camelot

UNDERSTANDING CHARGE, MASS AND HEAT TRANSFER IN FUEL CELLS FOR TRANSPORT APPLICATIONS

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DELIVERABLE REPORT

D5.3 – FFC BASED RECOMMENDATIONS OF NEXT GENERATION MEAS IN SRU GEOMETRY	
Due Date	M42
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PU	*Public*	***X***
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NATURE OF THE DELIVERABLE		
R	*Report*	***X***
P	*Prototype*	
D	*Demonstrator*	
O	*Other*	

SUMMARY	
Keywords	*Simulations, Performance, MEA, Single Repeating Unit*
Abstract	*Design recommendations from the MEA version of FAST-FC are implemented at the SRU level and simulated to assess the impact in achieving the targeted Beyond-SoA performance of >670mV at 2.7 A/cm2. It was found that some of the recommended changes did not yield improvements due to the along the channel effects at the SRU level and these changes were discarded while the remaining changes were implemented and then combined with operational levers to deliver a simulated performance that met the Beyond-SOA target at the SRU level. Design Recommendations were made based on these configurations for future experimental testing and investigation.*
Public abstract for confidential deliverables	

REVISIONS			
Version	**Date**	**Changed by**	**Comments**
1	Dec 18 2024	David Harvey	First Draft
2	February 28, 2024	David Harvey	Final Version

FFC BASED RECOMMENDATIONS FOR NEXT GENERATION MEAS IN THE SRU GEOMETRY

CONTENT

1 Introduction

Improving MEA performance has been the focus of the CAMELOT project, in this report the recommended MEA changes from WP2 which target the Beyond-SoA performance are investigated at the SRU level. The need to study the changes at the SRU level arise from the fact that the SRU adds the additional dimensional effects related to the flow channel and the reduction/increase in various parameters along the length; further the configuration of the flow between the anode and cathode (co-flow or counter flow) further influences these effects.

2 Scope

The work within this report is focused on the investigation of MEA performance as the SRU level for MEAs which were identified as design targets from WP2 in D2.4 entitled "Recommendations for Next Generation MEA Designs and Potential Design Route Maps". The report discusses the implementation of a 2-D SRU model in the FAST-FC COMSOL implementation and the discusses the analysis of the route maps which were explored in D2.4 but at the SRU level.

3 Discussion

3.1 2-D SRU FAST-FC Implementation

To implement FAST-FC into an SRU geometry a 2-D implementation was chosen to balance the computation requirements but provide the effect of the channel length on the performance. The equations that were used within WP2 were used directly in the 2-D implementation and additional physics were added to govern the flow for the anode and cathode compartments; the domain of the SRU with an arbitrary channel length is shown in Figure 1.

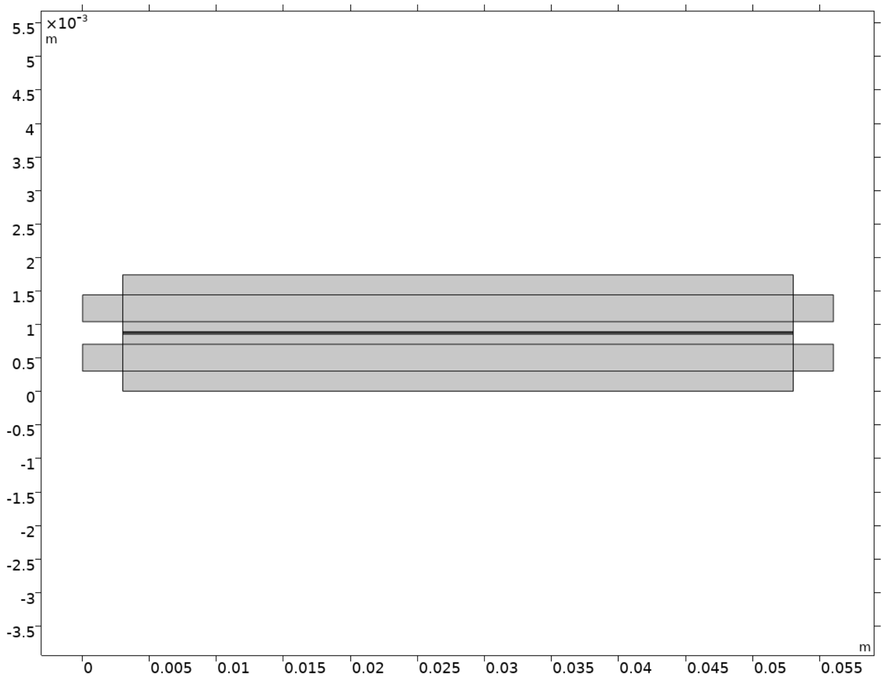

Figure 1: 2-D SRU Domain with an arbitrary channel length, domain is scaled 5:1 (length: height).

From the Figure 1, there were 4 extensions added to the core SRU at the inlets and outlets of the cell. These extensions are done to ensure that the boundary condition for flow is "pulled away" from the edge of the MEA were the source and sink terms in the MEA layers start and this was done for numerical stability reasons but also somewhat simulates that the flow enters via manifold at the plate level. Figure 2 shows a zoomed in region which highlights the MEA structure and denotes the flow direction of the simulations are counter flow.

