

Modelling of a Reversible SOC in Ansys Fluent

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Reversible Solid Oxide Cells (SOC) are quite susceptible to variations in operating parameters, and especially the switching of operating modes is not yet well understood. Effects like thermal stress from changes in the current density pattern, as well as carbon deposition and nickel oxidation can destroy SOC. Thus, in order to design a robust SOC system a SOC stack model has been built in ANSYS Fluent 17.0. In this work, this model is used to study the impact of operating mode transition from fuel cell to electrolysis on the stack. It is found that the thermal gradients resulting from switching operation modes are largely depending on the gas compositions fed during both operating modes. Therefore, at fixed operating temperature especially by adjusting the gas feeds thermal gradients can be flattened, so that their effect on the lifetime of the SOC can be significantly reduced.

Introduction

Solid Oxide Cells (SOC) are capable of converting fuel into electrical energy and reversing its operation to produce fuel for storage. Therefore, reversibly operated SOC represent a promising technology considering the compensation of intermittent electricity production from renewable energy sources, such as wind and photovoltaics. However, SOC are quite susceptible to variations in operating parameters, and especially the switching of operating modes is not yet well understood. Effects like thermal stress from changes in the current density pattern, as well as carbon deposition and nickel oxidation can destroy SOC almost immediately, or at least largely affect the lifetime via long-term degradation. Thus, in order to design a robust SOC system, these aspects have to be investigated in detail.

For this purpose a SOC stack model has been built in ANSYS Fluent 17.0. The SOC geometry and performance has been adjusted to fit experimental data. In this work, the model is used to study the impact of operating mode transition from fuel cell to electrolysis on the stack. In fuel cell (FC) mode, fuel gas is fed to the fuel electrode (FE) and air is fed to the oxidizer electrode (OE) to produce electrical energy via the oxidation of hydrogen into water. Other gases, such as methane can be alternatives as the fuel source as internal reforming is possible in the cell (1). In electrolysis (EC) mode, electrical energy is consumed to split water molecules into hydrogen and oxygen gases, which can be stored separately. Besides the common steam electrolysis, SOCs are capable of undergoing carbon dioxide electrolysis (co-electrolysis), meaning harmful

greenhouse gases can be eliminated and converted into useful fuel (2,3). Furthermore, the concept of SOC enables flexible switching between electricity generation mode and relatively easier storage in the form of fuel when there is no demand for electricity. When operated on biogenic fuels potentially even system configurations with negative net CO₂ emissions are possible (4,5).

This study aims to investigate the switching processes between fuel cell and electrolysis operating modes. Firstly, the SOC model in ANSYS Fluent is adapted to perform transient CFD simulations. Important settings and methods of carrying out transient simulations efficiently are tested and improved. An optimal set of settings and methods are determined to achieve balance between reasonable computational time and reliable results. Based on a readily available Fuel Cell and Electrolysis Module in Fluent, dynamic simulations are carried out to identify the critical parameters present in the mode switching processes. Suitable countermeasures are proposed and implemented to tackle the critical parameters to achieve stable operation for the SOC during switching processes between operating modes.

Fuel Cell Model in Ansys Fluent

The SOC stack is modelled as a stripe cut out of one cell/interconnect layer of a stack, since a stripe is the smallest repeating unit in an SOC stack. The calculation mesh is shown in Figure 1. Here, the section in red color represents the fuel channel (FC anode), while the section in light blue represents the oxidizer channel (FC cathode). As the cell type is fuel electrode-supported, the thicker porous fuel electrode is below the thinner porous oxygen electrode. The thin layer of electrolyte is sandwiched between the both. The electrolyte only allows transfer of ions and prevents the diffusion of gases. The transfer of electrons is facilitated by the external circuit via the current collectors, which are surrounding the gas channels respectively as shown in grey color in the figure.

