



# Investigation into SECCM proton reduction using COMSOL simulations.

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## Introduction

The investigation of proton reduction and understanding the formation of H<sub>2</sub> microbubbles and nanobubbles is an essential prerequisite to the development of safe hydrogen fuel cells. Simulations are incredibly useful in gaining a thorough understanding of exact dynamics in a given physical experiment, or in predicting possible outcomes.

In this study, COMSOL software was used to simulate the electrochemical parameters of a SECCM pipette performing proton reduction, in order to better grasp the influence of different microprocesses on H<sub>2</sub> microbubble formation.

## Theory

- Scanning Electrochemical Cell Microscopy is a valuable tool in R&D of fuel cells and batteries. Many papers have made use of the technique to map surfaces, determining areas of high electrochemical activity.
- Modelling this system is therefore useful as a resource for those wishing to understand unexpected or interesting results.
- H<sup>+</sup> in solution is reduced to hydrogen gas by electron transfer at an electrode-droplet interface, which is then transported by diffusion through the droplet, and escapes at the droplet-air boundary.

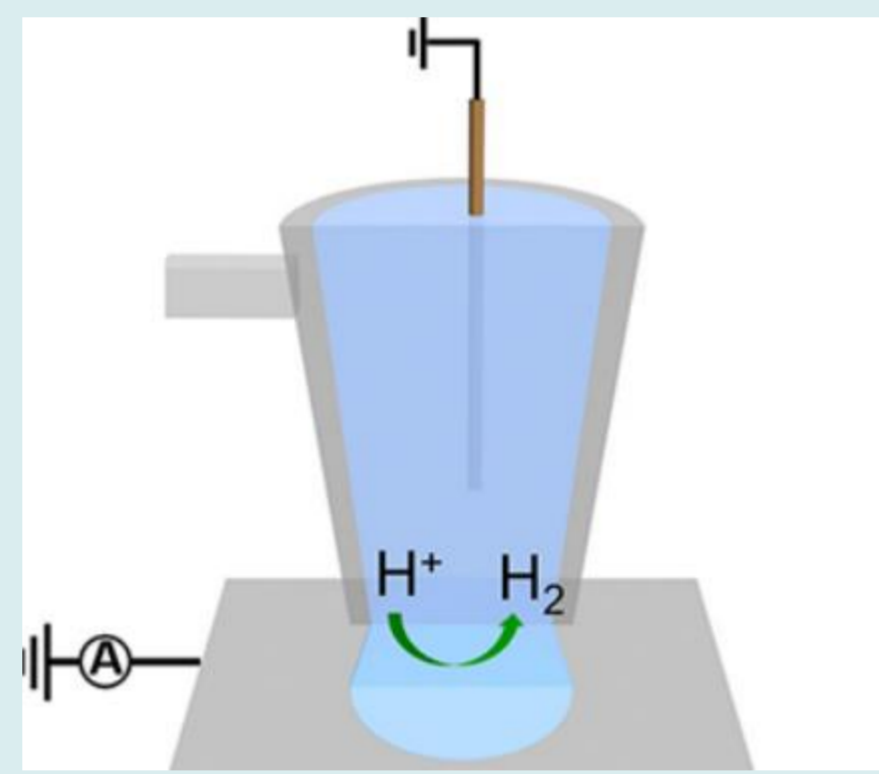
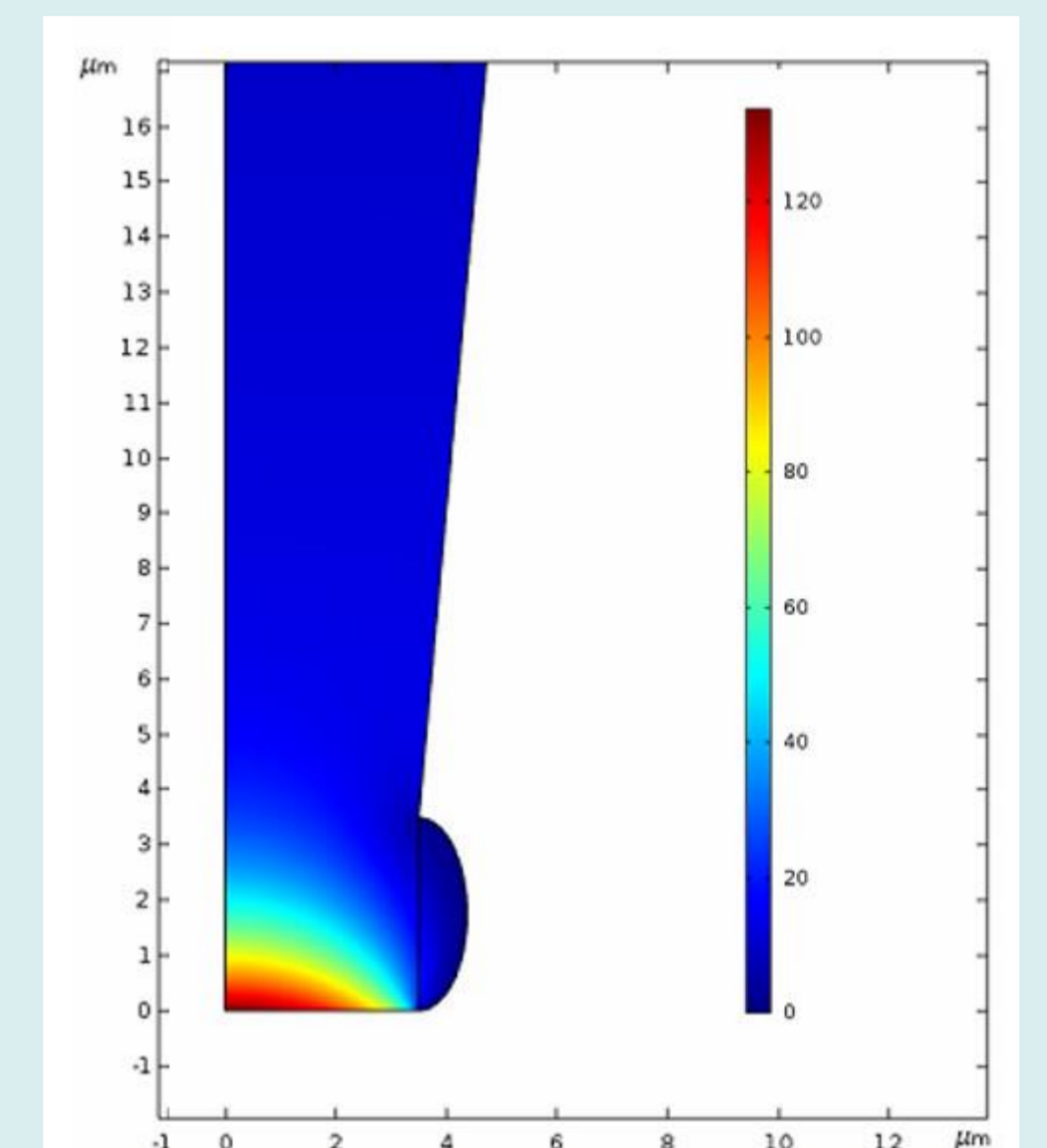


