \Delta I_{fc} + C_2 \Delta P_{H_2} + C_3 \Delta P_{O_2} + C_4 \Delta P_{H_2O} \right] \frac{1}{T_e} - \Delta I_{fc} \frac{1}{T_e} \quad (4.1)$$

$$\Delta \dot{q}_{H_2-in} = \left[ 2K_r \Delta I_{fc} - \Delta q_{H_2-in} U_{opt} \right] \frac{1}{T_f U_{opt}} \quad (4.2)$$

$$\Delta \dot{P}_{H_2} = \left[ \Delta q_{H_2-in} - 2K_r \Delta I_{fc} - \Delta P_{H_2} K_{H_2} \right] \frac{1}{T_{H_2} K_{H_2}} \quad (4.3)$$

$$\Delta \dot{P}_{O_2} = \left[ \Delta q_{O_2-in} - K_r \Delta I_{fc} - \Delta P_{O_2} K_{O_2} \right] \frac{1}{T_{O_2} K_{O_2}} \quad (4.4)$$

$$\Delta \dot{P}_{H_2O} = \left[ 2K_r \Delta I_{fc} - \Delta P_{H_2O} K_{H_2O} \right] \frac{1}{K_{H_2O} T_{H_2O}} \quad (4.5)$$

Where,

$$C_1 = -r$$

$$C_2 = \frac{N_0 RT}{2F} * \frac{1}{P_{H_2}}$$

$$C_3 = \frac{N_0 RT}{4F} * \frac{1}{P_{O_2}}$$

$$C_4 = -\frac{N_0 RT}{2F} * \frac{1}{P_{H_2O}}$$

The Jacobian matrix evaluated from the linearized model

$$\begin{bmatrix} \Delta \dot{I}_{fc} \\ \Delta \dot{q}_{H_2-in} \\ \Delta \dot{P}_{H_2} \\ \Delta \dot{P}_{O_2} \\ \Delta \dot{P}_{H_2O} \end{bmatrix} = \begin{bmatrix} \left( \frac{-P_{fc-ref} C_1}{V_{fc_0} T_e} - \frac{1}{T_e} \right) & 0 & \frac{-P_{fc-ref} C_2}{V_{fc_0} T_e} & \frac{-P_{fc-ref} C_3}{V_{fc_0} T_e} & \frac{-P_{fc-ref} C_4}{V_{fc_0} T_e} \\ \frac{2K_r}{T_f U_{opt}} & -\frac{1}{T_f} & 0 & 0 & 0 \\ -\frac{2K_r}{T_{H_2} K_{H_2}} & \frac{1}{T_{H_2} K_{H_2}} & -\frac{1}{T_{H_2}} & 0 & 0 \\ -\frac{2K_r}{T_{O_2} K_{O_2}} & \frac{1}{T_{O_2} K_{O_2}} & 0 & -\frac{1}{T_{O_2}} & 0 \\ \frac{2K_r}{K_{H_2O} T_{H_2O}} & 0 & 0 & 0 & -\frac{1}{T_{H_2O}} \end{bmatrix} \begin{bmatrix} \Delta I_{fc} \\ \Delta q_{H_2-in} \\ \Delta P_{H_2} \\ \Delta P_{O_2} \\ \Delta P_{H_2O} \end{bmatrix}$$

By calculating eigenvalues from above Jacobian Matrix, the stability of the system can be determined.

# Chapter 5

## Simulation & Results

### 5.1 Steady State Characteristics

#### 5.1.1 Steady state curves generated for constant flow rate

The stack model can be used to generate voltage–current and power–current curves at constant fuel flows. The results are displayed in Fig-5.1 and Fig-5.2

