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Validation of Engineering FEA Predictive Sintering Models of Steel Supported SOFCs

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Abstract

Ceres Power has a unique low temperature, metal supported SOFC design (the SteelCell™) based predominantly around the use of ceria. This unique architecture allows for a robust, low cost, subsidy free fuel cell product, whilst retaining the advantages of fuel flexibility, high efficiency and low degradation.

Predicting the evolution of thermal stress during fuel cell manufacture processing is important in the design and manufacture of metal supported SOFC. Catering for thermal stresses during manufacturing enables higher process yields; and during the cell and stack design processes, results in more mechanically robust modules for higher performance and improved durability.

In a collaborative project between Ceres Power and Lancaster University, funded by Innovate UK, an engineering FEA model has been developed to understand the role of thermal stresses in the manufacturing processes. In such a model, material properties, such as the thermal expansion coefficient, Young's modulus, layer densification rates and creep, are very important. These properties, when interacting with the applied thermal processes, give rise to stresses within the fuel cell layers, resulting in permanent deformation and residual stresses at room temperature at the end of the processing steps.

Experimental validation of such models is important to ensure their predictive capability. This work is a follow-up investigation of a sintering model previously presented and consists of a series of validation experiments that were performed for this purpose. More specifically, varied boundary conditions were applied in both the simulations and the experimental environment resulting the different deformed shapes. The results were compared to prove there is good degree of confidence in the results.

Introduction

The combination of low operating temperature (and thus the ability to use low-cost materials in the stack and balance of plant (BOP)), metal support and careful optimisation of the microstructure of the ceramic layers in the SteelCell™ allows for low cost stack and BOP components and state-of-the-art robustness to real-world operating conditions, whilst maintaining high efficiency using real world fuels.

More specifically, the SteelCell™ consists of a ferritic stainless steel foil, which is perforated to create a gas permeable central region surrounded by an impermeable outer region. A thick-film cermet anode is deposited over the perforated region of the substrate, but not on the impermeable surround, delimiting the active area of the cell. An electrolyte is deposited over the anode and overlaps onto the surrounding steel, forming a seal around the edge of the anode. The electrolyte is a composite structure consisting of a thick-film CGO layer, which provides mechanical integrity and gas-tightness, a thin-film electron blocking layer to block electronic conductivity through the mixed-conducting CGO, and a thin film CGO layer providing a barrier layer between the composite electrolyte and the cathode. The cathode has a conventional structure of a thin active layer where the oxygen reduction reaction occurs and a thicker bulk layer for current collection. The cathode electro-catalyst and current collector are perovskites; the exact choice of perovskites contributes significantly to the outstanding stability of the cells to thermal cycling. The combination of these materials allows the SteelCell™ to operate at low temperatures (500 – 620 °C) compared to conventional SOFCs, but also have great mechanical robustness, whilst maintaining high volumetric power density (Figure 1).

One of the main reasons that the SteelCell™ is so robust is its unique manufacturing process. The combination of materials preparation and processing give the SteelCell™ high mechanical stability and performance. Understanding the stress evolution and distribution during manufacturing as well as the residual stresses after is very important, because it gives an insight to how the cell will behave under the desired operating conditions, further enhancing the rapid development of the Ceres Power products [1, 2].

For this work, thermal treatment of the SteelCell™ was simulated by means of Finite Element Analysis. The aim was to understand how the cell deforms under different constraints when exposed to high temperatures.

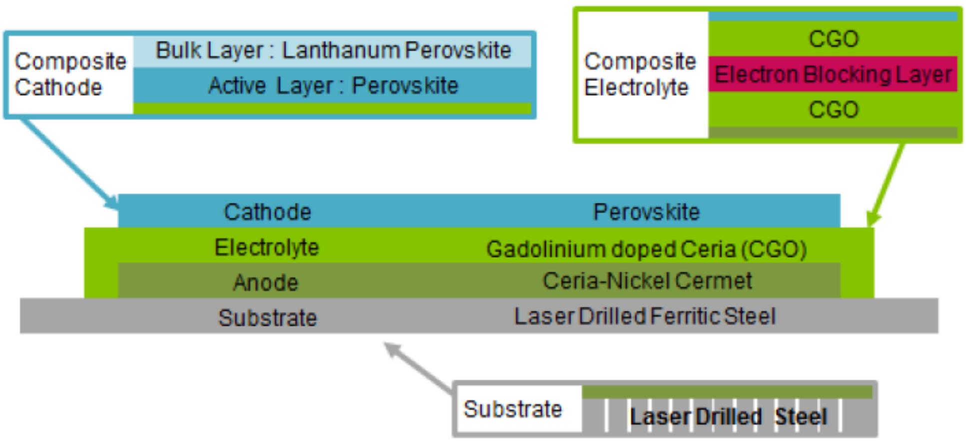

Figure 1 Schematic representation of a Ceres Power SteelCell™.