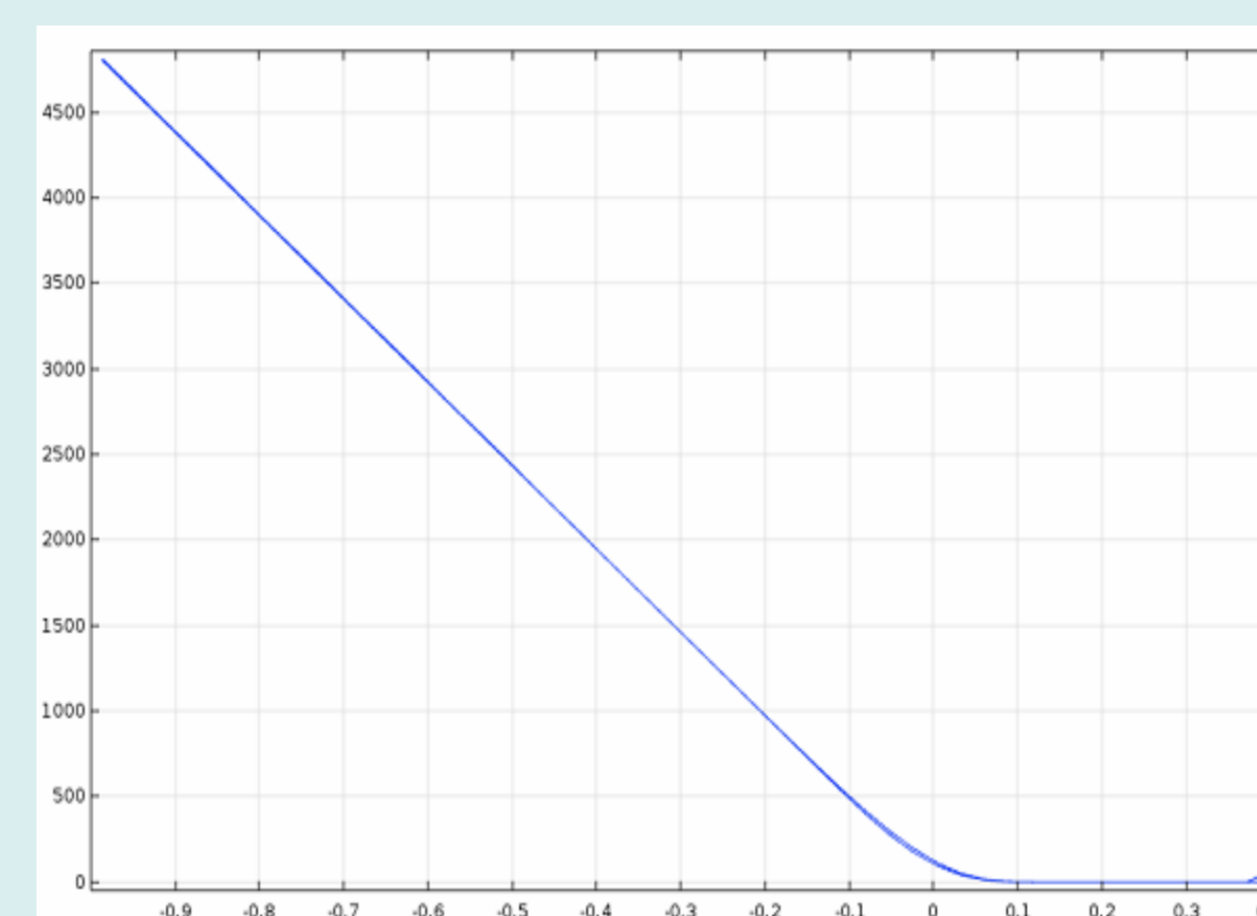
Diagram illustrating physical experimental setup [1]

## Results & Discussion

- Many simulations were run using the parameters replicating physical experiments previously carried out in the lab.
- The surface of H<sub>2</sub> concentration, when the droplet boundary was set to 0 to simulate the escape of hydrogen gas, was centred around the electrode-droplet interface.



