Thesis project

Thesis title: Investigating bubble nucleation in water electrolysis using the lattice Boltzmann method
Supervisors: Arvind Pari (daily supervisor), Dr. R.M. Hartkamp, Prof.dr.ir. J.T. Padding
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Theme: Energy
Is an external organization involved? No
The thesis involves: Modelling
Prerequisite courses and/or knowledge: Transport phenomena (multiphase systems), Fundamentals of Electrochemistry and Electrochemical processes, Programming languages (preferably C++ or Python)

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)) contribute to mass and heat transfer limitations, making their study vital for the design of more efficient electrolysers.

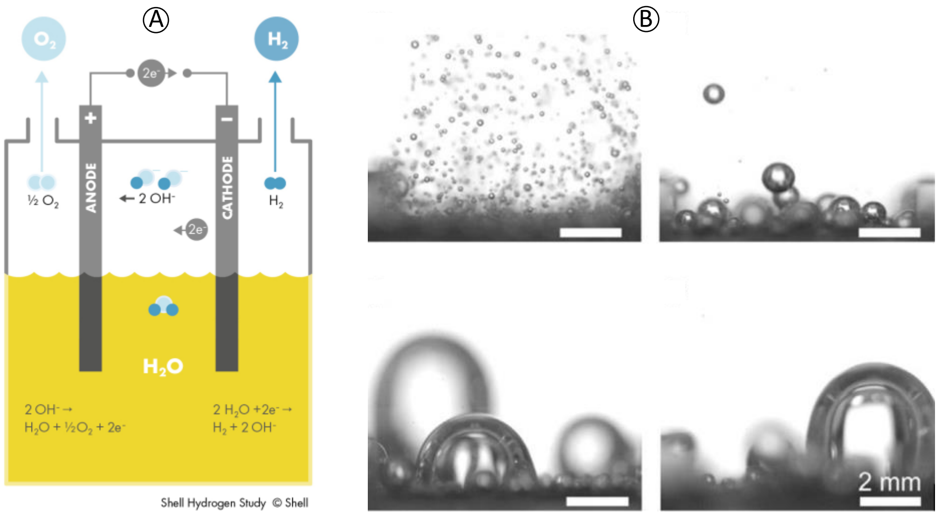

Fig. 1: (A) Schematic representation of a water electrolyser. (B) Side view of oxygen bubbles produced on the surface of the anode during alkaline water electrolysis[1].

The life of a gas bubble at an electrode typically consists of three stages[2]: nucleation, growth, and detachment (see Fig. 2(A)). The first step, bubble nucleation, is still surrounded by its fair share of enigma. It is known that nucleation usually occurs on cracks and crevices in the electrode surface, which results in the formation of a cluster of gas molecules from a solution supersaturated with dissolved gas. After nucleation, the bubble continues to grow by taking up more dissolved gas molecules. As it grows, the buoyant force on the bubble increases. When the buoyant force is strong enough to counter the adhesion force that keeps the bubble on the electrode surface, the bubble is lifted and then detaches from the electrode surface.

This study will investigate bubble nucleation on the surface of an electrode in an electrolyser using the lattice Boltzmann method (LBM). Similar studies on bubble evolution from heated walls have already been carried out using LBM (see Fig. 2(B)). The study would (sequentially) involve:

- Learning the fundamentals of LBM and applying it to simulate simple single-phase systems
- Exploring the different existing methods for modelling multi-phase systems[3] such as the free-energy, the Shan-Chen pseudopotential, and the colour-gradient method
- Simulation of simple multi-phase systems with LBM
- Identification of a suitable multiphase LBM model for the simulation of bubble nucleation on the surface of a solid electrode

The LBM code for these purposes will be developed (preferably) in either C++ or python. Therefore, a strong command of either one of those two programming languages is highly recommended.

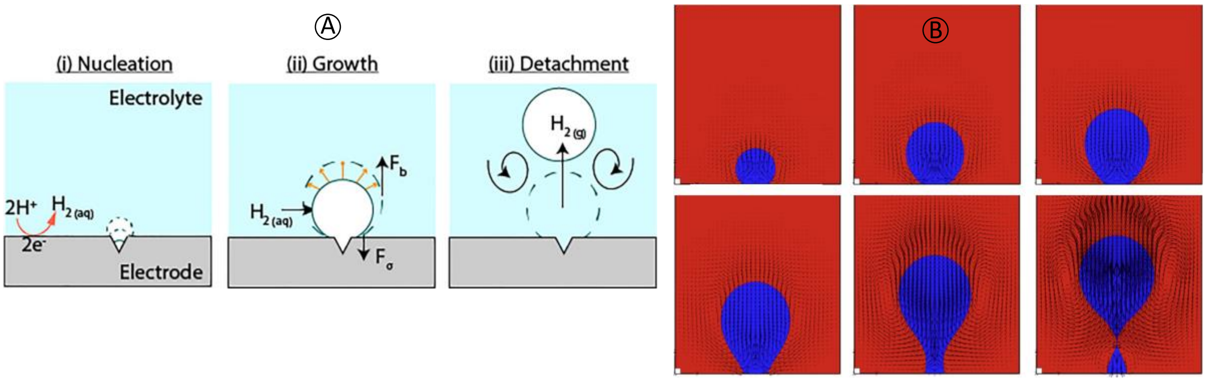

Fig. 1: (A) The stages of bubble evolution on electrode surface: (i) nucleation, (ii) growth, and (iii) detachment[4]. (B) The evolution of bubble from a heated wall and the associated velocity vectors with time[5].

References

[1] Iwata, R., Zhang, L., Wilke, K. L., Gong, S., He, M., Gallant, B. M., & Wang, E. N. (2021). Bubble growth and departure modes on wettable/non-wettable porous foams in alkaline water splitting. *Joule*, *5*(4), 887–900. https://doi.org/10.1016/J.JOULE.2021.02.015

[2] 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

[3] H. Huang, M.C. Sukop, X.Y. Lu, Multiphase Lattice Boltzmann Methods: Theory and Applications (Wiley-Blackwell, Hoboken, 2015)

[4] Angulo et al., Influence of Bubbles on the Energy Conversion Efficiency of Electrochemical Reactors, Joule (2020), https://doi.org/10.1016/j.joule.2020.01.005

[5] Sun, T., & Li, W. (2013). Three-dimensional numerical simulation of nucleate boiling bubble by lattice Boltzmann method. *Computers and Fluids*, *88*, 400–409. https://doi.org/10.1016/j.compfluid.2013.10.009