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Production, simulation and design of an anode supported SOFC

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Abstract
Environmental consciousness of today's society requires the renewable energy industry to provide clean energy solutions that are cost effective and implementable in different scenarios. Solid oxide fuel cell is one the technologies that has the potential to be leading the market in the race of clean energies. This report focuses on three main subjects. First is the production of a sample fuel cell using the most common methods of powder compression and screen printing. The test cell is made using the powders of the materials and then sintered in a furnace before other layers are added to complete the cell. The result is a solid cell that is ready to be tested under different open circuit voltages. The second is the validation of a simulation model using the experimental data available from a commercialised fuel cell. The model was validated with good agreement between the simulation results and the experimental data. The last aspect of this research shows the theoretical I-V curve of the designed cell which can produce a maximum theoretical power density of 0.41 W/cm^2.

Keywords: Solid oxide, fuel cell, anode supported, simulation, fluent

1 Introduction
In the past few decades there has been a huge improvement in terms of human awareness towards the alarming rate the global society is consuming fuel and using energy. More than 80% of the energy used in 2010 was produced from fossil fuels such as oil, coal and gas (The world bank, 2012). These resources are finite and are slowly but inevitably running out, causing the price of fossil fuels to rise. There is also a concern about the global warming and the effect of fossil fuels on the situation which has sparked a movement towards clean energy solutions. These circumstances require us to establish other methods to produce energy from sources which are either infinite or more sustainable than current fuel types. One of the methods that has been established in the field of renewable energy is the use of fuel cells to produce electrical energy. Fuel cells are electrochemical devices capable of converting the chemical energy of a fuel directly into electrical energy in a continuous catalytic process (McGraw-Hill, 2007). The chemical reaction produces heat as a by-product which can then be used in hybrid systems to initiate another phase of energy production. Solid oxide fuel cell (SOFC) is considered a good candidate for electrical power plants and combined heat and power systems because of its high conversion efficiencies and environmental compatibility, which is important in a society motivated to reduce the pollution. In the recent years, there has also been more research focused on Proton Conducting SOFC which is said to be able to run at lower temperatures compared to normal SOFC (Kreuer, 2003).

SOFCs are produced commercially mainly for stationary applications because of their high operating temperatures and there is a need for more research into this field to

optimize these devices for applications other than what was mentioned earlier. The field of research on SOFCs expands from small scale electricity generating plants to combined heat and power production. The strategy in this research is to build a new simulation model which is validated with a commercialised cell and apply the model to the cells designed and produced in the lab to evaluate their performance.

2 Methodology

The test cell was produced based on the materials used by H. C. Starck (H.C. Starck, 2008). This fuel cell is classified as an anode-supported SOFC and is comprised of five layers, anode electrode/catalyst (NiO/YSZ, 3:1 weight ratio), electrolyte (YSZ, $(ZrO_2)_{0.97}(Y_2O_3)_{0.03}$), cathode catalyst (YDC, $Ce_{0.8}Y_{0.2}O_{1.9}$) and cathode electrode (LSCF, $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_3$). The anode electrode and catalyst layer were made in one stage since both layers have identical porosity and use the same material.

The anode substrate was made using a hydraulic press operated manually with a hand pump and has a maximum operating pressure of 15 tonnes. The dye used in production of the anode has a diameter of 30mm. Since the production is done under normal operating temperatures, the pellets made with thickness of <2mm are fragile even after the sintering process. The pellet was sintered at a temperature of 1000°C with a starting temperature of 150°C for 6 hours (Figure 1). The resulting anode measured 2mm in thickness. Scanning electron microscope (SEM) was used on the cell in order to show the arrangements of the particles, the porosity of the pellet and the size of the crystals.