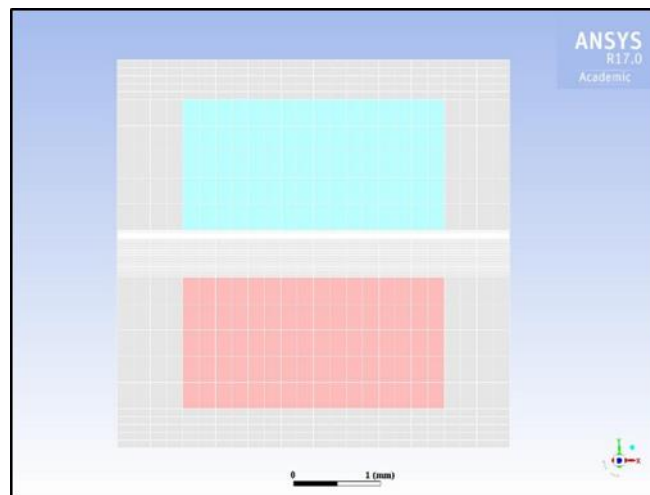


Figure 1. Cross-section view of the SOC stripe model.

Fuel and oxidizer gas streams are set up in a counter-flow arrangement. Previous studies showed that counter-flow yields a more uniform temperature profile along the flow direction. As an assumption the boundary conditions are set as adiabatic. The

respective geometry parameters, which are typical for anode supported SOFCs, are provided in Table I.

Via an implemented User Defined Function (UDF) calculating volumetric reaction kinetics retrieved from Boder et al. and Habermann et.al., the model is capable to perform internal steam reforming of methane, as well as the water gas shift reaction (6,7).

TABLE I. Dimensions of the Fuel Cell Stripe Components.

Parameter	Value	Unit
SOC Cell Stripe Length	100	mm
SOC Cell Stripe Width	3	mm
FE Diffusion Layer Thickness	0.3	mm
FE TPB Layer Thickness	0.01	mm
Electrolyte Thickness	0.012	mm
OE Diffusion Layer Thickness	0.04	mm
FE TPB Layer Thickness	0.01	mm
Current Collector Thickness	0.3	mm
FE Flow Channel Height	1	mm
OE Flow Channel Height	1	mm
FE Flow Channel Width	2	mm
OE Flow Channel Width	2	mm

Uniform inlet flow perpendicular to the boundary is assumed. Boundary conditions such as gas mole fractions, inlet gas temperature and mass flow rates are defined at the anode and cathode inlets. The current density and cell voltage can also act as manipulating variables to influence the cell operation.

The electrochemical model parameters have been adjusted to obtain the performance of typical SOC stacks from Blum et. al. (8). A comparison for the fuel cell operation at identical operating conditions is shown in Figure 2. As can be seen the performance matches well with the experimental results for all operating temperatures between 650-800°C.

Operation at Steady State

Before the transient operation steady states for both, FC and EC operation are simulated. These serve as starting point for the transient operation, as well as to verify that the transient has been completed.