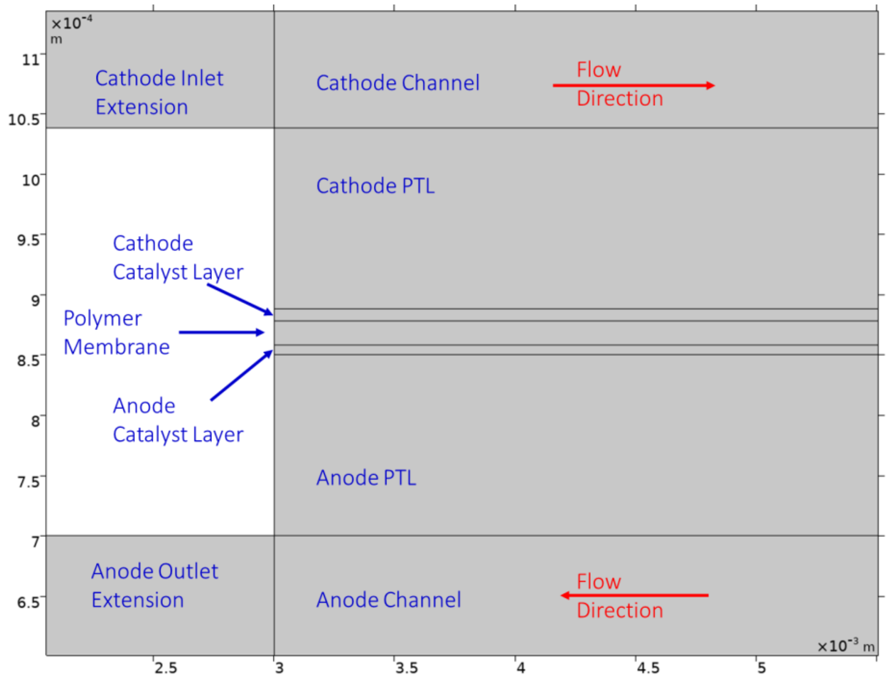

Figure 2: 2-D SRU Domain showing MEA region and counter flow arrangement.

The computation mesh was split into two types, a coarse mesh (Figure 3) and a fine mesh (Figure 4). The course mesh was used to get initial solutions which were then used as the starting guess for the simulations on the fine mesh to improve convergence.

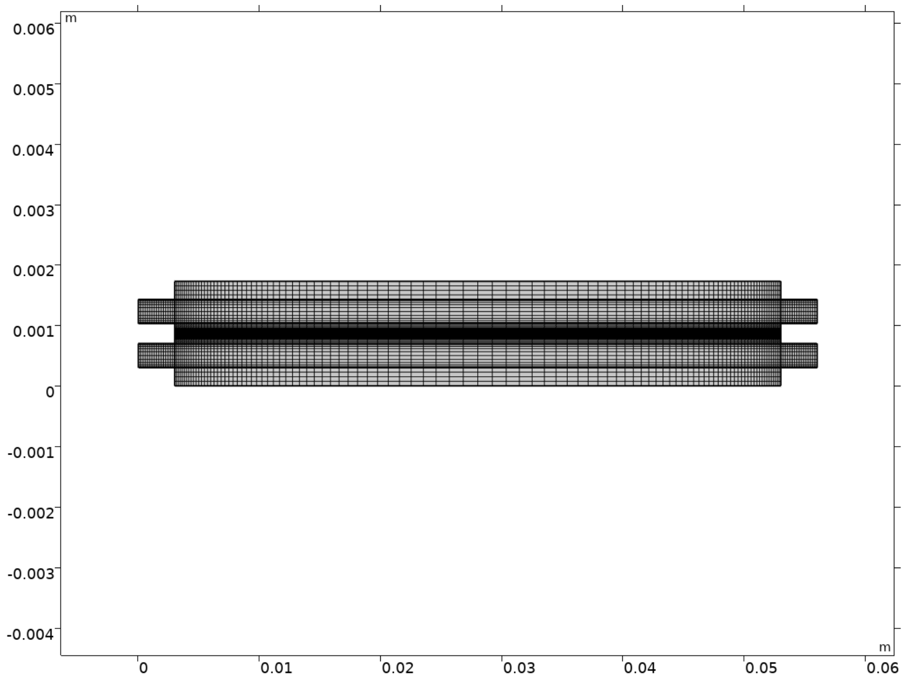

Figure 3: Coarse Mesh used for Initial Guess Simulations at the SRU Level

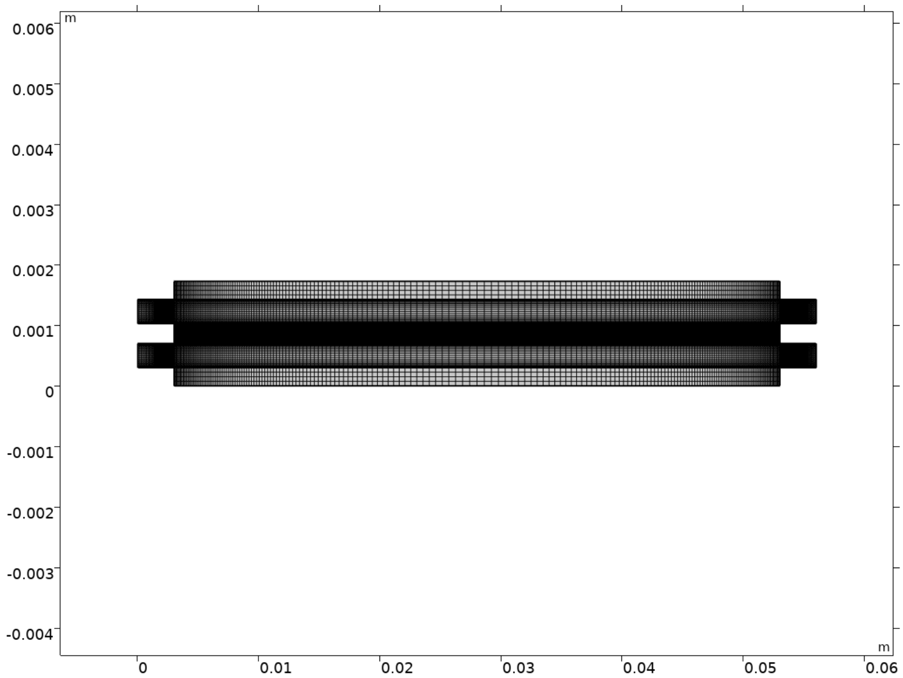

Figure 4: Fine Mesh used for Final Simulations at the SRU Level

Counter flow was applied within the experimental testing and therefore was used within the 2-D model to provide the closest comparison to the data based on the actual physical testing arrangement.