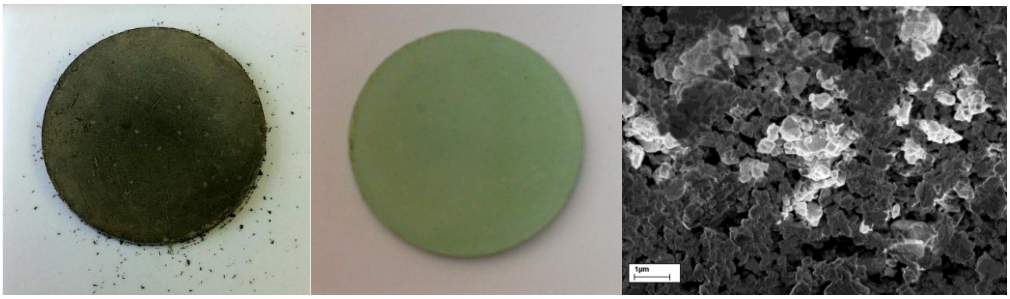

Figure 1. Anode substrate before (left) and after (centre) the sintering process and the SEM picture in 1µm scale.

The electrolyte layer was deposited on the anode substrate using the screen printing method. An organic compound consisting of 20% hydroxypropylcellulose and 80% hexanol was mixed with yttria stabilized zirconia (YSZ) powder with ratio of 3:1. The mixture was then put in a centrifuge for 1 min at 3500 turns per minute. Using an stencil, the slurry was deposited as a thin layer on the substrate, left to dry for 10 minutes at 150°C and then sintered at 1100°C for 2 hours, stopping at 450°C to remove the organic compounds for an hour (Figure 2).

Figure 2. Electrolyte layer before (left) and after (right) the sintering process

The cathode catalyst and electrode were deposited one after another using the same technique as the electrolyte. However, the ratio of powder to organic compound was changed to 2:1 in order to produce a more viscous solution and achieving a thinner layer after sintering. The drying and sintering method were followed in the same manner (Figures 3 & 4).

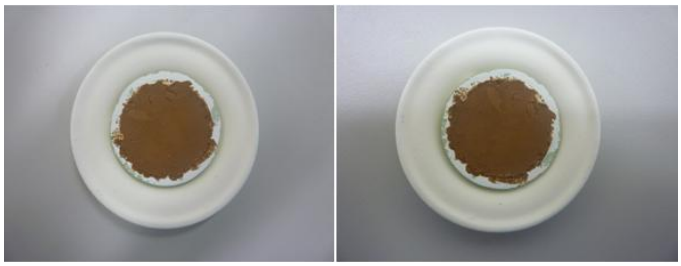

Figure 3. Cathode catalyst layer before (left) and after (right) the sintering.

Figure 4. Cathode electrode layer before (left) and after (right) the sintering.

The thickness of the layers were: electrolyte (0.1mm), cathode catalyst (0.24mm) and cathode electrode (0.3mm). The overall thickness of the cell was 2.64mm which was used in designing the simulation model.

2.1 SOFC Computational Model

Two computational models have been generated for the purpose of simulation based on the test cell that was built and SOFC that is currently being produced by H.C. Starck. The only difference between the two models used is their geometry which affects the rate of diffusion of hydrogen and oxygen and the overall resistance of the cell. The model based on the commercial fuel cell is primarily used to validate the computational model and thus allowing us to estimate the performance of the designed cell.

The channel design for this simulation is based on a research by Kakac et al. (Kakac & Pramuanjaroenkij, 2007). The active area of the simulation for the test cell was designed to be 4.9cm^2, which corresponds to a pellet with a radius of 1.25cm. The active area of the Starck's cell is set to 1.33 cm^2. The fuel cell consists of seven different sections. These include gas channels, current collectors, anode electrode and catalyst, cathode electrode and catalyst and electrolyte. Figure 5 shows the different sections of the simulation model and their arrangement.