1. Simulation Approach

There has been a lot of FEA development on predicting mechanical conditions of SOFC stacks in large scale trials, as rapid failure, thermal cycling intolerance and step change in electrochemical performance have been observed, which seemed to be linked to poor mechanical structure [3]. However, most of these models assume stress-free initial conditions, leading to inaccurate results.

The use of Finite Element Analysis is very important for understanding SOFC development. Since the SteelCell™ is a combination of a metal substrate and ceramic layers with different thicknesses, it is essential to have an insight of how these materials behave at high temperatures. The results of such simulations can be used as an input to large scale models resulting in better accuracy.

The model was built to successfully converge and also be computationally efficient. The layers that are simulated are the substrate, anode and thick-film electrolyte layer. These layers constitute the most significant parts of the cell, the successful formation of which largely dictates its overall form. Therefore, the simulation primarily concentrated on the formation of these layers and the results presented here exclude the remaining processing steps towards the full cell.

The models created to predict such distortion [2], were modified to represent a SteelCell™. More specifically, the geometry was edited and different boundary conditions were applied. The validation was focused on measuring permanent deformation of the cell and compare it with simulation results.

2. Simulations

The software used for the presented simulations is ABAQUS.
The details of the model's setup are presented below.

<u>Geometry / Assembly</u>

A simplified SteelCell™ geometry (Part) was imported in the software, where all round entities and minor details were removed.

The Part was placed on a flat rigid surface through the whole simulation.

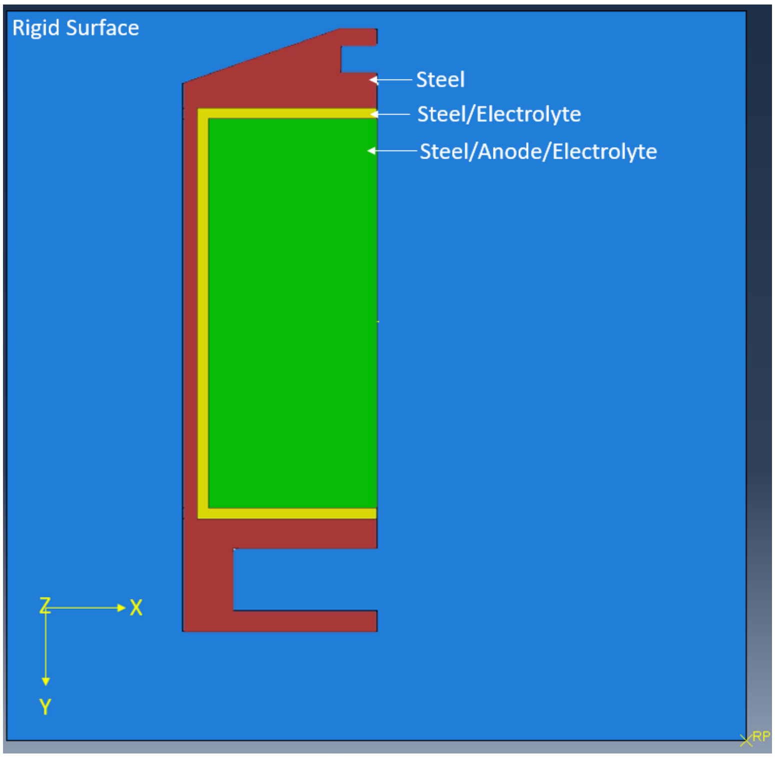

Figure 1 Simulation assembly.

Steps

As the ceramics become denser during high temperatures, it is very important to understand how the steel behaves during this process. To ensure that the simulation runs without computational problems, in this modelling experiment the end temperatures are achieved in steps. This is a sample thermal treatment to validate the engineering model, rather than the actual cell manufacturing process.

Interactions

ABAQUS captures the frictional interaction and hard contact between the cell and the rigid surface that the cell is placed on during processing.

Boundary Conditions

To minimise the need for computational resources, symmetry boundary conditions were applied on the Y axis (half symmetry) for all the simulations.

