Analysis of polymer electrolyte water electrolysis by numerical modelling and simulation

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BACKGROUND

Market penetration of renewable energy is limited by the intermittency and unpredictable nature of energy sources such as solar and wind power. Large scale energy storage is needed to store generated energy during peak supply and release it during peak demand.
Hydrogen production using PEM water electrolysis technology offers a number of advantages in this area such as GWh scale storage capabilities and fast response times but suffers from high cost and durability issues.

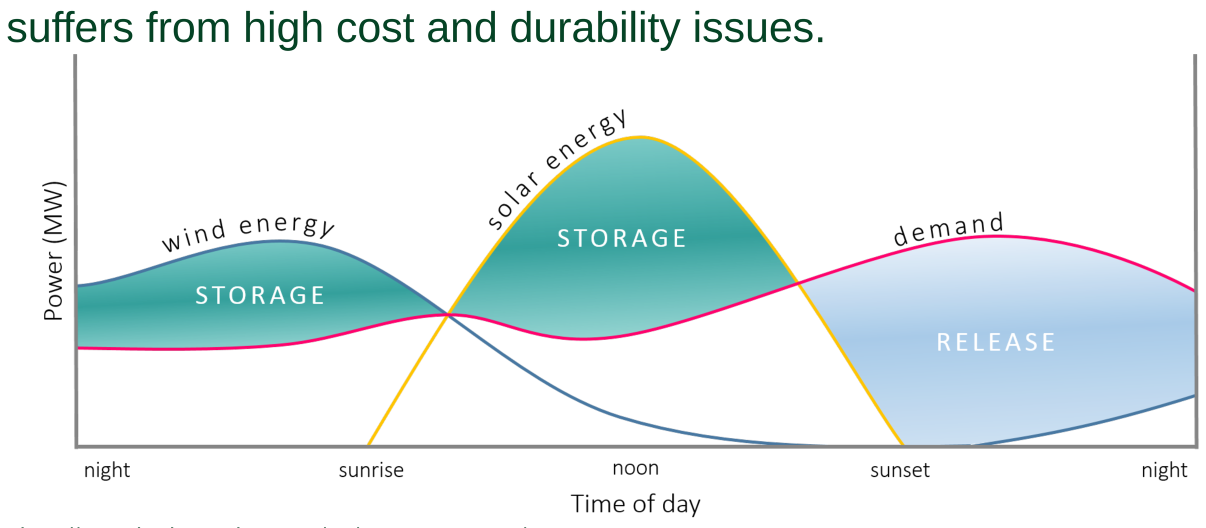


Image taken from: http://www.hydrogenious.net/en/energy-storage/

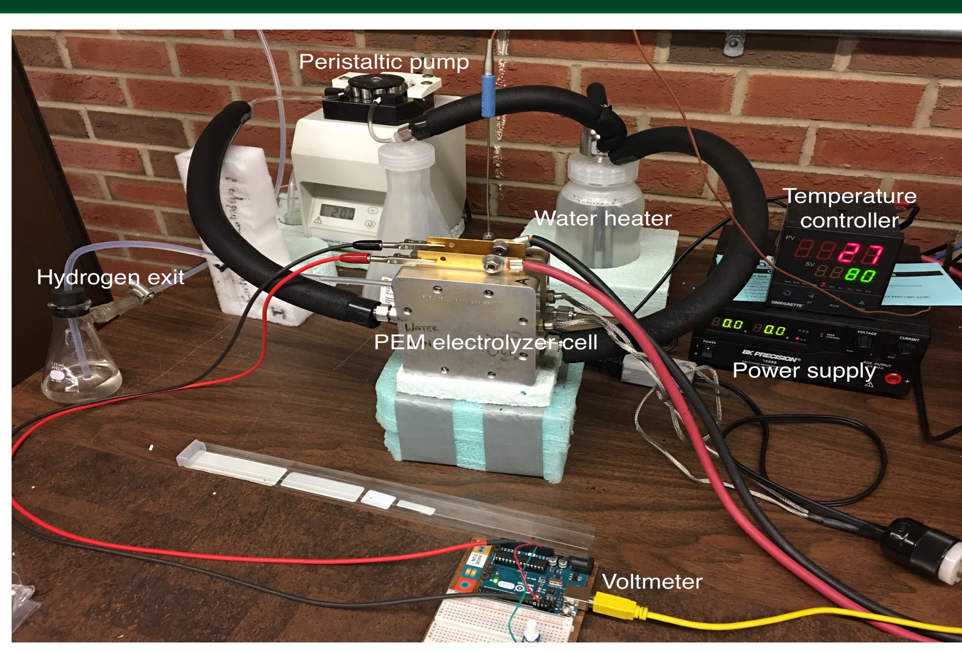
AIMS AND OBJECTIVES

The principal aim of this work is to develop a numerical model of a PEM water electrolyser cell to help improve our understanding of the processes occurring within the cell and in interpreting experimental data produced in-house. Ultimately, the model should be of sufficient accuracy to allow for the future design and optimisation of electrolysers, allowing manufacturers to reduce costs and improve durability.