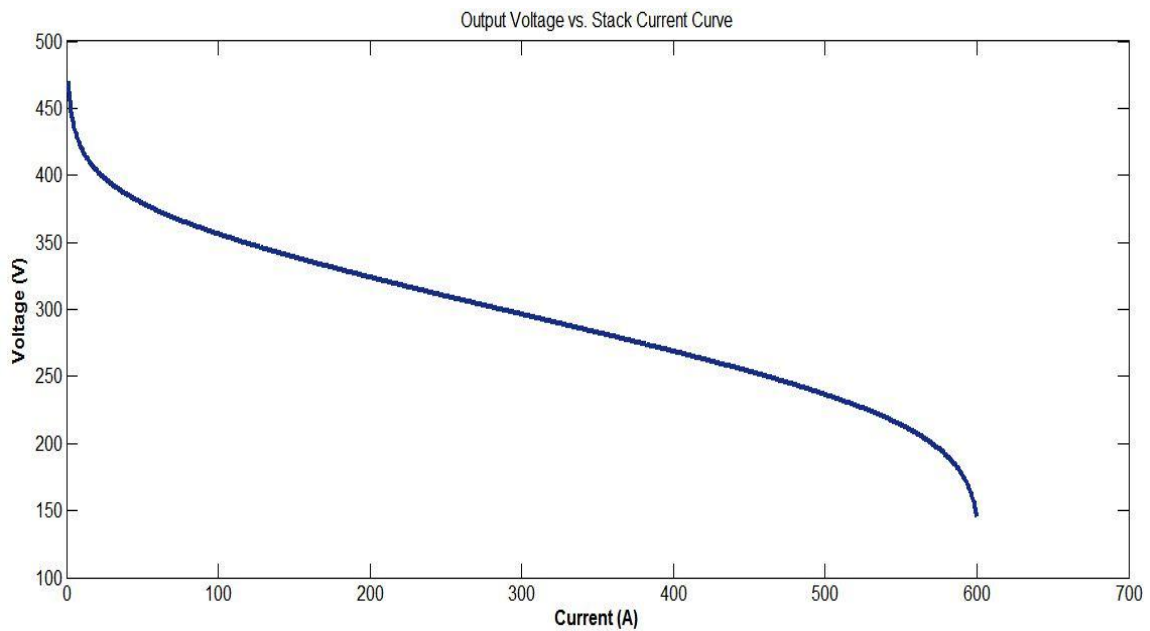


Fig-5.1: Voltage-Current steady-state characteristics ( $q_{H_2}=1.2 \times 10^{-3}$  kmol/s)

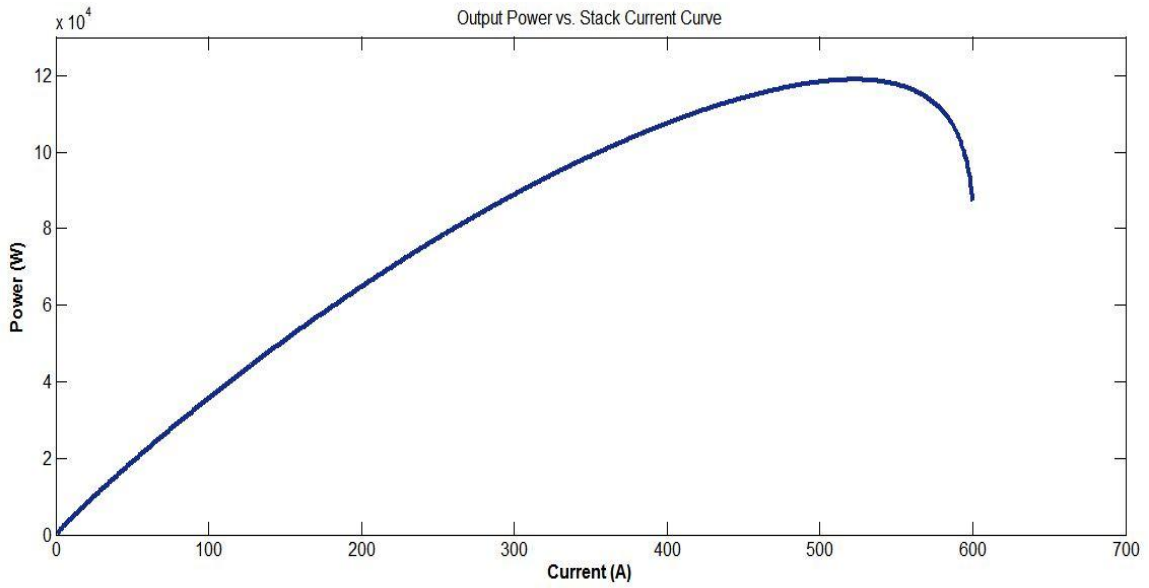


Fig-5.2: Power-Current steady-state characteristics ( $q_{H_2}=1.2 \times 10^{-3}$  kmol/s)