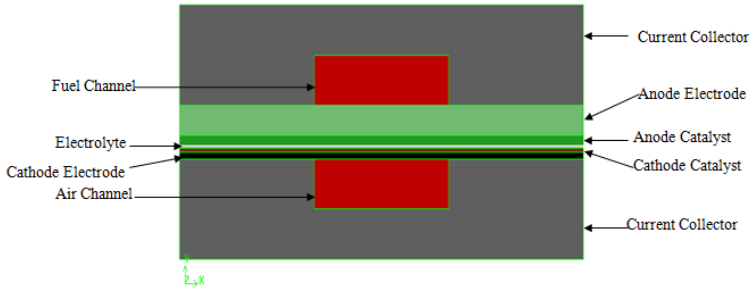

Figure 5. Fuel cell computational model arrangement

The dimensions of the current collectors were inspired by the simulation done by Kakac et al. (Kakac & Pramuanjaroenkij, 2007)and the thickness of the test cell were taken from the produced test cell. Figure 6 outlines the dimensions of the fuel cell and the values of dimensions are given in table 1.

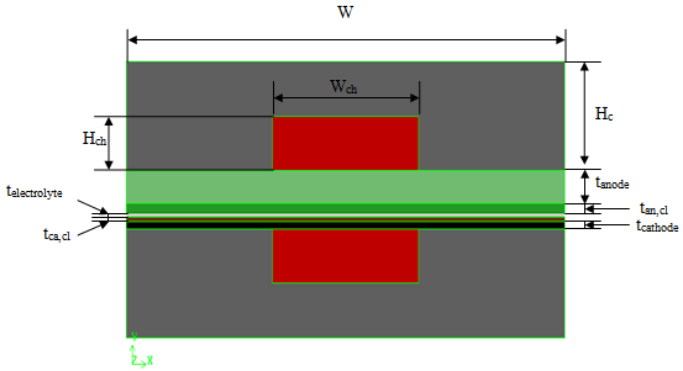

Figure 6. Fuel cell dimensions

Table 1. Dimensions of the modelled SOFCs

Symbol	Component	Size (mm)	
		Designed cell	Starck's cell
L	Cell Length	50	125
W	Cell Width	30	3.2
H	Cell Height	22.64	2.955
H_{cc}	Current Collector Height	10	1.20
H_{ch}	Channel Height	5	0.6
W_{ch}	Channel Width	10	1.0666
t_{anode}	Anode Electrode thickness	1.5	0.51
$t_{cathode}$	Cathode Electrode Thickness	0.3	0.045
$t_{electrolyte}$	Electrolyte Thickness	0.1	0.005
$t_{an,cl}$	Anode Catalyst Thickness	0.5	0.0075
$t_{ca,cl}$	Cathode Catalyst Thickness	0.24	0.003

The inlet boundary conditions are based on the published results by H.C. Starck (H.C. Starck, 2008). The difference between the active fuel cell areas has been taken into account when setting the mass flow rates for the test cell. The test cell has an active area of 3.75 times bigger than the Starck's cell and therefore the flow rates have been increased to compensate. The simulation assumes the reactions inside the fuel cell happen under atmospheric pressure and at a constant temperature of 700°C.**Error! Reference source not found.**

Table 2. Boundary conditions of the channels' inlets

	Mass Flow Rate ($kg\ s^{-1}$)		Initial Gauge Pressure (Pa)	Temperature (K)		Species Mass Fraction	
	Designed Cell	Starck's Cell		Designed Cell	Starck's Cell	Test Cell	Starck's Cell
Fuel Inlet	13.26e-6	3.538e-6	101325	973	973	H_2: 1	H_2: 0.40 H_2O:0.05
Air Inlet	15.47e-6	4.129e-6	101325	973	973	O_2: 1	O_2: 0.21

Material properties such as specific heat, thermal conductivity and electrical resistivity which was measured experimentally and properties of the species used in the simulation can be found from another research by the author (Azmin, 2010).