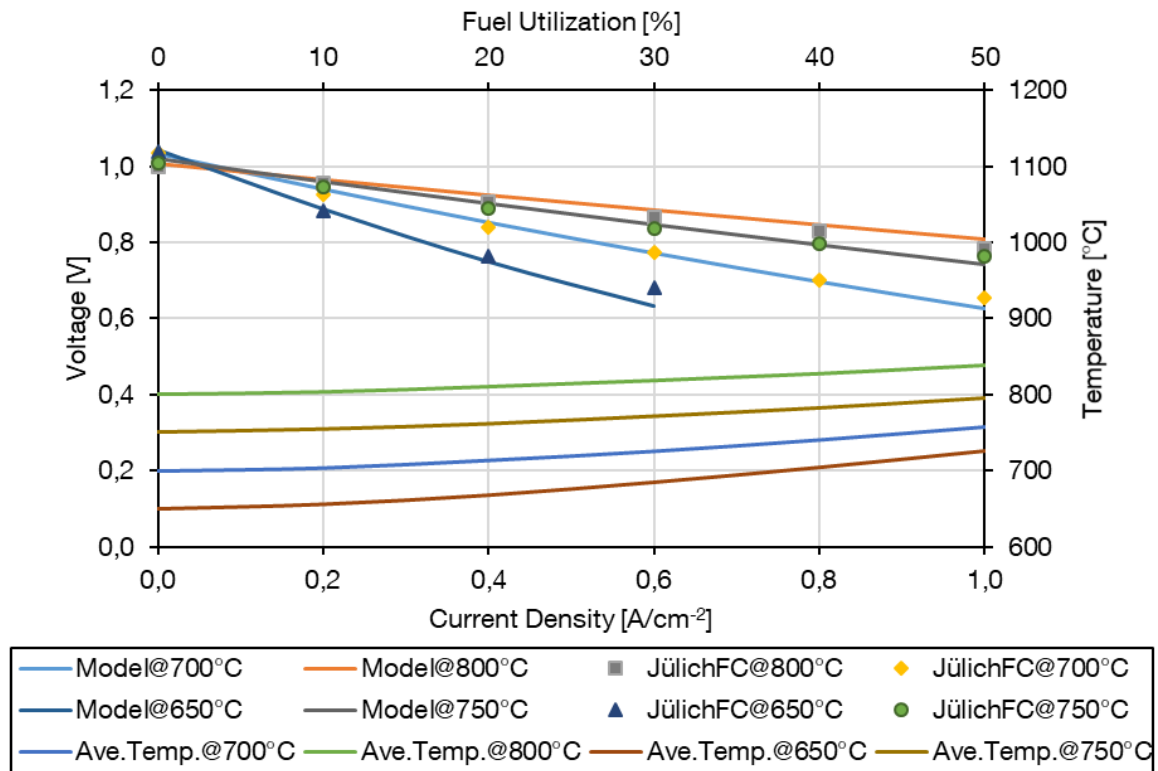


Figure 2. Electrochemical performance validation of the SOC model against real stack data from Blum et. al. (Jülich) (8).

Fuel Cell Operation

In the FC mode, the SOC is fed with a fuel mix containing mainly methane and steam, representing typical operation on natural gas. It is found that for stability reasons some hydrogen has to be added because otherwise the simulation does not converge well, since the gas composition changes dramatically due to the internal reforming near the inlet. Table II displays the fuel cell operating conditions.

TABLE II. Operating Conditions for the RSOC Model in Fuel Cell Mode.

Parameter	Value	Unit
Hydrogen	12	mol-%
Water	60	mol-%
Methane	28	mol-%
Carbon Monoxide	0	mol-%
Carbon Dioxide	0	mol-%
Oxygen (OE, Rest N ₂)	21	mol-%
Inlet Temperature FE	973	K
Inlet Temperature OE	973	K
Inlet Fuel Mass Flow Rate	1.39E-07	kg/s
Inlet Air Mass Flow Rate	4.50E-06	kg/s
Cell Voltage	0.82	V
Current Density	0.50	A/cm ²
Fuel Utilization	0.7023	-

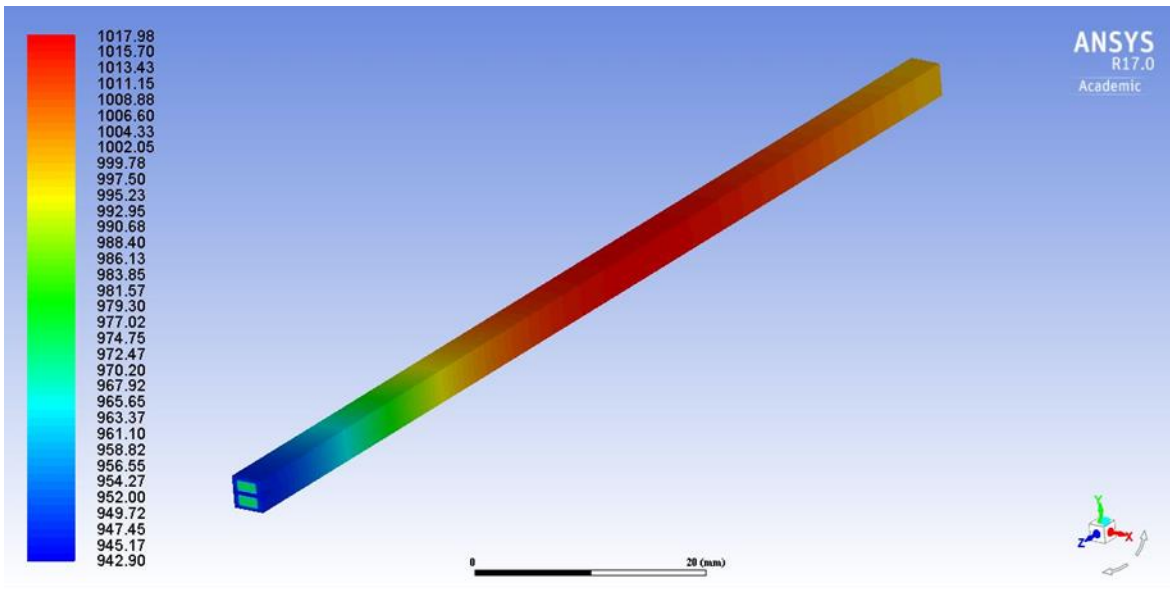


Figure 3. Temperature profile of the stripe during fuel cell operation. FE inlet and OE outlet are located on the left side, temperatures are given in K.