### 5.1.2 Steady-State curves generated different flow rate

The stack model can be used to generate voltage-current and power-current curves at different fuel flows. The results are displayed in Fig-5.3 and Fig-5.4

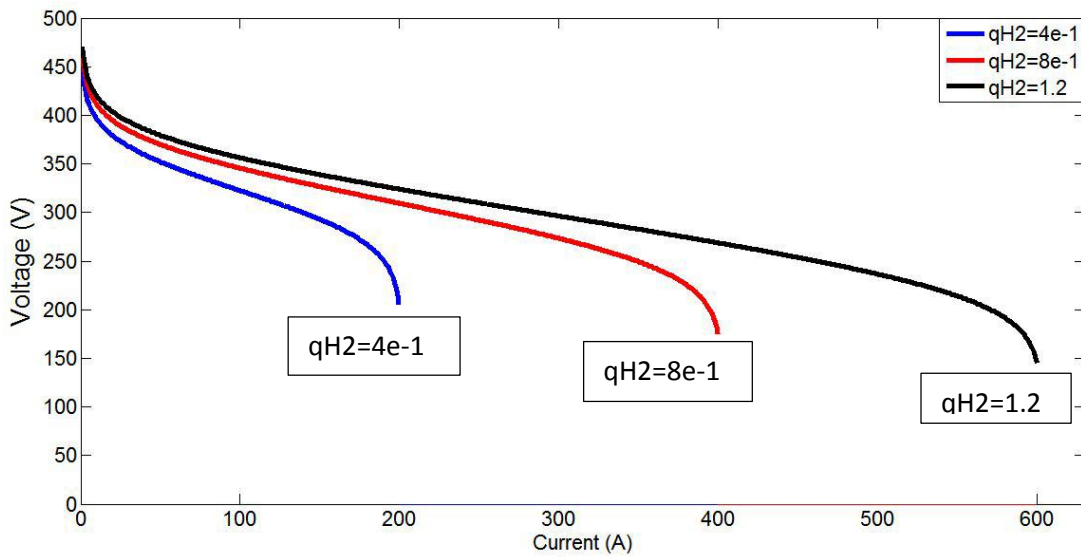


Fig-5.3: Voltage-Current steady-state characteristics of the SOFC stack model.

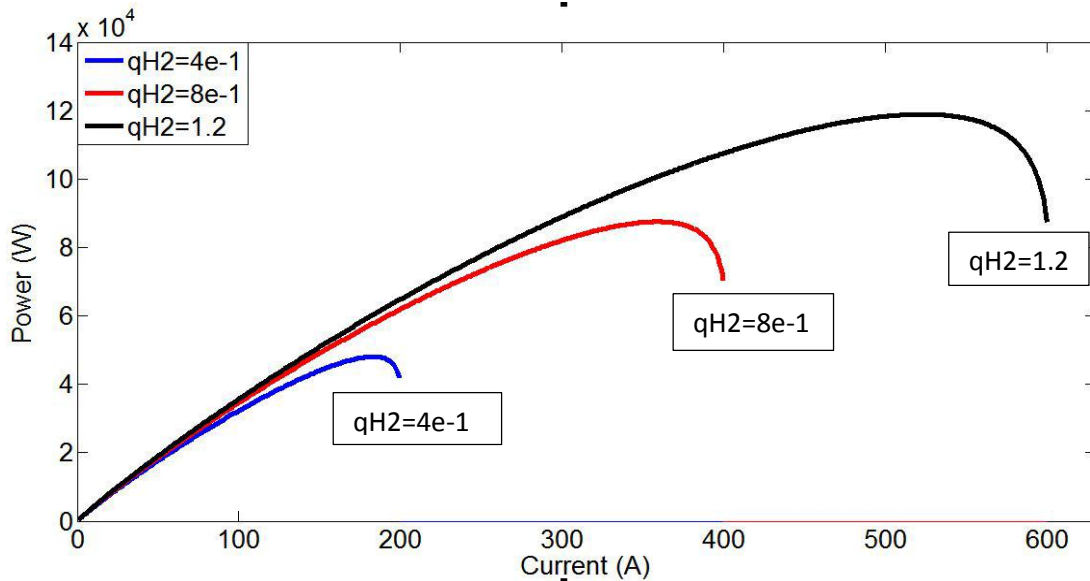


Fig-5.4: Power-Current steady-state characteristics of the SOFC stack model

### 5.1.3 Operational Limits of the Plant

In order to make clear some of the functions that the plant controller should implement, Fig-5.3 has been envisaged as an interesting way to define what the safe operating areas of the plant are. As an example, three different limits have been set for Fig-5.3