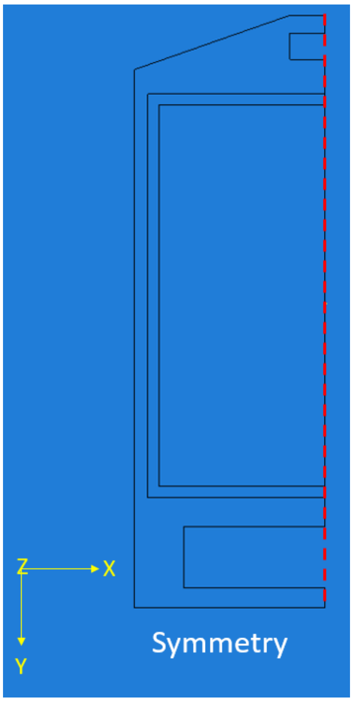

Figure 2 Boundary condition.

Different boundary conditions were applied to understand how constraints affect distortion when non-densified thin ceramic layers are fired at high temperature and to enable improved validation of the model. More specifically, three different constraints were applied as shown below.

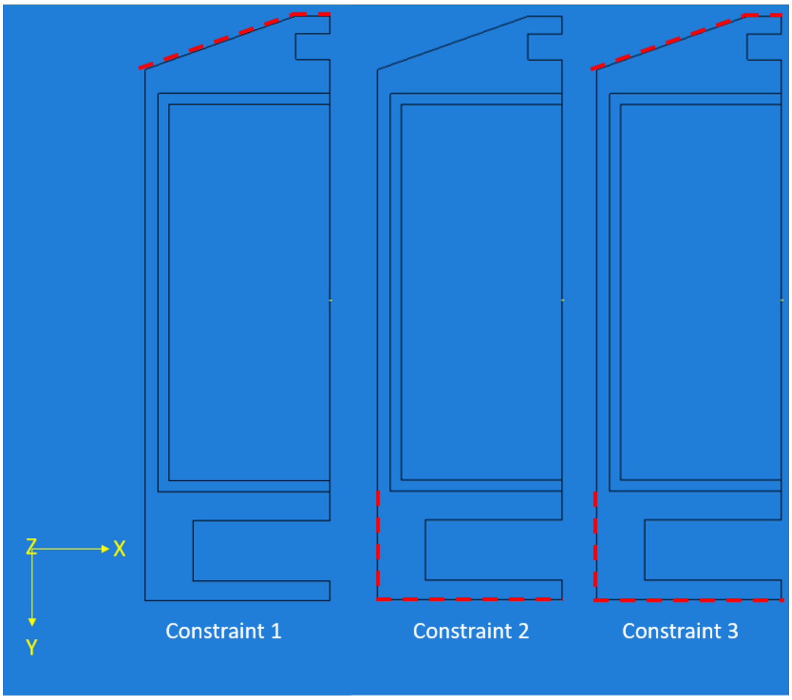

Figure 3 Constraints.

Materials

By identifying the critical material properties this simulation effectively captures the evolution of layer deformation during firing. For the purposes of this work the properties of the following materials were measured using proprietary techniques:

- Anode: CGO based NiO ceramic
- Electrolyte: CGO based ceramic
- Substrate: Ferritic steel [2].

3. Experiments

To validate the predictability of the described model, cells were placed in a chamber furnace and fired to the temperature profile used for the simulations.

The same constraints as in the simulations were applied. A suitably capable measurement process was applied to produce 3D surface graphs. These graphs were used to map the distortion of the real parts and compare it with the simulation results.

4. Results

The permanent deformation of the cell after a thermal process was studied, as this result can easily be used for correlation purposes. As mentioned above, the simulations were run for the three different constraint sets, which were applied on real test parts. 3D surface graphs of the whole part were created from the data gathered after the experiments. Due to the complexity of the measurements, not all noise could be removed from the experimental graphs.

The following figures show that the experimental data is in good agreement with the simulation results.

In Figure 4 the constraint is applied at the upper end (side marked as A) of the cell, which results in displacement of the outer side and the lower end (side marked as B). This is also shown in the 3D surface graph obtained from the experiments.