Figure 3 shows the temperature profile of the stripe in FC mode. At the entrance of the fuel channel, fuel gas flows in with an initial temperature of 973 K and immediately shows a sharp temperature drop, mainly due to endothermic effects of the internal methane reforming reactions. The temperature then steadily rises to a peak at around the middle of the cell and gradually decreases flowing out towards the end of the fuel channel. The second temperature drop is caused by the cooling effect of the incoming air from the opposite direction.

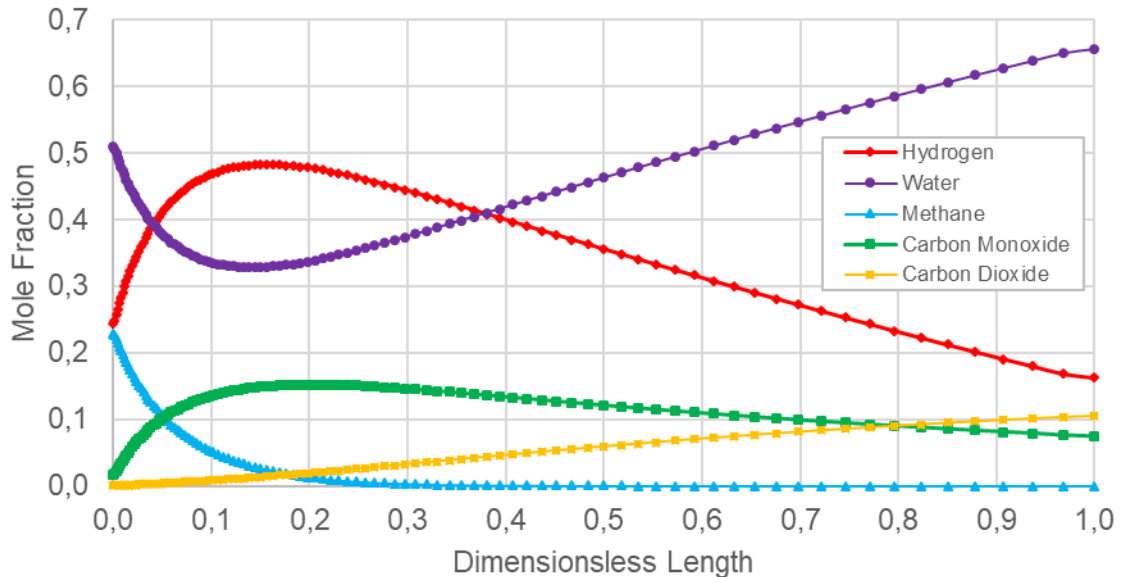


Figure 4. Gas composition along the fuel channel during fuel cell operation.

Figure 4 displays the mole fraction distributions along the cell. At the entrance of the fuel channel the endothermic internal reforming reactions dominate the evolution of species concentrations, which corresponds to fast methane and water consumption. When

the methane is depleted, oxidation and water-gas-shift reactions take the lead, resulting in the formation of water and the conversion of carbon monoxide into carbon dioxide.

Electrolysis Operation

Figure 5 depicts the temperature profile along the cell during electrolysis. The standard configurations including operating temperatures, fuel utilization, current densities and cell voltages can be seen in Table III.

TABLE III. Operating Conditions for the RSOC Model in Electrolysis Mode.

Parameter	Value	Unit
Hydrogen	10	mol-%
Water	70	mol-%
Methane	0	mol-%
Carbon Monoxide	0	mol-%
Carbon Dioxide	20	mol-%
Oxygen (OE)	100	mol-%
Inlet Temperature FE	973	K
Inlet Temperature OE	973	K
Inlet Fuel Mass Flow Rate	1.00E-06	kg/s
Inlet Oxygen Mass Flow Rate	1.00E-08	kg/s
Cell Voltage	1.30	V
Current Density	1.1755	A/cm ²
Oxygen Utilization	0.4378	-

Both channels receive an inflow of gases with an initial temperature of 973 K. In comparison to fuel cell mode no air is fed and pure oxygen is formed at the OE. The much lower mass flow of oxygen gas does not provide a significant cooling effect. Hence, the temperature of the cell retains its increasing trend from the FE entrance to the outlet.