- **Underused fuel:**  
If the fuel utilization drops below a certain limit 70% in this example, the cell voltage would rise rapidly.
- **Overused fuel:**  
If the fuel utilization increases beyond a certain value 90% in this example, the cells may suffer from fuel starvation and be permanently damaged.
- **Under voltage:**  
If the stack voltage output drops beyond certain point, the power conditioner will lose synchronism with the network and the whole plant will have to be disconnected.

## 5.2 Dynamic Operation

### 5.2.1 Response of the plant to constant load

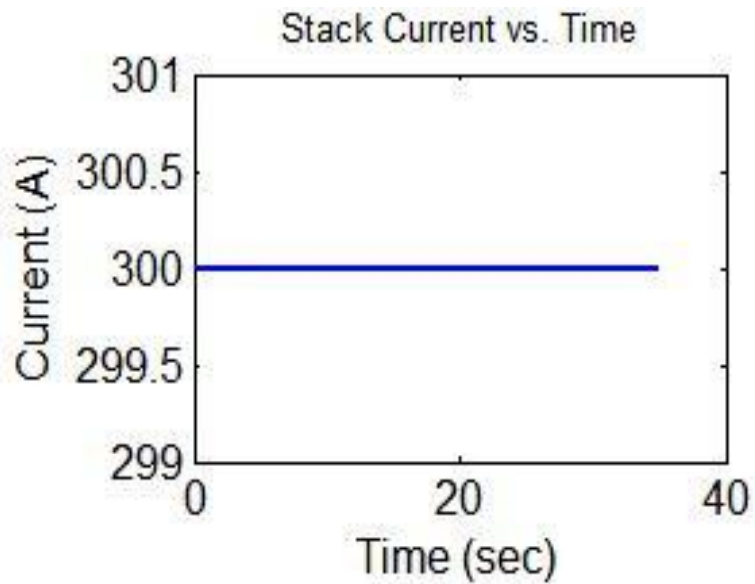


Fig-5.5: Stack Current for constant load

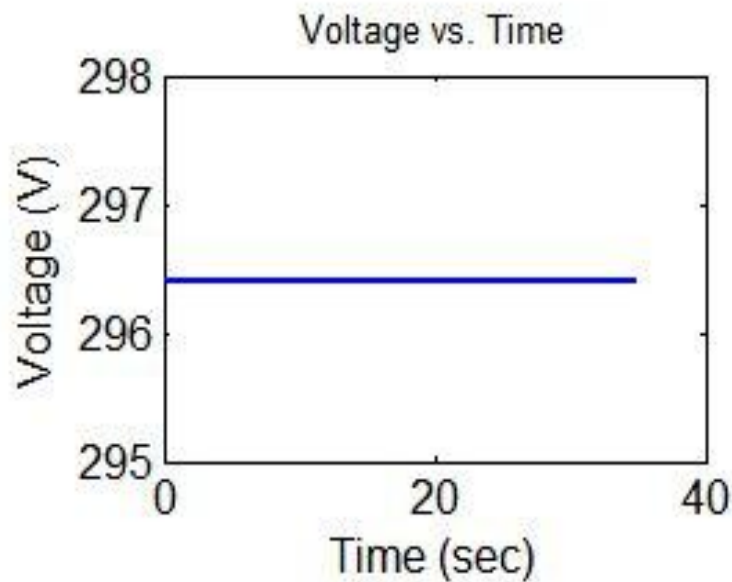


Fig-5.6: Stack voltage for constant load



## 5.2.2 Response of the plant to load changes

The stack model allows the simulation of the event of a load change to the stack. Fig. shows a change in the stack current from 300 A to 500 A in 5 s. This change is backed up with proportional changes in the fuel and airflows. It can be seen that during the decrease of the current, the stack starts following the nominal voltage curve, but soon the response transit beyond the nominal values. In some situations, the voltage output may be situated outside the safe operating area.