3 Results and Discussion

Figure 7 demonstrates the I-V curve found through simulation on the two designs compare to the values that were gathered through experiments by H. C. Starck. Comparing the results from Starck's cell operating at 700°C to those of ASC4 (experimental values) at 700°C, there is a clear agreement with a slight offset which is due to the fact that not all of the simulation values have been fine tuned. However, these results validate the use of the simulation model in order to estimate the performance of the new cells. Power density is by far the most important factor that judges the effectiveness of a fuel cell and figure 8 shows the I-V and the power density curve of the two simulated models. At its peak power density (0.47 W cm^{-2}), Starck's cell has a current density of 0.855 A cm^{-2} while the designed cell has a power density of 0.413 W cm^{-2} while it produces a current density of 0.827 A cm^{-2}. This results in a difference of 3.38% between the power density of the two fuel cells.

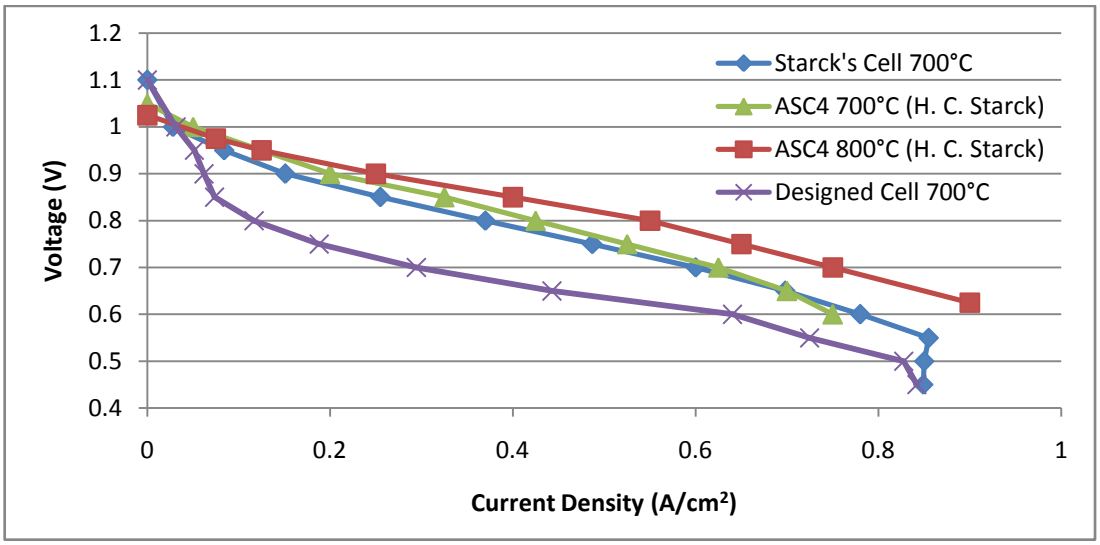

Figure 7. Comparison of the I-V curves from the experimental results and the simulation results