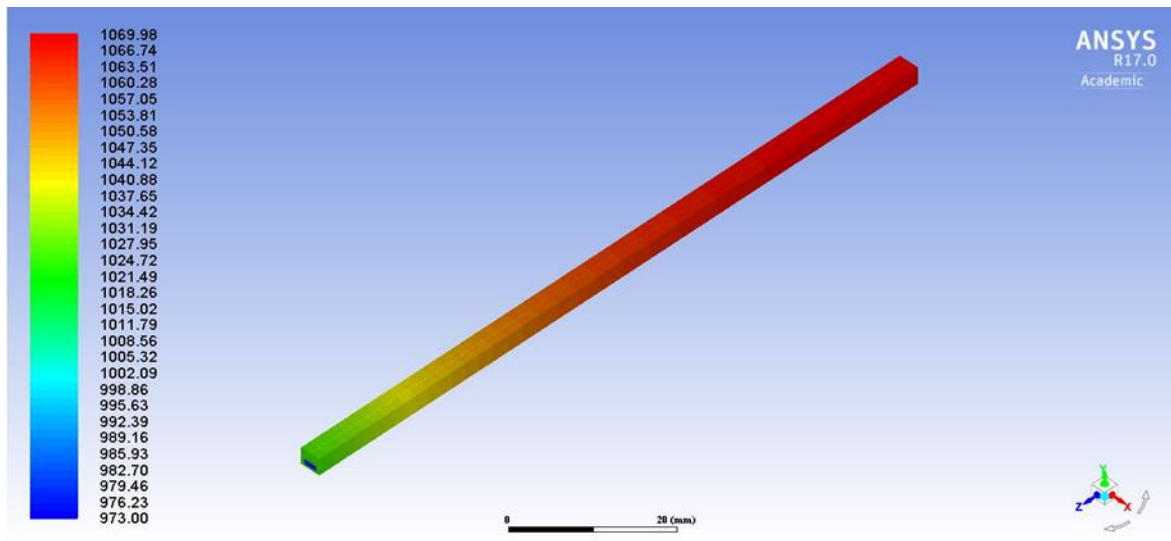


Figure 5. Temperature profile of the cell stripe during electrolysis operation.

Figure 6 presents the mole fraction distributions of the gases along the cell. During co-electrolysis, the gas consisting mainly of water and carbon dioxide is converted into hydrogen, oxygen and carbon monoxide. The steadily decreasing concentrations of water and carbon dioxide along the cell validate the occurred reactions.