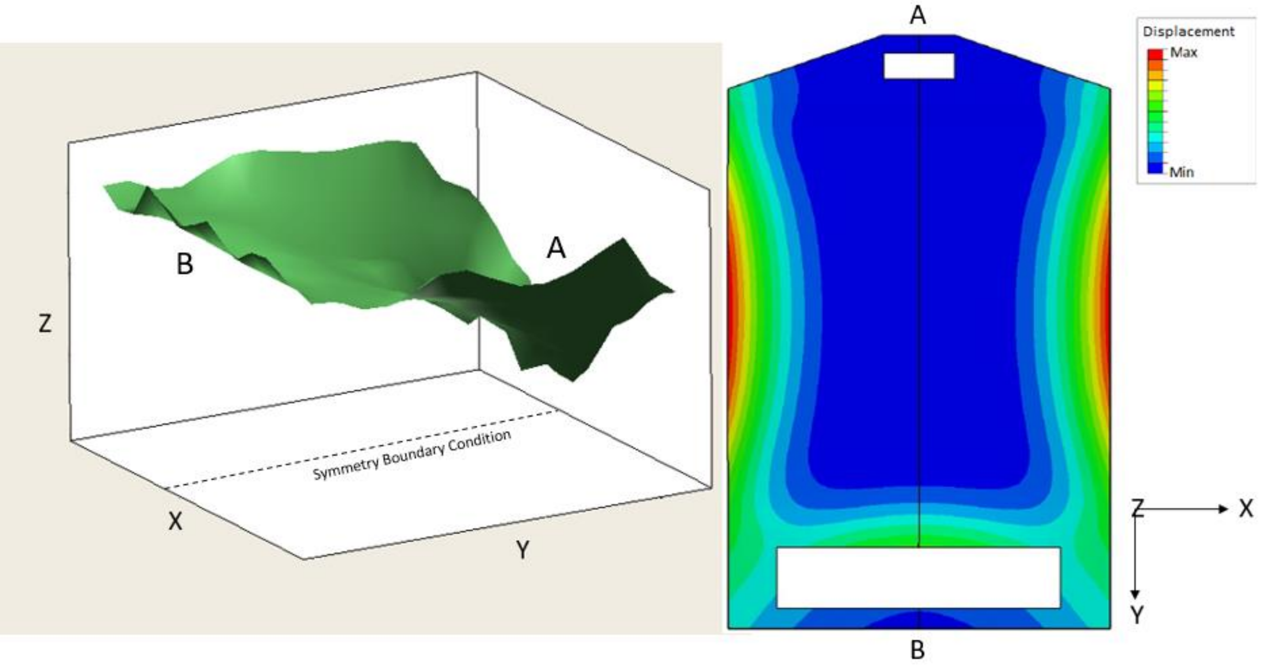

Figure 4 Constraint 1: 3D surface plot and simulation results.

Similarly, in Figure 5 the outer side, as well as the upper end (A) of the cell are distorted. Finally, in Figure 6, where both the ends of the cell (A and B) are constrained, only the outer sides of the cell are distorted.

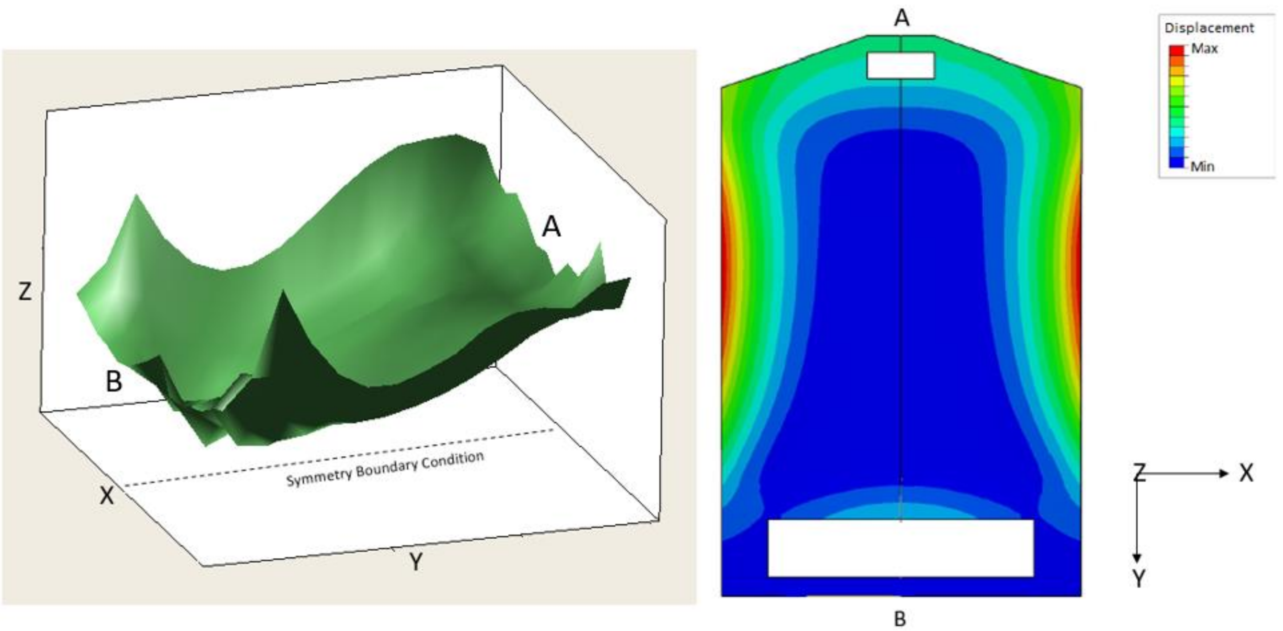

Figure 5 Constraint 2: 3D surface plot and simulation results.