As initial checks that the model configuration was working correctly, the plots of the velocity profiles are shown in Figure 5 and Figure 6. We see that the profiles appear fully developed as expected towards the inlet side, the cathode remains relatively constant which reflects that it does not substantially lose mass during the polarization sweep, and that the anode appears to decelerate which is consistent with a loss of mass due to the reaction of hydrogen and the associated swing in the mixture density.

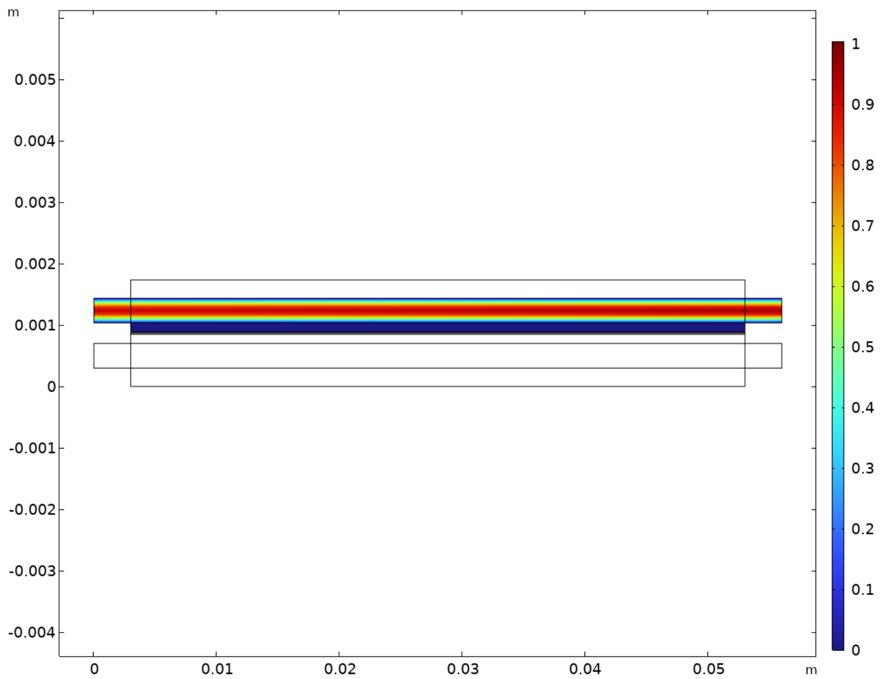

Figure 5: Example Velocity Profile on the Cathode, Scaled 5:1 (Length: Height).

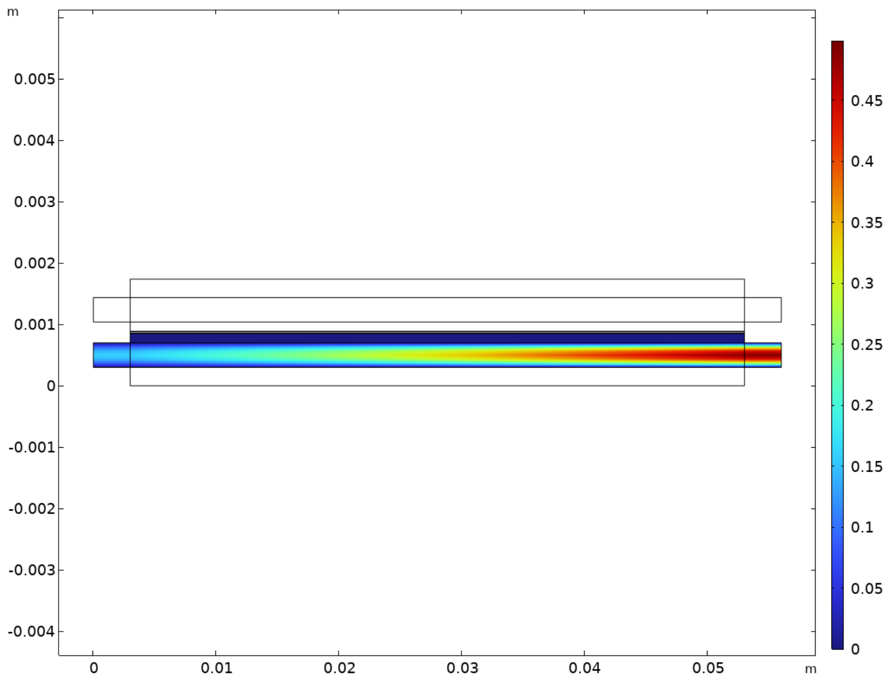

Figure 6: Example velocity Profile on the Anode in Counter Flow, Scaled 5:1 (Length: Height)

Further, exploring the change in the mass fractions we see that the oxygen is depleted along the length of the channel leading to a concentration boundary layer behaviour, shown in Figure 7, and the same behaviour is observed in the water vapor along the cathode channel length, Figure 8.