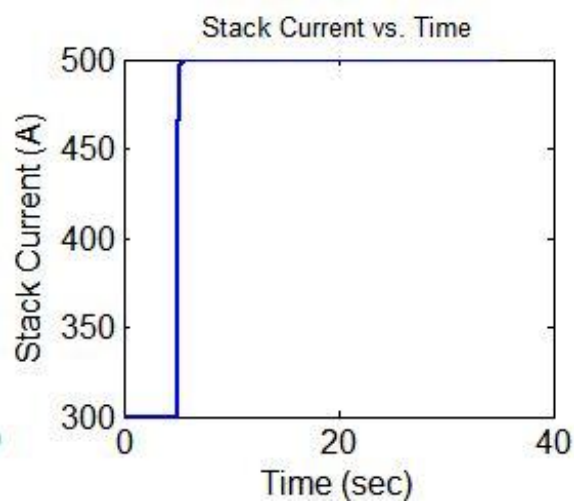


Fig-5.7: Stack current change in 5s

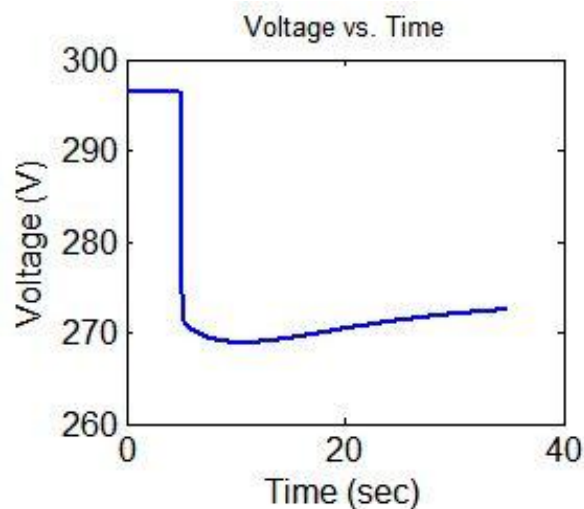


Fig-5.8: Stack voltage after current ramp from 300 A to 500 A in 5 s

In simulations similar to the example, some conclusions have been reached:

- When the output current changes, the mere observation of the voltage profile is not sufficient to anticipate the possible consequences of this current change. Some additional variables might have to be monitored.
- If the stack problems associated with a current change are null, the control system may satisfy the demands of the network.
- If the current change indicates stack problems, the network will have to be satisfied at a pace that is sustainable by the stack. This operating mode coincides with what has been proposed by.

The purpose of the plant control system will be to identify the likely dangers that any network transients bring, anticipating the transient response that will take place inside the stack, and providing the network with any available power.

### 5.3 Simulation of D.C Current Load Following of SOFC

The SOFC dynamic model is tested with step changes in the load. The changes of the load current, the load voltage are shown in Fig. Figures show variations of quantities in a test period of 35 seconds.

The waveform of SOFC output currents for DC loads can be seen from Fig. The variations at the stack voltage in the system are given in Fig. The increasing in the load current causes a decrease in the output voltage.