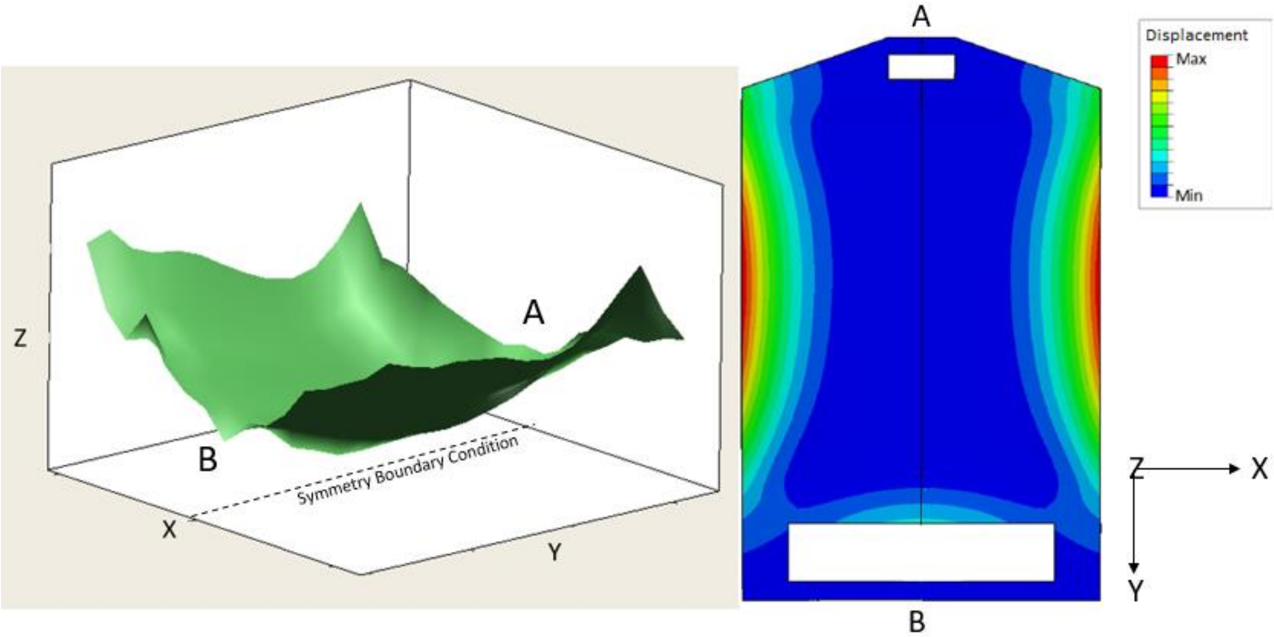

Figure 6 Constraint 3: 3D surface plot and simulation results.

As the ceramic particles sinter together, the ceramic layers shrink, causing residual stresses, leading to permanent deformation of the steel. Depending where the constraints are during a thermal process the distortion differs, but the centre of the cell remains un-distorted in all three examples. These are examples of how this modeling tool can be used to predict distortions of the SteelCell™ from the manufacturing processes used.

5. Conclusions

In summary, this paper demonstrates the predictive capability of the developed FEA engineering model using experimental data performed to validate the presented simulations. This model has huge advantages in enhancing and understanding the behaviour of the SteelCell™ at high temperatures. The demonstrated capability can be used towards the optimisation of thermal processes, such as manufacturing, as well as feeding into future process and cell designs. Such models and techniques are being developed at Ceres Power and are used towards next generations of steel cells to reduce process waste in a lean manufacturing environment.

6. Further Work

To further enhance the predictability of the presented model, further measurements and experiments can be performed. More specifically, the stresses in ceramic layers after thermal processing are of great interest to improve the validity of the model. By validating the residual stresses predicted from simulations, this predictive tool becomes more valuable as it will increase the confidence and accuracy of the results for any future cell and manufacturing design.

Acknowledgments

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