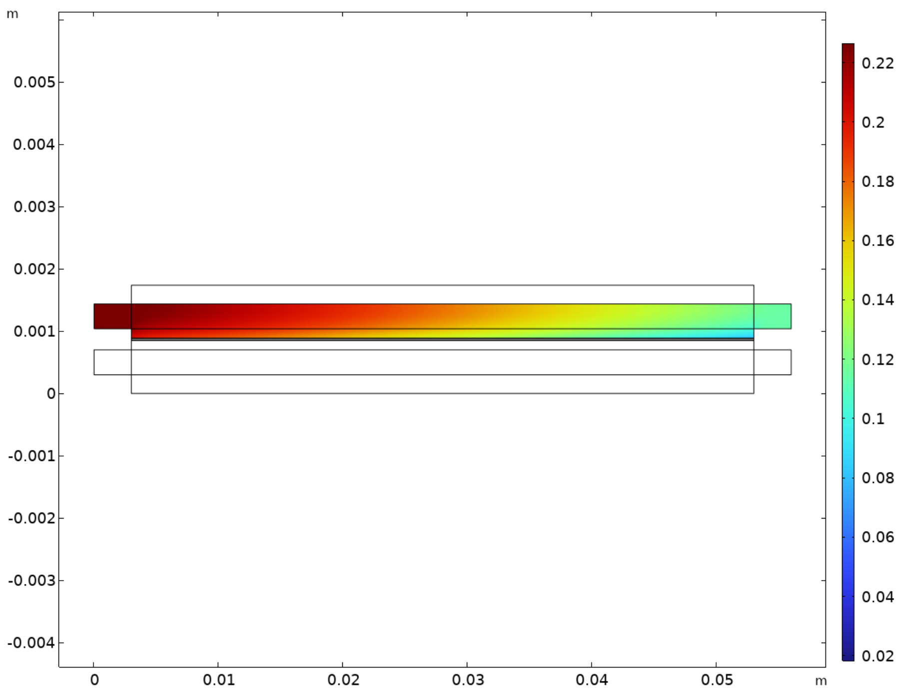

Figure 7: Oxygen Mass Fraction along the length of the Cathode Channel in Counterflow, Scaled 5:1 (Length: Height)

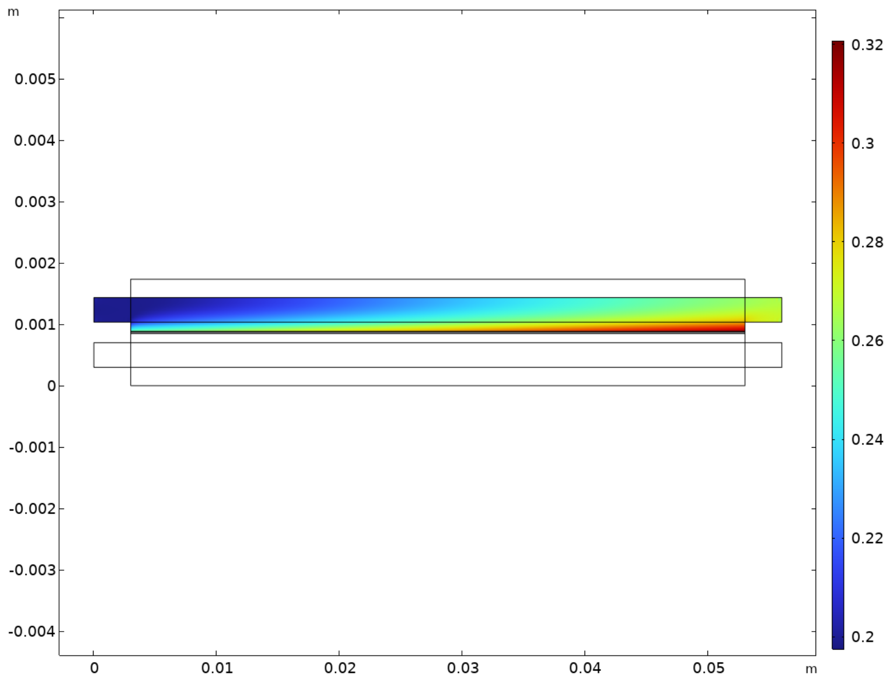

Figure 8: Water Mass Fraction along the length of the Cathode Channel in Counterflow, Scaled 5:1 (Length: Height)

Initially the performance comparison to the experimental SoA data from WP5 showed an overprediction and required adjustment of the coupling between the liquid phase mass fraction and the gas diffusion transport parameters. Figure 9 shows the overprediction and Figure 1 shows the comparison once the