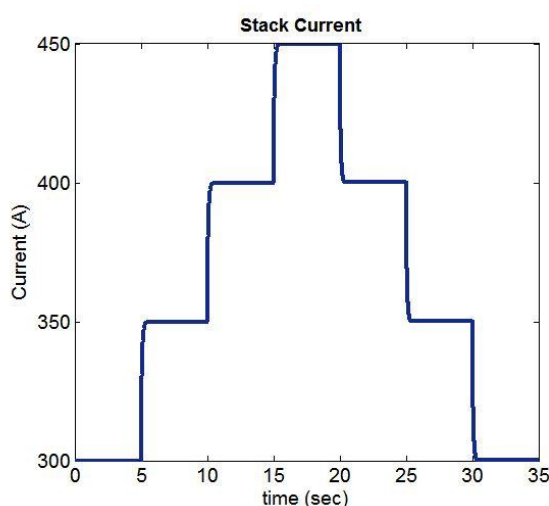


Fig-5.9: SOFC DC output current

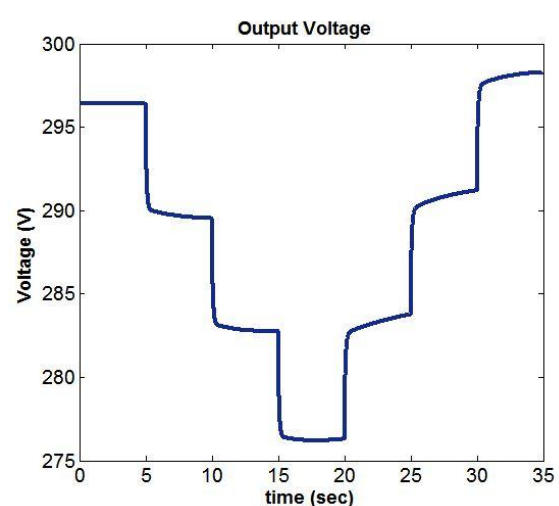


Fig-5.10: SOFC DC output voltage

## 5.4 Stability

### 5.4.1 Without considering concentration loss and activation loss

Eigen values:

-10.9142

-0.3326

-0.2022

-0.0118

-0.0397

### 5.4.2 Considering concentration loss and activation loss

Eigen values:

-10.9817

-0.3327

-0.2022

-0.0118

-0.0397

All the eigenvalues in both cases are negative. So, our system is driven back to steady state value (Stable).

# Conclusion

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This thesis investigates design, operation and control of solid oxide fuel cell (SOFC) which can be used for small signal and stability studies. The proposed SOFC system has fast dynamic response for the load variations. DC load tracking capability of the system is good. Simulation results produced by the dynamic SOFC model are similar to those obtained by the studies.

Fuel cells are dynamic devices and their penetration into the distribution system will affect the behavior of this system, but control of these devices can enhance the stability of the overall system. Further work in this area will address the ways in which a plant controller can solve these problems. The model provides a foundation for continued work in modeling and controlling SOFC.

Solid Oxide Fuel Cells can operate on hydrogen, carbon monoxide, or a mixture of both fuels. The capability to operate on carbon monoxide allows SOFC's to operate directly on reformed hydrocarbon fuels. A transient reformation model could be incorporated into the model described in this paper. The steam (water) necessary for reformation can be obtained by recirculating a portion of the depleted fuel as it exits the cell. Reforming of natural gas should be investigated for utility applications of SOFC's. Reforming of liquid fuels such as methanol, gasoline, and diesel fuel should be modeled for transportation applications.

# Appendix

## Fuel Cell Operating Data

Rated power	100 kW
Rated stack voltage	286.3V
Rated stack current	300 A
Number of cells	384
Number of stacks	1
Open circuit voltage for each cell	0.935 V
Input fuel flow (Fuel)	1.2e-3 kmol/s
Input air flow (Air)	2.4e-3 kmol/s
Tafel slope(b)	0.11
Tafel constant (a)	0.05
Cell area	1000cm <sup>2</sup>
Operating point cell temperature (TH2)	1000° C
Ohmic resistance constant ( $\beta$ )	-2870
Ohmic resistance constant ( $\alpha$ )	0.2
Constant temperature (T0)	923 <sup>0</sup> C
Thickness ( $h_{eff}$ )	5 mm
Thermal conductivity (ls)	15 W/ (m K)
Efficiency (eta)	80%
Density (ro)	7000 kg/m <sup>3</sup>
Limiting current (iL)	0.8 A/m <sup>2</sup>
KH2	8.43e-4 kmol/(atm s)

## Values of Constants

Parameter	Value	Unit
$N_0$	384	
$K_{H_2}$	8.43e-4	kmol/(atm s)
$K_{H_2O}$	2.81e-4	kmol/(atm s)
$K_{O_2}$	2.52e-3	kmol/(atm s)
$\tau_{H_2}$	26.1	s
$\tau_{H_2O}$	78.3	s
$\tau_{O_2}$	2.91	s
$r$	0.126	$\Omega$

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