Surface of H<sub>2</sub> concentration in mM

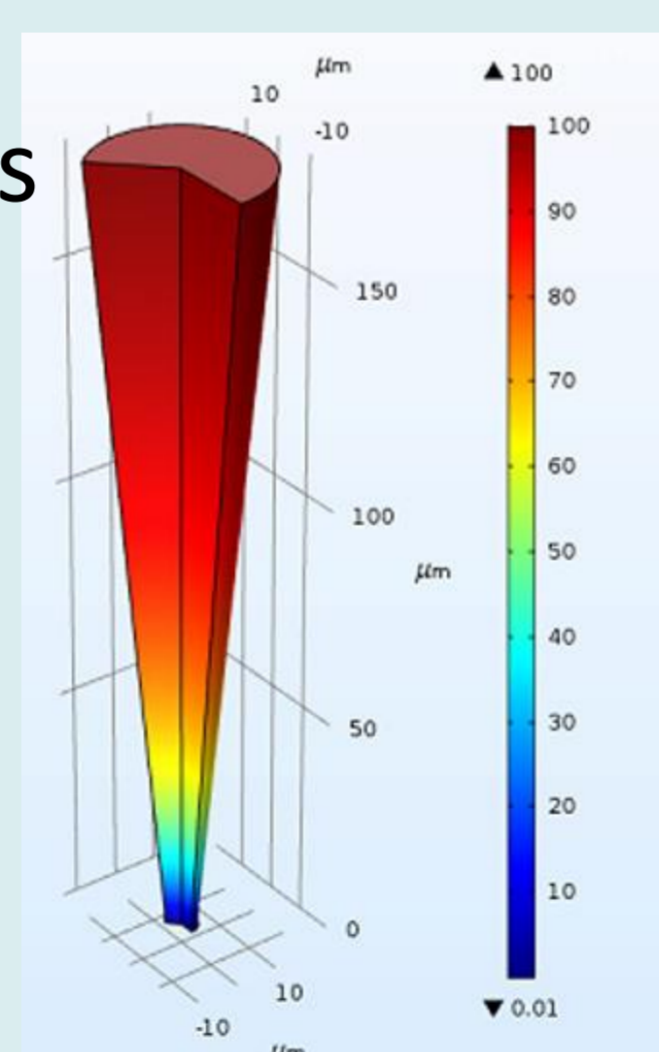


Current vs voltage across electrode-droplet interface

- In order to obtain currents in the range of the physical experiments, migration contributions were key – Multiphysics was used to achieve these results