The objectives of the research are as follows:

- Development of 0-D basic electrolyser model to help assess potential areas of research
- Development of 2-D finite element model to investigate additional physical phenomena such as catalyst degradation, mass transport, transient and two-phase flow effects
- Validation of model against in-house experimental data
- Extension of model to solid oxide electrolysis

EXPERIMENTAL SETUP



- In-house electrolyser test station
- MEAs manufactured in-house using inkjet printing
- Tests include polarisation curves, stability tests, electrochemical impedance spectroscopy and cyclic voltammetry

FUTURE DIRECTIONS

MODEL DEVELOPMENT

The model will now be further developed with its inclusion in the OpenFCST code, an open source, finite element framework, developed in house. This will allow for modelling in 2-D and the inclusion of additional physics such as transient, two-phase flow or thermal effects.

The kinetics of the OER will be further studied, requiring the use of a more advanced model and experimental studies to determine reference states. In addition, the study of the degradation of the catalyst will require the implementation of new kinetic models in OpenFCST and the inclusion of transient effects.

Moving to a 2-D model will allow for the calculation of the reaction distribution within the electrode and the inclusion of two phase flow. It will then be possible to study the movement of oxygen bubbles at the reaction sites and any subsequent reduction in active area.

RESULTS

0-D MODELLING

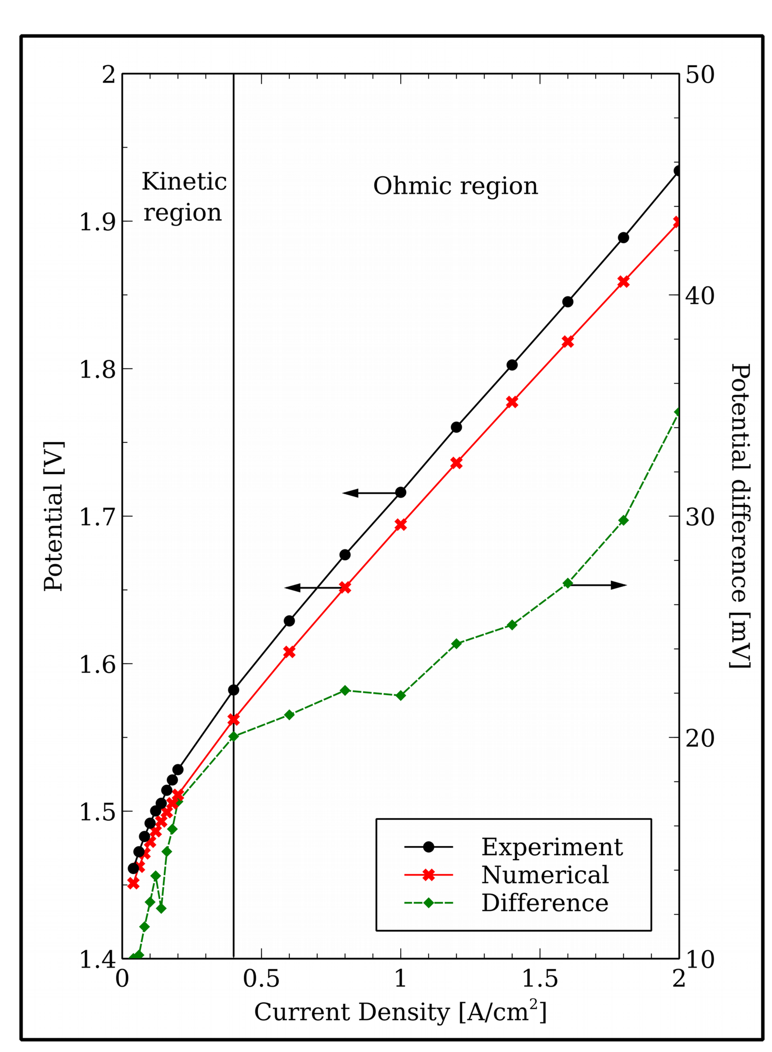
A preliminary study has been performed using a basic 0-D model that accounts for the reaction kinetics of the OER and the ohmic resistance of the cell. Key parameters for the model were determined in-house experimentally using a 5cm^2 cell. A polarisation curve from the same cell was modelled and the results show inaccuracies in the kinetic region and ohmic region.