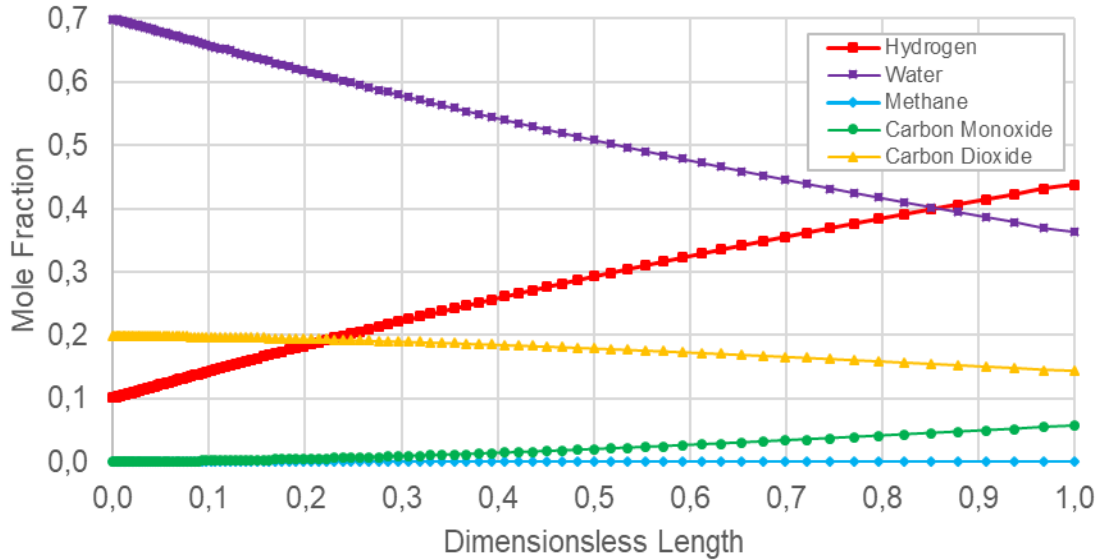


Figure 6. Gas composition along the fuel channel during electrolysis operation.

Comparison of Steady States

During transient mode switching the temperature profiles are expected to change from the initial to the respective final steady state. Therefore, first of all the two steady states are compared in terms of the difference in temperature along the cell. Figure 7 displays the difference in temperature (averaged in the x-y-plane) along the cell between electrolysis and fuel cell steady states. It can be seen that there is a significant difference, especially at the FE outlet/OE inlet side of the cell stripe. Thus, large temperature gradients should be expected at this position.

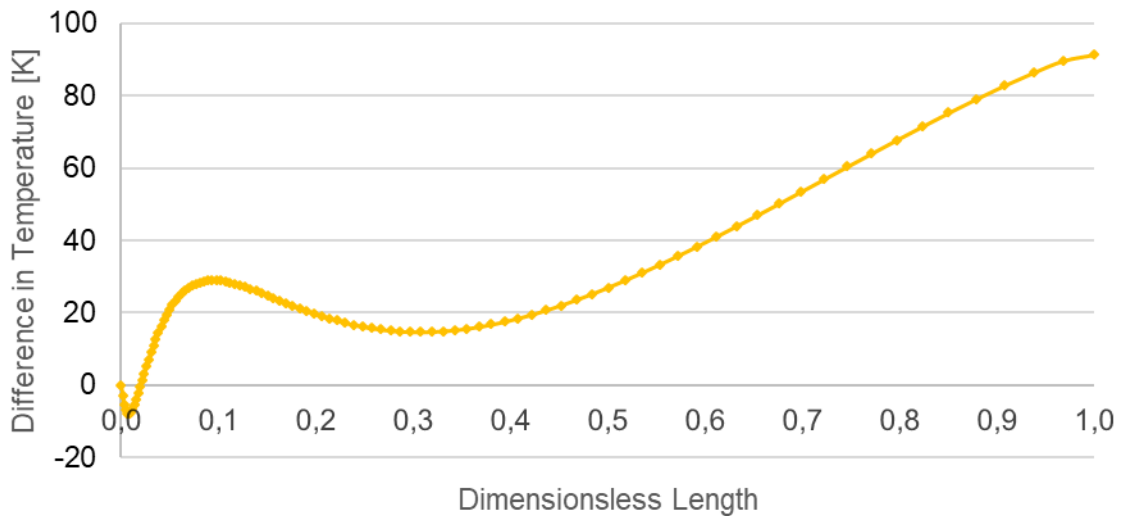


Figure 7. Deviation of temperature along the cell stripe comparing fuel cell and electrolysis operation.

Transient Simulation of Switching Operating Modes

Peak Temperature Evolution

Figure 8 shows the evolution of maximum temperatures of the FE (denoted as Anode) and OE (denoted as Cathode) gas channels during the switch from FC to EC. It is noteworthy that both gas channels exhibit the same maximum temperature from the beginning of the mode switch until reaching the EC steady state after around 1200 s. Initially the maximum temperature drops about 10 K, which is followed by a gradual increase until about 1105 K.

