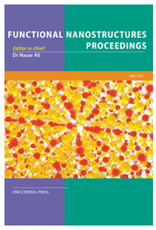
ONECENTRAL PRESS

Available online at www.onecentralpress.com

One Central Press

proceedings webpage: www.onecentralpress.com/functional-nanostructures-proceedings



A model for internal phenomena in a ceramic nanocomposite fuel cell

Riina Jokiranta[1,], Muhammad Imran Asghar[1] and Peter Lund[1]*

[1]New Energy Technologies Group, Department of Applied Physics, Aalto University, P.O. Box 15100, Fi-00076 Aalto, Finland.
[*]corresponding author

ABSTRACT

All the complex phenomena and processes in ceramic fuel cells are not yet fully understood. For example the degradation processes affecting fuel cell performance are still somewhat unclear and there are some stability problems with the cells. These phenomena need to be studied in detail to enable better performance and durability of fuel cells.

Fuel cell modelling is a valuable tool for understanding the electrochemical reactions and internal phenomena of fuel cells. With the help of modelling and validating the model with experimental data, new technologies can be developed and fuel cell operating conditions can be optimized.

A general 2D fuel cell model was created with COMSOL Multiphysics ® to simulate the behavior of an operational fuel cell. The model includes ion and electron transport, reaction kinetics, gas diffusion and thermal considerations at a moderate level of accuracy. In addition, a simplified engineering model with fundamental equations was created for comparison.

In the future, the 2D model will be developed further to account for degradation phenomena, temperature dependencies of the parameters and the composite nature of the electrolytes. Experimental data will also be gathered for use in validating the model and developing it further.

I. INTRODUCTION

The increasing global energy demand and the massive use of fossil fuels requires immense actions on renewable energy production. However, renewable sources are usually very unpredictable and thus need balancing power from other energy sources for large scale utilization to be possible. Fuel cells are one option for balancing the production, because they are reliable, efficient and produce no additional emissions when operated on hydrogen. They can be used for large-scale production as well as for smaller applications. [1]

Some obstacles still remain between fuel cells and commercialization, and conquering them requires a deep understanding of the fuel cell processes. Fuel cell modelling helps in building a bridge between theoretical knowledge and real life measurements.

II. FUEL CELL MODELLING

The constructed model consists of four different computational parts that each model a different real-life phenomenon and are coupled together to simulate the interactions of the parts. The cell is assumed to be in stationary state and thus no time-dependency is implemented.

One of these computational parts is the electrochemical model, which captures the electrochemical reactions at the electrodes, which produce an electric current. The cell potential is estimated and charge transfer kinetics considered thoroughly.

Mass is constantly generated and consumed at the electrodes, because the electrochemical reactions cause a flux of matter. Hydrogen is consumed and water is generated at the anode and oxygen is consumed at the cathode. Concentration gradients also cause mass transfer by diffusion. Mass transfer model considers these phenomena.

The cell is operated at 800 degrees Celsius, but heat is also generated in some parts of the cell due to exothermic cell reactions and ohmic heating. Conduction and convection are the routes of heat transfer, but in this model only conductive transfer is considered. Heat transfer model simulates this.

Boundary conditions. To match the real life situation as closely as possible, boundary conditions corresponding to measurement data are set to the cell geometry and modelling regions. In this way, a solution to the governing equations can be found. Some of the model parameters are from real measurements, and the rest are gathered from literature and are chosen to represent our reference case as accurately as possible.

Equations. Cell potential is calculated with

$$V = E_{OCV} - \eta_{ohm} - \eta_{act} - \eta_{conc}. \quad [2] \qquad (1)$$

The Butler-Volmer equation used for estimating the current is

$$i = i_0\left(exp\left(\frac{\alpha_a F \eta_{act}}{RT}\right) - exp\left(\frac{-\alpha_c F \eta_{act}}{RT}\right)\right), \quad [3] \qquad (2)$$

and the Nernst equation for SOFC is stated as

$$E = E^0 + \frac{RT}{2F}\ln\left(\frac{P_{H_2,a}P_{O_2,c}^{\frac{1}{2}}}{P_{H_2O,a}}\right). \quad [1] \qquad (3)$$

Structure. The modelled 2D cell consists of three layers: anode, cathode and electrolyte. The electrodes are separated by the electrolyte and the air and fuel inlets are modelled as fine meshes. The 1D cell in the engineering model is modelled as a series of simple resistors.

Materials. The materials used in the reference measurements are common SOFC materials. The electrolyte is SDC, the anode 50% SDC and 50% NiO and the cathode 50% SDC and 50% LSCF. The model assumes the electrodes to be only from the electrode material without the electrolyte SDC.

III. RESULTS AND DISCUSSION

The modelled cell open circuit voltage is higher than in real life, and this is due to the ideality of the model. Many losses are neglected for simplicity is this model version. Figure 1 shows the ionic potential distribution in the cell. The cathode has a lower voltage and the direction of the current is from anode to cathode. This seems to be the opposite of a normal SOFC, which might indicate a different charge carrier, for example H+, but this needs to be studied in more detail to know for sure.