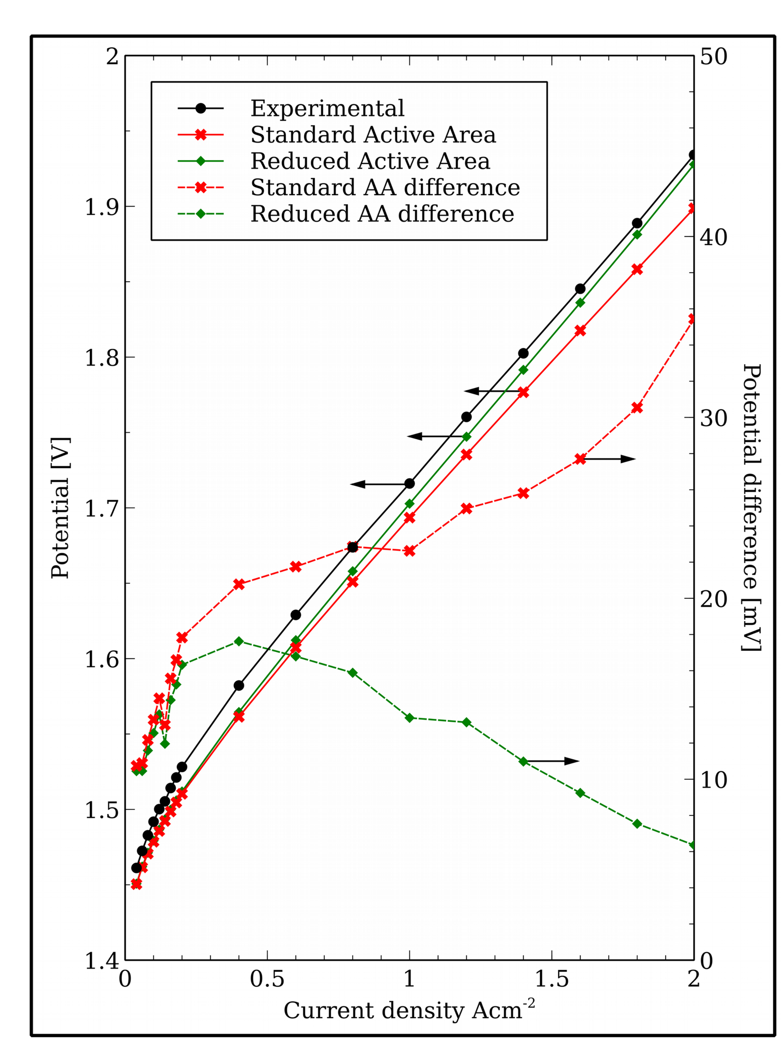
KINETIC REGION

The kinetic region was modelled by the Tafel equation, which is the most commonly used model in the literature. A study of the kinetic parameters used showed that the Tafel equation cannot accurately capture the kinetic region and highlighted the difficulty in measuring the reference potential. A more accurate kinetic model is needed.

OHMIC REGION

The ohmic region is characterised by the ohmic resistance of the cell, which is measured directly in the lab using EIS. Despite this, the experiment shows a different slope compared to the model. A study of the reduction in active area with increasing current density showed that this can produce an apparent ohmic resistance. This active area reduction could be brought on by oxygen bubbles blocking the active sites in the electrode, which would require the modelling of mass transport within the cell. This is generally neglected in the literature.





FES PROJECT OVERVIEW

T06-P04 – Grids and Storage

New technologies enable us to exploit renewable energy resources, but truly harnessing their energy requires the ability to control and adapt to the complex interaction between multiple sources and users. Smart grid technology will enable systems that can adapt to the variation in supply that is common from renewable sources, while new storage technologies will make it possible to retain energy generated during peak times to be withheld for later use. Developing hybrid grids that can accommodate both AC and DC power, accommodating distributed generation and energy storage, and effectively interface with legacy grid systems will be essential to our energy future.

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