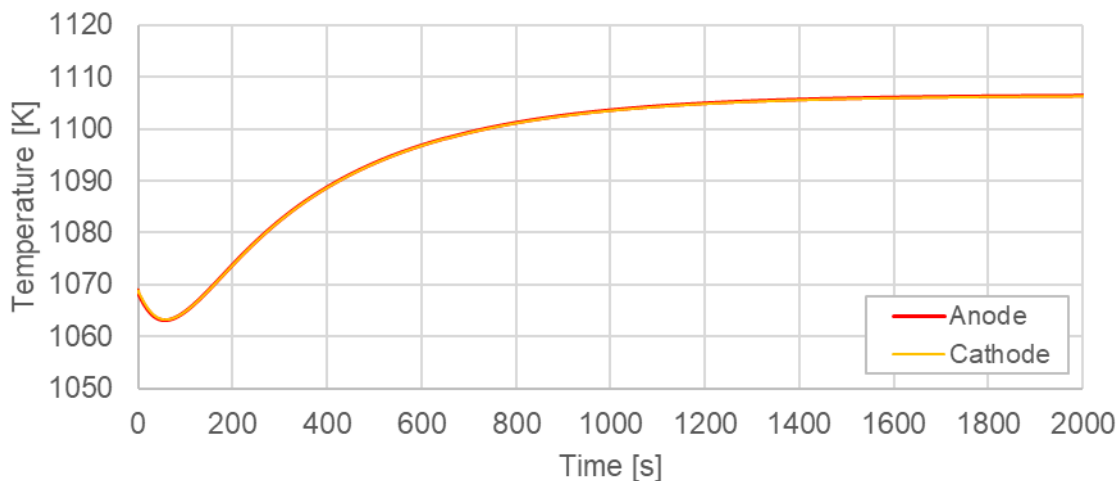


Figure 8. Evolution of the maximum temperature of the FE (Anode) and OE (Cathode) channels during transition from FC to EC operation.

This is due to a shift of the temperature peak from the mid to the FE outlet of the cell stripe. While the mid of the cell cools down because of the higher FE mass flow, thus initially decreasing the maximum temperature, the FE outlet temperature rises, surpasses the mid-channel temperature and therefore becomes the maximum temperature. Overall, the temperature gradients observed in the gas channels are higher than the maximum gradients of 1-3 K/min usually stated as tolerable for SOC stacks.

Temperature Gradients in SOC Functional Layers

Therefore, the evolution of the average temperatures of the major individual cell components of the SOC is also studied during the transient simulation of switching from FC to EC mode. These include the catalysts, current collectors and gas channels of FE and OE, and also the electrolyte layer separating both gas channels.

Figure 9 displays the results for only the first 0.2 seconds after mode switching (where the gradients are largest) for a clearer comparison of the temperature changes. It is discovered that most cell components, with the exception of FE catalyst in this case, experience relative smaller changes in temperature despite big variations in the gas channels. The temperature of the FE support layer (Catalyst_A) shows a similar trend to that of the FE gas channel (Channel_A). Due to their high respective heat capacity and thermal conductivity the current collectors (C.C._A/C) are not affected very much by the transient.

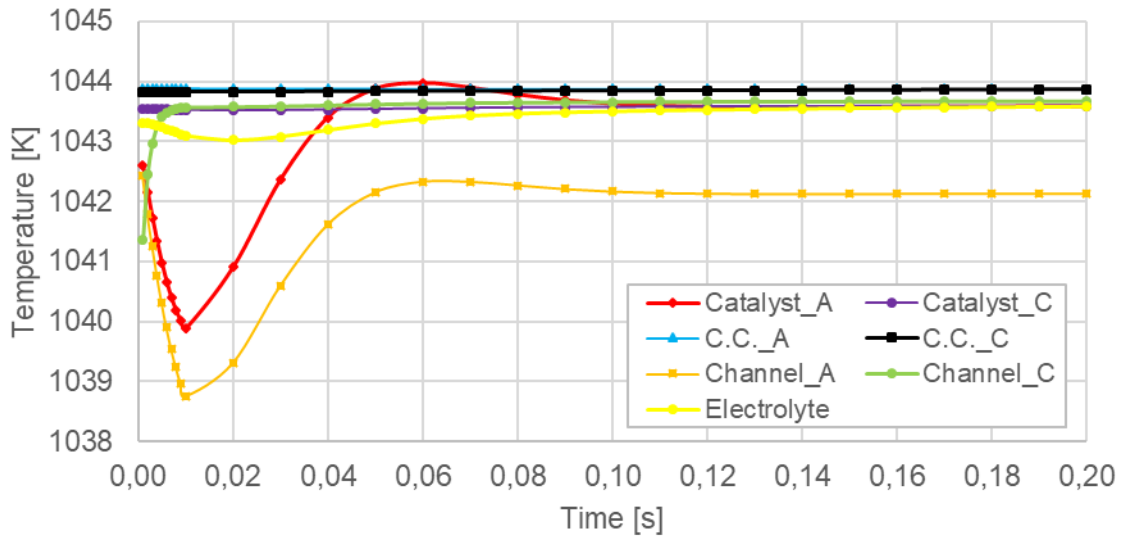


Figure 9. Evolution of the average temperature in the different cell layers during the initial 0.2 seconds of mode switching from fuel cell to electrolysis.

