Thesis project: Investigation of the influence of dynamic gas bubbles on the electrical conductivity of the electrolyte in a water electrolyser using COMSOL

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Theme: Energy
Is an external organization involved? No
The thesis involves: Modelling
Prerequisite courses and/or knowledge: Fundamentals of Electrochemistry and Electrochemical processes, COMSOL Multiphysics® (not necessary but recommended), Programming language (preferably Python) for any pre- or post-processing

Project description:

The energy transition towards renewable sources has created a new avenue for research: How to efficiently convert and store the excess electrical energy generated during off-peak hours? This is one of the reasons why water electrolysers have been getting attention in the recent years. Water electrolysers (see Fig. 1(a)) powered by a renewable source of energy could be employed to produce hydrogen, which is a dense energy carrier that can be used as fuel later on (during peak hours) for re-electrification. During water electrolysis, the gas bubbles produced at the electrodes (see Fig. 1(b) and (c)) contribute to mass and heat transfer limitations, making their study vital for the design of more efficient electrolysers.

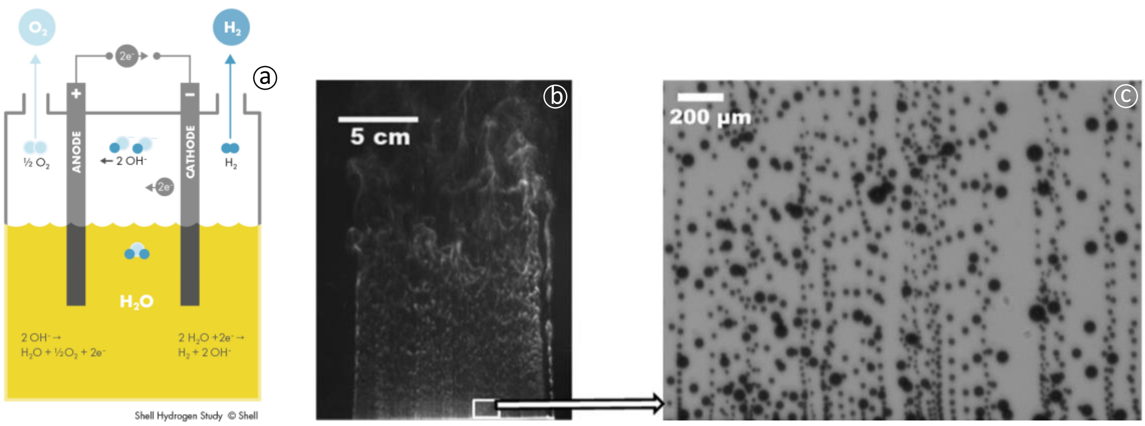

Fig. 1: (a) Schematic representation of a water electrolyser. (b) Planar view of a typical hydrogen bubble plume produced during water electrolysis [1]. (c) Magnified view of the plume originating from the horizontal electrode surface [1].

The presence of a large number of gas bubbles near the electrode surface affects the local transport phenomena and the effective physical properties of the system, for instance the local electrolytic conductivity. This has been studied and theoretical models have been developed for very idealized cases (see Fig. 2(A) and (B)) which quantify the electrical conductivity as a function of the bubble gas fraction [2-3]. These models assume the bubbles to be **static** that neither mover nor grow, which is of course far from reality.

Consequently, this study will investigate the influence of **dynamic** gas bubbles on the electrical conductivity of the electrolyte in a water electrolyser, wherein the bubbles could be growing, moving or rupturing, and subsequently attempt to answer questions including but not limited to:

- If and how the dynamics of bubble growth or movement affects the electrolytic conductivity, especially in comparison to static bubbles
- How does the lifetime of bubbles affect the said conductivity?

This investigation will be carried out using COMSOL Multiphysics®, specifically making use of the Electrochemistry and Electrolyser modules.

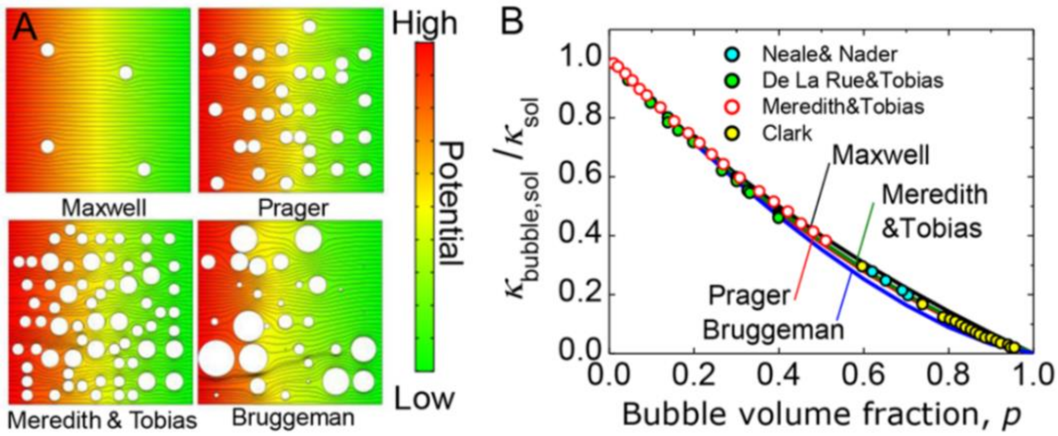

Fig. 1: (A) Illustration of the theoretical models for predicting the conductivity of dispersions in a solution used by Maxwell, Prager, Meredith and Tobias, and Bruggeman [3]. (B) Comparison between experimental data and theoretical predictions of solution conductivity as a function of the bubble volume fraction [3].

References

[1] Chandran, P., Bakshi, S., & Chatterjee, D. (2015). Study on the characteristics of hydrogen bubble formation and its transport during electrolysis of water. *Chemical Engineering Science*, *138*, 99–109. https://doi.org/10.1016/J.CES.2015.07.041

[2] Meredith, R. E., & Tobias, C. W. (1961). Conductivities in Emulsions. *Journal of The Electrochemical Society*, *108*(3), 286. https://doi.org/10.1149/1.2428064

[3] Zhao, X., Ren, H., & Luo, L. (2019). Gas Bubbles in Electrochemical Gas Evolution Reactions. *Langmuir*, *35*(16), 5392–5408. https://doi.org/10.1021/acs.langmuir.9b00119