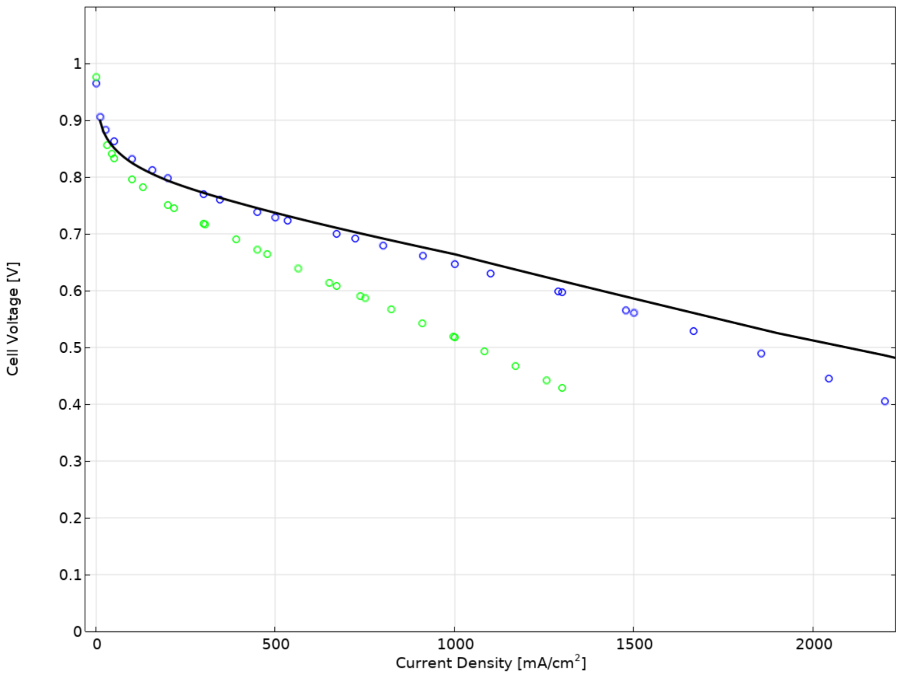

Figure 9: SRU Prediction before adjustment of liquid phase coupling to gas phase transport, Black Line = Model Simulation, Blue Circles = Cold & Wet SRU Data, Green Circles = Hot & Dry SRU Data.

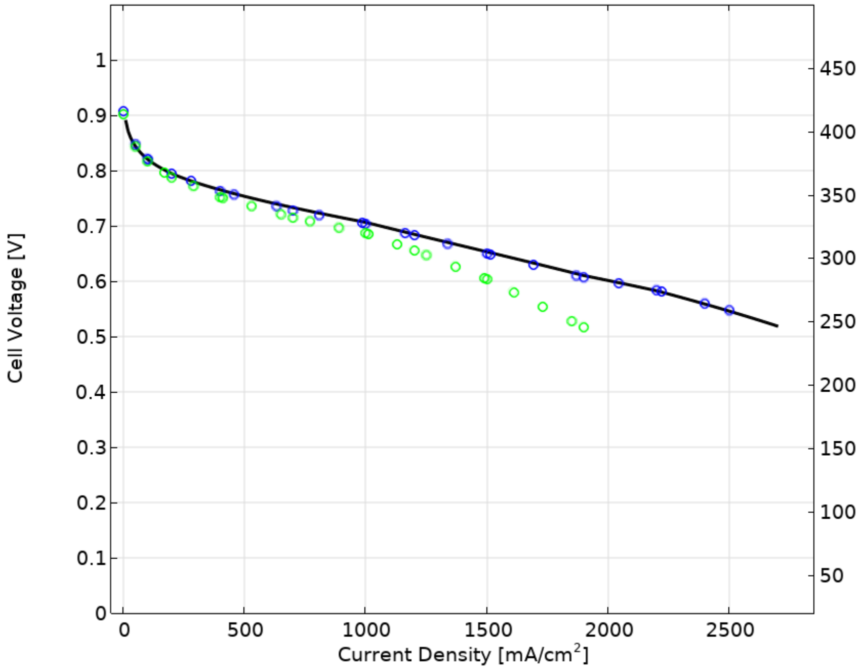

Figure 10: SRU Prediction after adjustment of the liquid phase coupling to gas phase transport, Black Line = Model Simulation, Blue Circles = Cold & Wet SRU Data, Green Circles = Hot & Dry SRU Data.

Based on these adjustments the model is now matching the experimental SoA dataset under cold & wet conditions as the starting point to investigate recommendations for Next Generation MEAs at the SRU level.

3.2 Beyond-SoA Performance Study

From WP2, recommendations for beyond-SoA MEAs included the following:

Table 1: Beyond SoA MEA Recommendations from WP2.

Description of Change	Changed Value
PTL Thickness Reduction	50 µm
Graded CCM	0.2 mg/cm^2 Average
Thinner Membrane	5µm
Thinner Membrane	7µm
Increased Cathode EPSA	180
Relative Humidity & Temperature	75% RH at 70 C
Operating Pressure & Temperature	1.5 barg at 70 C

From these recommendations, the combination was tested at the SRU level and assessed to determine if the impact was similar between simulations at the MEA level and those at the SRU level where the effect of channel length and the SRU architecture would influence the outcome.

A similar process to D2.4 was followed in that each change shown in Table 1 was implemented sequentially to determine if the performance provided an uplift to the SRU or a reduction.

Starting with the PTL Thickness reduction to 50µm, shown in Figure 11, it was found that the performance gain seen at the MEA level was greater than that observed at the SRU level. This appears to be the result of liquid water accumulation along the length of the channel which leads to a negligible overall effect.