While the electrolyte, as the most critical layer, shows minimal substantial temperature changes, the other cell components show no immediate response to these changes in temperatures of the gas channels. This is essential, as it demonstrates that material damage caused by thermal stress may still not be very likely, even when strong changes in gas temperatures occur in a very short span of time.

Temporary Fuel Starvation

However, another critical aspect may originate from the fuel channel composition. As can be observed in Figure 10, during switching from EC to FC operation, an initial starvation of hydrogen and carbon monoxide can occur in the fuel channel. This may lead to a short period of absence of the reducing environment and may therefore lead to nickel oxidation, potentially resulting in irreversible damage of the FE structure.

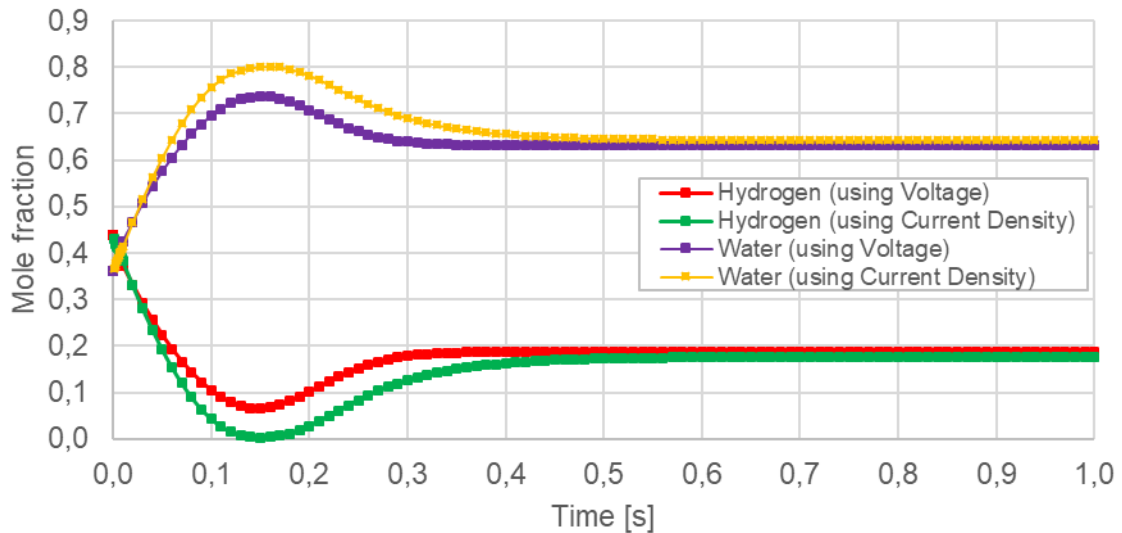


Figure 10. Evolution of the average H_2 and H_2O concentrations in the fuel channel during the first second of mode switching from EC to FC.

As is shown in the figure, this problem can only occur when the switching is done into a galvanostatic (current density controlled) state. If a potentiostatic (voltage controlled) switching is performed, this problem can be avoided, since in this case the current density will be reduced for a short period of time, while the FE gas is exchanged to the FC composition.

Summary

The main objective of this work was to study the transient processes occurring during the switch of operation between fuel cell mode and electrolysis mode in a SOC by means of CFD simulation. Based on a stripe cell model, transient simulations have been carried out using an adapted version of the Fuel Cell and Electrolysis Module in ANSYS Fluent.

Dynamic simulations of switching operation modes between fuel cell and electrolysis modes were then performed using typical operating conditions. The transient simulations were done with reference to acquired results of steady state simulations of both operation modes. It could be shown that continuous monitoring of the important parameters, such as temperature of cell components, mole fractions of gas components along the cell, cell voltage, and current densities is of a high priority to ensure safe operation of the SOC. By adjusting the operating conditions during switching critical situations, such as high temperature gradients or temporary fuel starvation can potentially be avoided.

Acknowledgements

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