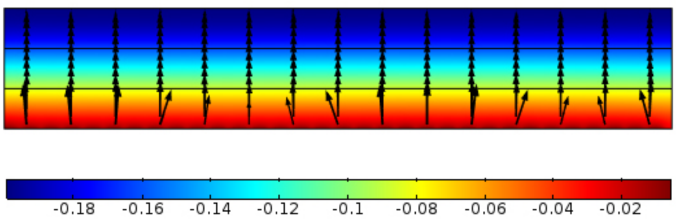


Figure 1 Ionic potential distribution (V) and ionic current density vectors in the 2D simulation (cell potential 0.6V).

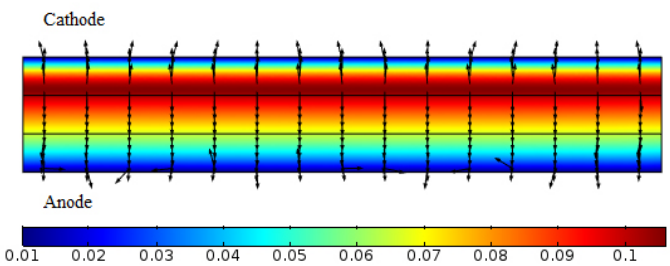


Figure 2 Temperature distribution (K over 800C) and total heat flux vectors in the 2D simulation (cell potential 0.6V).

Figure 2 shows the temperature distribution in the cell. The temperature differences seem to be very small, but there is an exothermic reaction taking place at the cathode near the border of the electrolyte. This might be due to the hydrogen ions combining at the cathode instead of the oxygen ions at the anode.

The validation of the models is done by comparing the cell JV curves as illustrated in Figure 3. The 2D model fits the experimental results [4] quite well, even though it is a bit optimistic. The 1D model has very little losses and is therefore further from the experimental data.

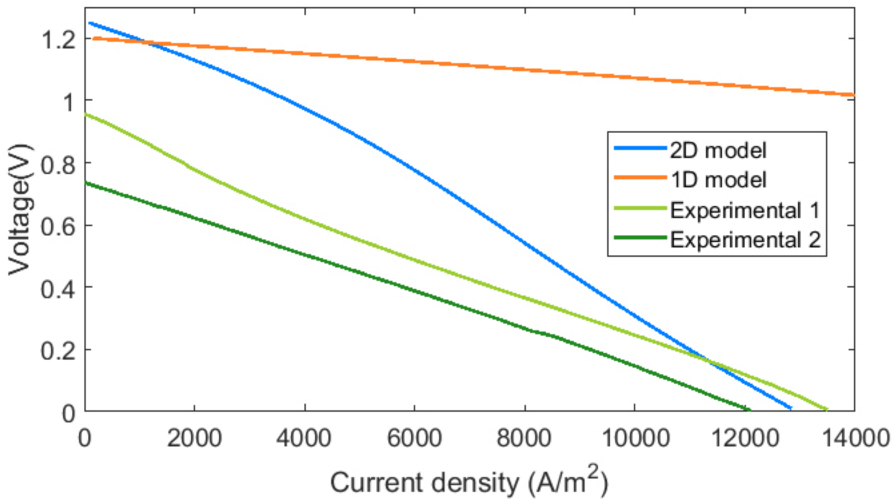


Figure 3 Comparison of the modelled and experimental JV curves from 1D and 2D simulations and nanocomposite cell measurements.

In the future, the model parameters need to be adjusted to the measurement conditions better and the simplifications made in the model need to be corrected to better correspond to reality. Degradation phenomena, cell losses and more accurate diffusion mechanics need to be added and the composite nature of the electrodes has to be taken into account. Tertiary current distribution can be used, and thermal expansion phenomena, cracking of the cells and penetration depth of gases should be studied.

IV. SUMMARY

Fuel cell modelling helps in understanding the complex cell phenomena and in designing new technology and predicting cell behavior. Modelling can be used to do the groundwork before putting resources into measurements.

The 2D model gave some fairly good results which are in line with the experimental data, even if a bit optimistic due to neglected losses. The 1D model also captured the essential behavior of the cell and will be used to test parameters and cell configurations quickly and suggestively. The 2D model will be developed in the future to account for the simplifications made in this version.

V. ACKNOWLEDGEMENTS

The authors especially thank Academy of Finland for their financial support (Grant No.13282962) with the framework of EU New Indigo programme.

VI. REFERENCES

[1] Ryan O'hayre et al. Fuel cell fundamentals. John Wiley & Sons, 3rd edition, 2016.

[2] Subhash C. Singhal and Kevin Kendall. High-temperature Solid Oxide Fuel Cells – Fundamentals, Design and Applications. Elsevier Advanced Technology, Oxford, 2003.

[3] Allen J. Bard and Larry R. Faulkner. Electrochemical methods: fundamentals and applications. Wiley, 2nd edition, New York (N.Y.), 2000.

[4] Asghar, M. I., Heikkilä, M., Lund, P. D., Advanced low-temperature ceramic nanocomposite fuel cells using ultra high ionic conductivity electrolytes synthesized through freeze-dried method and solid-route, accepted in Materials Today Energy, 2017.