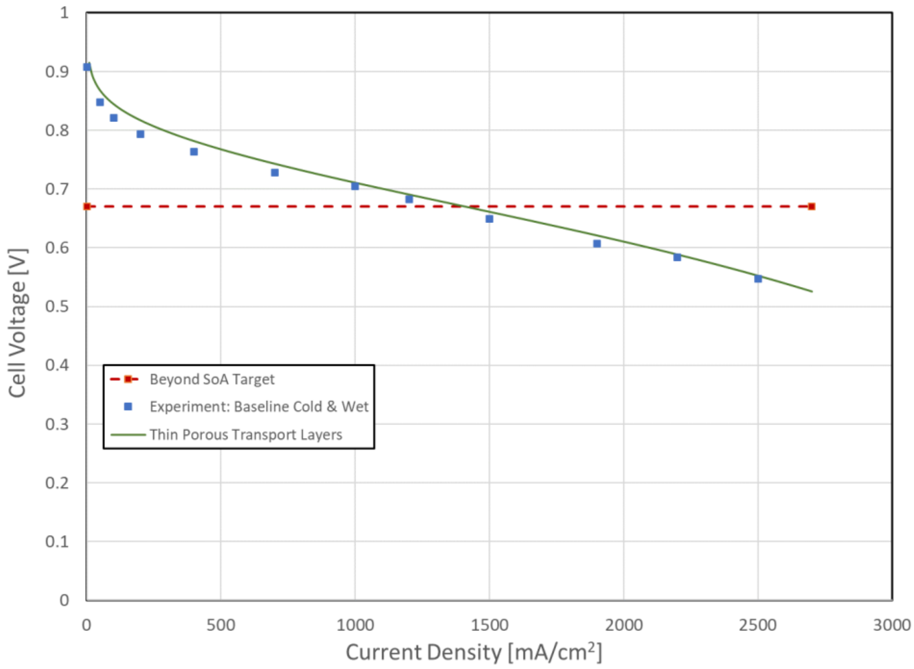

Figure 11: Effect of Thin Porous Transport Layers at the SRU Level.

The graded CCM appears to provide an impact which is consistent with that observed in the MEA level simulations. A drop can be seen in the kinetic region due to the reduced loading but the utilization of the layer over the length of the cell is improved and results in an increase in overall performance.

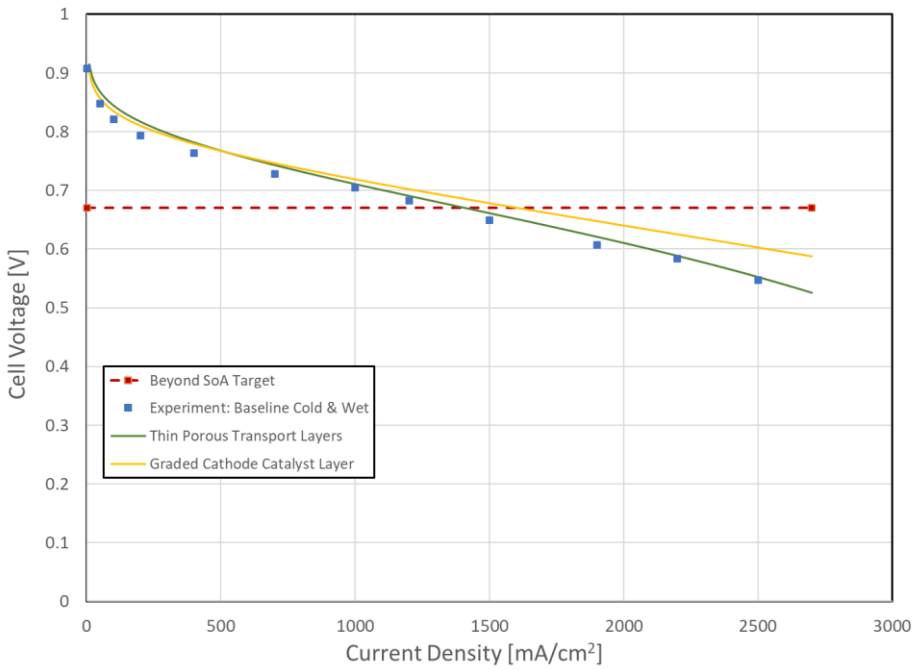

Figure 12: Effect of Graded CCL at the SRU Level

From Table 1, the next step from WP2 was the consideration of the thinner membrane materials. The significantly thinner membrane was bypassed and the 7um suggested thickness evaluated. In the counter flow case there was observed some change in the hydration profile of the membrane from inlet to outlet on the cathode and the respective outlet to inlet on the anode. This led to profiles that were somewhat complicated to investigate, however the overall performance trend showed an uplift in performance but not to the same amount that was observed at the MEA level; the performance comparison is shown in FIGXX as a cumulative effect with the Graded Cathode Catalyst Layers.

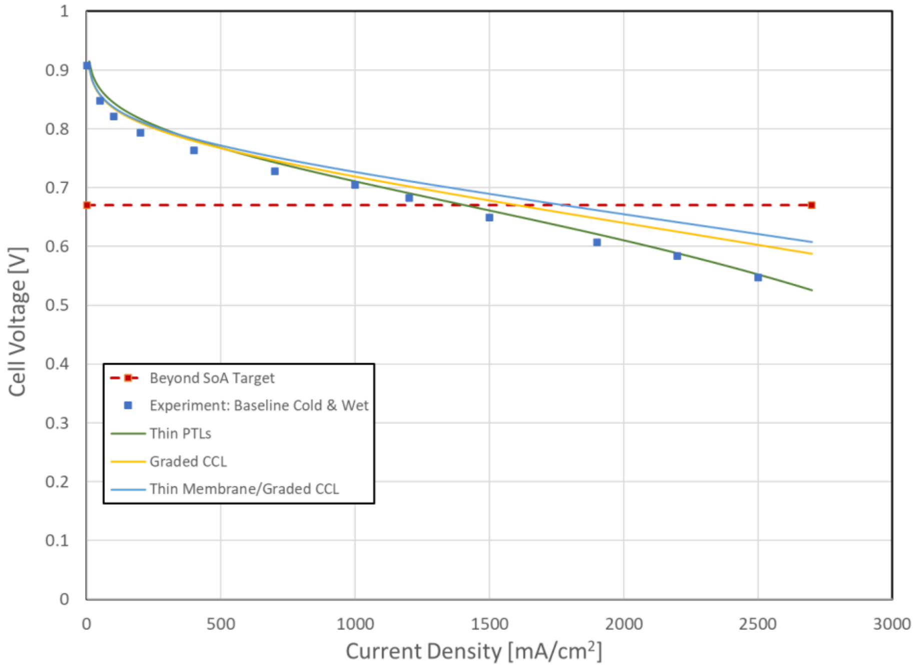

Figure 13: Effect of Thin Membrane Materials coupled with the Graded CCL layer at the SRU Level.