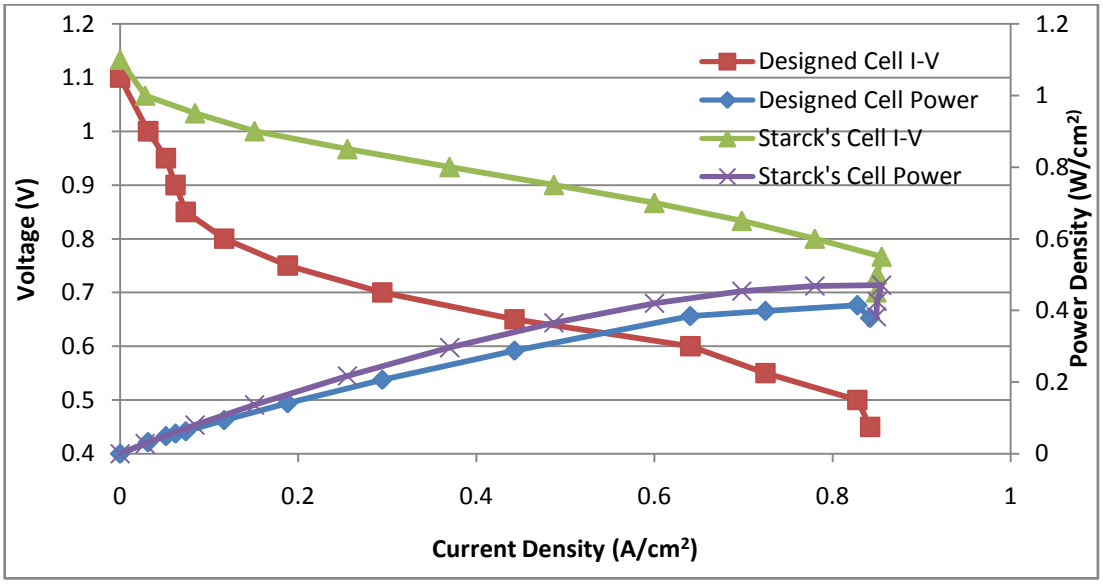

Figure 8. Comparison of the I-V and power curves from the simulation results

Although the thickness of the cell does not affect the power density by a considerable amount, it has to be mentioned that the simulation is only taking place over one channel and for a fuel cell stack this would amount to a larger difference between the power densities. The thickness of the cell also affects the diffusion of the hydrogen through the electrode/catalyst layer as expected which is shown in figure 9 in comparison to normal hydrogen diffusion rate.

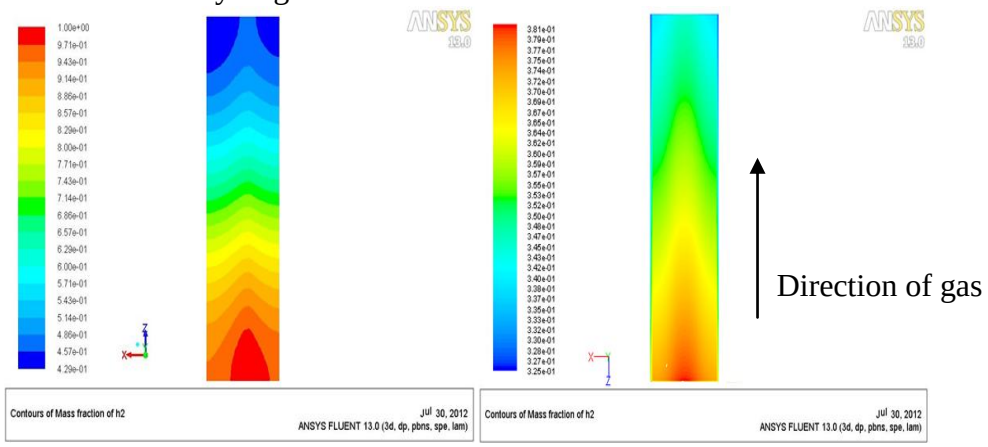

Figure 9. Mass fraction of hydrogen on the anode electrode/catalyst interface (Right: Starck's cell, Left: Designed cell)

4 Conclusion

The aim of the research was to demonstrate the ability to produce a solid oxide fuel cell capable of being a candidate for practical tests and to prepare and validate a simulation model which could be used to assess the reliability of newly designed cells. The fuel cell was successfully produced from powdered materials with the screen printing method. The dimensions of the produced fuel cell were used to create a simulation and assess its viability. The simulation results were in agreement with the experimental results and thus validating the model. However, the model could be still be fine tuned to decrease the gap between the experimental and simulation results. The maximum theoretical power density of the designed cell was simulated to be 0.413 W cm^{-2}. Based on the results further work is advised into using different methods to produce the fuel cell in order to be able to produce thinner cells capable of producing equivalent current densities with lower temperature.

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