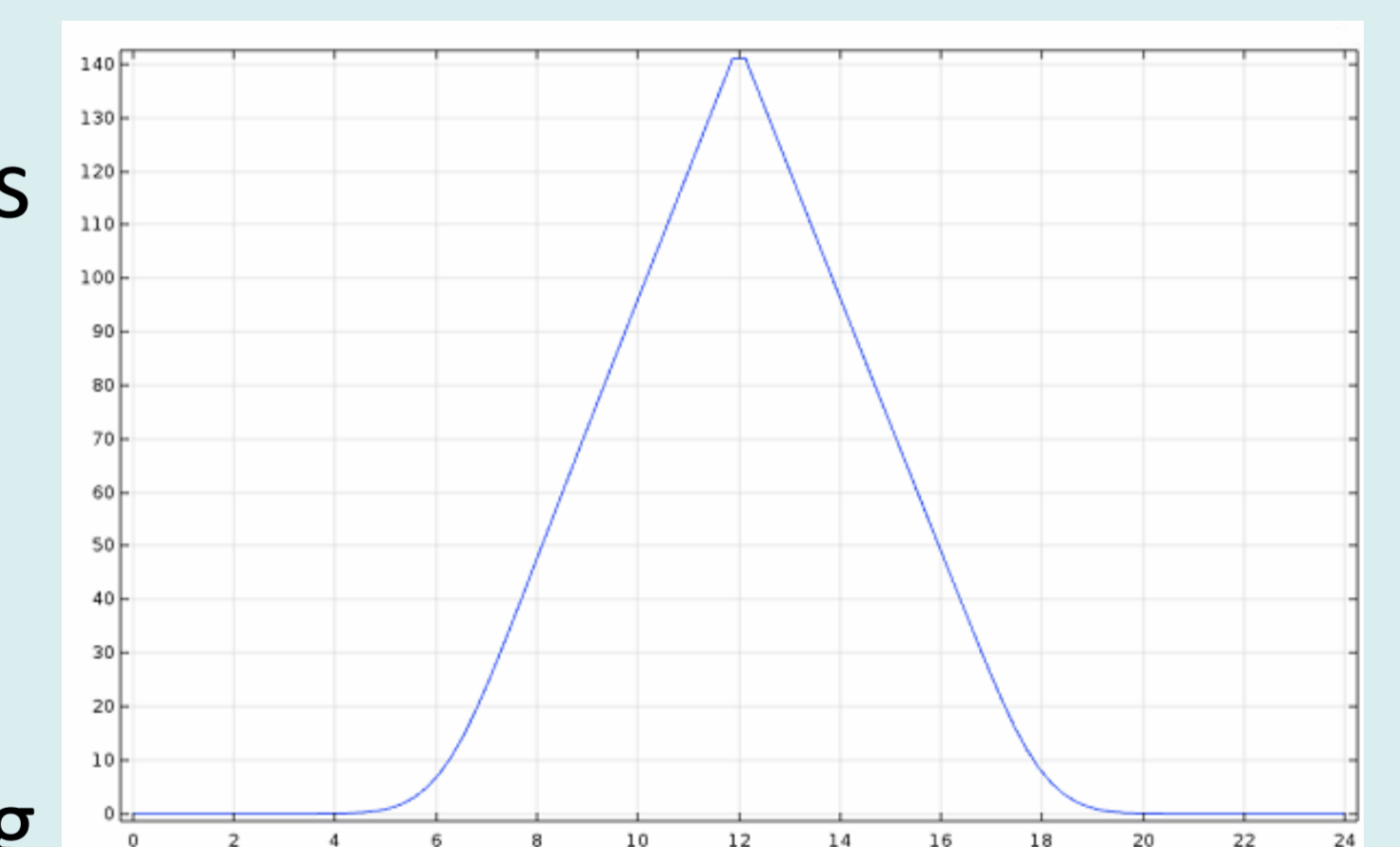
## COMSOL parameters

- Physics used: Transport of Dilute species, Electrostatics
- Initial concentration of H<sup>+</sup>: 100mM
- Initial concentration of H<sub>2</sub>: 0 mM
- Boundary conditions:
  - [H<sup>+</sup>] in bulk = 100mM
  - No Flux boundary at the pipette wall, droplet boundary set to 0.
  - [H<sub>2</sub>] dependent on [H<sup>+</sup>] at the electrode.
- Axial symmetric geometry:  $r = 3.5 \mu\text{m}$ ,  $\theta = 5^\circ$



SECCM pipette geometry. Surface indicates H<sup>+</sup> concentration in mM

- The concentration of hydrogen at the centre of the electrode as a result was above the 100 mM necessary to reach saturation<sup>[2]</sup> and form microbubbles of H<sub>2</sub>.
- Time varying investigation allowed a deeper understanding of the dynamics of the bubble formation.



H<sub>2</sub> concentration vs time at centre of electrode-droplet interface

## Conclusions

This project aimed to develop a framework for the use of COMSOL in modelling physical SECCM experiments, in order to better understand the processes occurring at the microscale.

The simulation parameters were developed based on previous physical experiments and testing lead to adjustments of the initial set up, including the addition of new physical models to incorporate migration of charged species, which proved to be essential for an accurate reflection of the current predicted by experiment.

This model could be used in the future to determine the microscale dynamics of other SECCM experiments, and could contribute to further development of zero carbon fuel cells for the future.

## Reference

- [1] White, Chen, Visualization and Quantification of Electrochemical H<sub>2</sub> Bubble Nucleation at Pt, Au, and MoS<sub>2</sub> Substrates, ACS Sensors, 2020  
[2] Whita, Luo, Electrogeneration of Single Nanobubbles at Sub-50-nm-Radius Platinum Nanodisk Electrodes, Langmuir, 2013.

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