The increase in the platinum surface area was undertaken by reducing the particle size and keeping the utilization equation from the MEA version of FAST-FC. This meant that the EPSA changed over the thickness of the electrode based on a predefined profile for the grading along with the other structural parameters. The increased ECSA yielded an increase at the SRU level, reported in Figure 14, for the overall performance as would be expected, the particle size used was approximately 2.7nm as the diameter of the platinum particle.

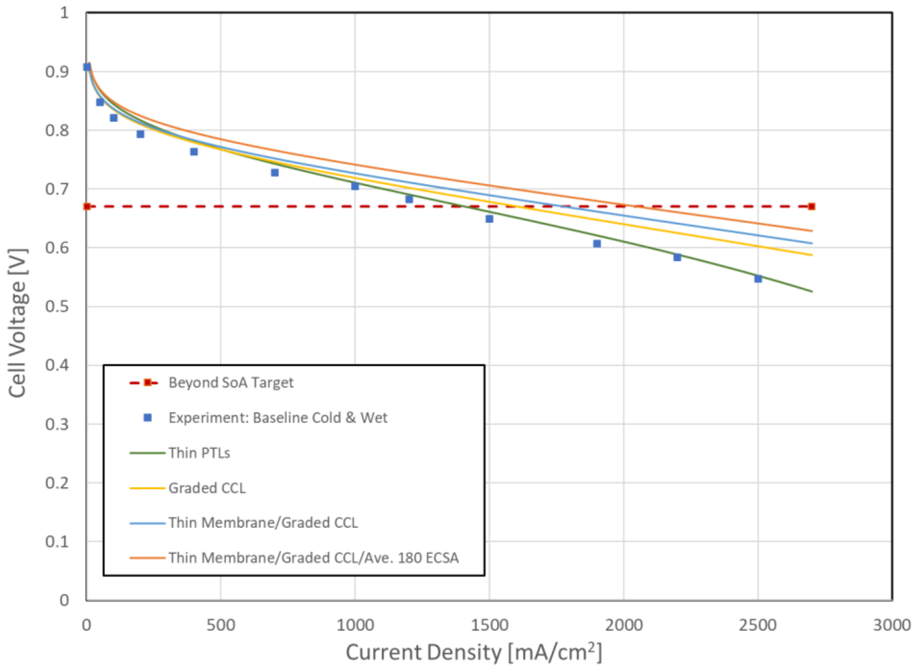

Figure 14: Effect of Thin Membrane Materials, a Graded CCL, and a reduction in the platinum particle size to 2.7nm (average ECSA of 180).

At this point the gap in performance from the SRU performance and the Beyond-SoA targets was about 42mV.

To investigate the effect of temperature, we reduced the cooling rate on the boundary condition between the bipolar plate (anode and cathode) to the cooling channels which increase the temperature rise along the cell to about 12 degrees; Figure 15.

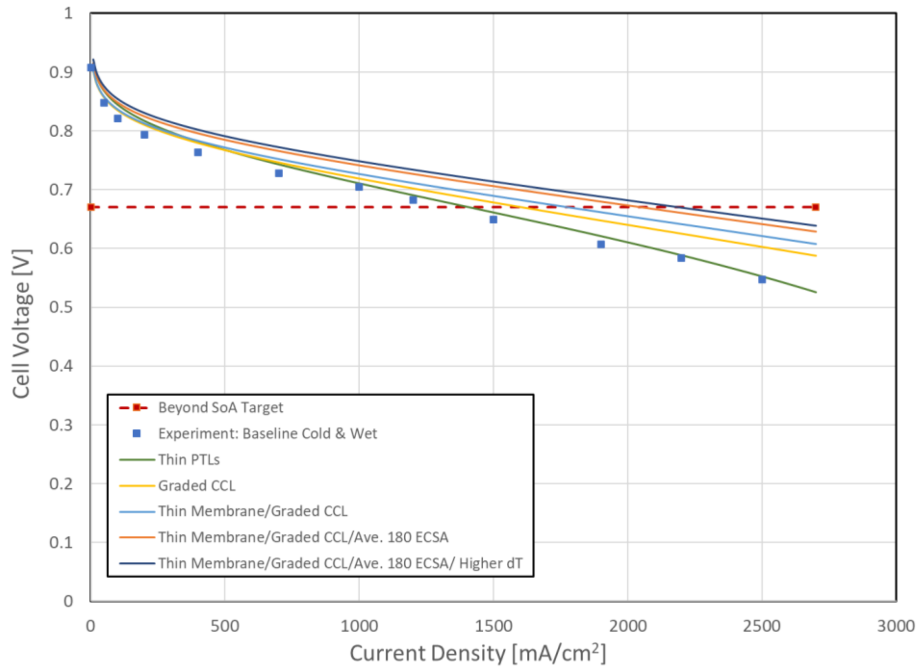

Figure 15: Effect of a higher dT on the SRU Performance using the MEA configuration from Figure 14.

The higher dT did not significantly increase the performance and this may have been due to additional drying to the anode due to the counter flow operation as the water content average for the membrane appeared to be reduced in the area towards the anode outlet and the cathode inlet where there was a significant flux due to electro-osmotic drag.

Both Stoichiometry and Inlet pressure were options to use as levers to consider making up the remaining millivolts to the beyond-SoA target. Following from table1, the increase in the operating pressure to 2.5 bara or 1.5 barg served to be almost sufficient to meet the difference in the performance target, however, it fell slightly short due to the differences between the MEA model which had no channel pressure losses and the 2-D model which included the channel pressure loss effects. As a result, the pressure increase required was to reach about 3 bara to meet the performance target for the beyond-SoA MEAs without a corresponding increase in operating RH; **Error! Reference source not found.**. The pressure drops for the corresponding flow are shown in Figure 17 for the higher current density of 2.7 A/cm^2.

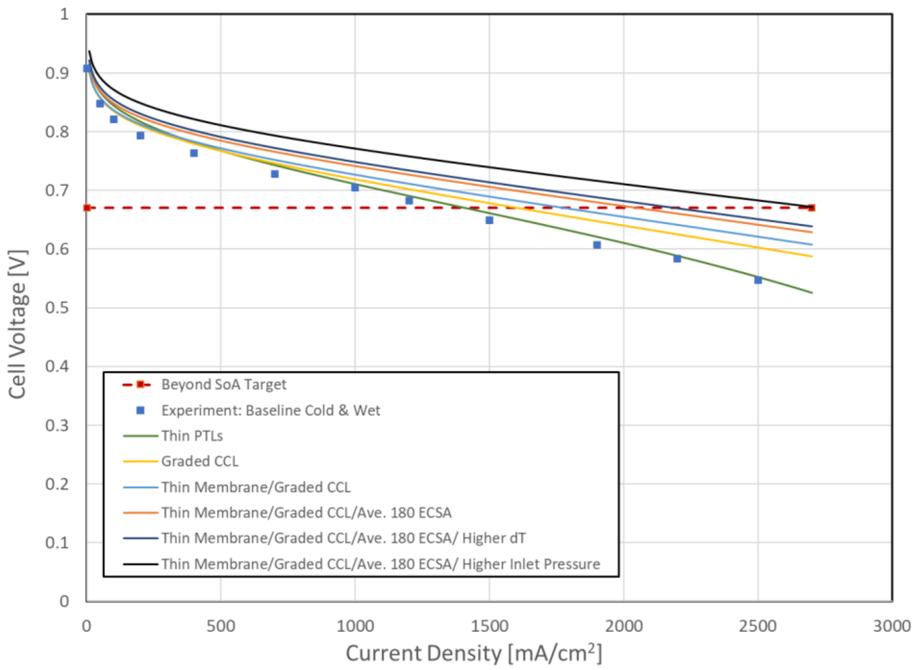

Figure 16: Effect of a higher inlet operating pressure (3 bara) on the SRU Performance using the MEA configuration from Figure 12.

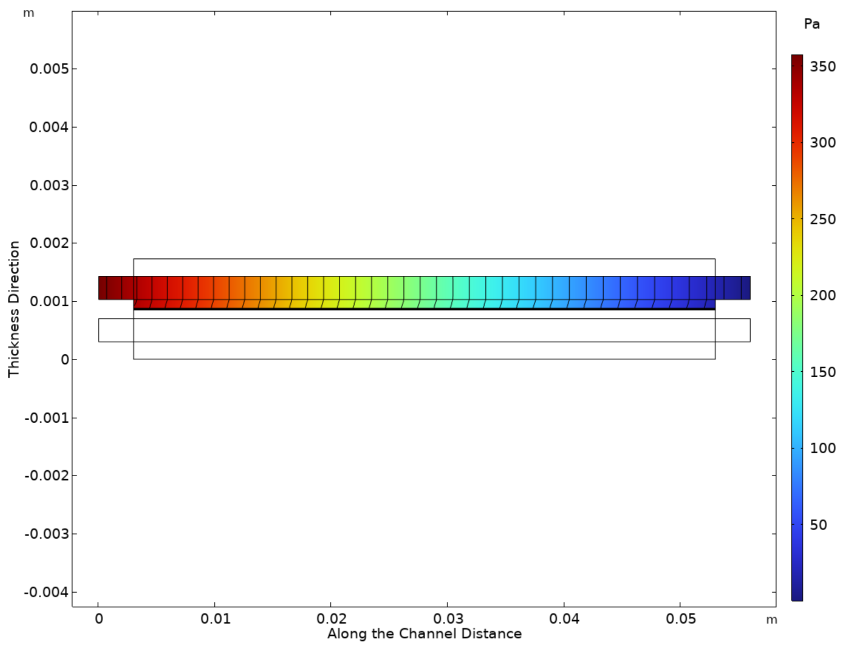

Figure 17: Cathode Pressure Drop (gauge pressure) [Pa]

4 Conclusions and Future Work

The design recommendations to achieve Beyond-SoA performance at the SRU level are based on the results in Section 3.2 where the MEA recommendations from WP2 were implemented at the SRU level. It was found that the decrease of the PTL thickness did not result in a measurable performance increase based on the simulations results. The Graded CCL structure (through the thickness) along with the thinner membrane, reduction is platinum particle size, and use of a higher inlet pressure were sufficient to increase the performance of the SRU to >670mV at 2.7 A/cm^2. Given that these changes resulted in a configuration which might meet the performance target it is recommended that these configurations be explored experimentally in future research efforts.

Further work on improving the similar is recommended with respect to the pressure drop in two-phase flow as the pressure drops predicted do not appear to be consistent with experimental data and it is unclear how this will skew the recommendations. Furthermore, the capillary pressure curves used are representative of Porous Transport Layers and are not likely equivalent for the catalyst layers; currently the model applies the same relationship for both layers.

5 References

6 Appendix

This project has received funding from the Fuel Cells and Hydrogen 2 Joint Undertaking (now Clean Hydrogen Partnership) under grant agreement No 875155. This Joint Undertaking receives support from the European Union's Horizon 2020 Research and Innovation program, Hydrogen Europe and Hydrogen Europe Research.

Clean Hydrogen Partnership

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