Numerical Investigation of bubble growth and detachment characteristics in electro-chemical systems

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Chemical process industries are energy intensive, with energy often being obtained from fossil fuels. Therefore, an electrolyzer represents a sustainable and cost-effective alternative for synthesis process. In the case of the electro-organic Shono-reaction, hydrocarbons are oxidated at the anode, while hydrogen is produced at the cathode. Evolving hydrogen generates gas bubbles and hence affects the species transport in the liquid electrolyte. The limiting transport mechanism in such electrolysis cells is the diffusion of the educts to the respective electrodes. While a bubble is attached to the electrode, educts are hindered from getting in contact with the electrode and thus the cell's productivity is reduced. To increase productivity, the two-phase flow and in particular the hydrogen bubble dynamics require further research. For the Shono-reaction oxidation occurs at the anode and the produced, long-chained hydrocarbon molecules dissolve in the electrolyte. Since the effect of the motion of these molecules on the species transport is yet to be determined, a simplified water electrolysis cell was chosen to examine the two-phase flow. Thereby, the simulation domain is firstly based on an existing design of a membrane-less electrolysis cell to enable validation in a later step [1].

This study focuses on the modelling of two-phase flow of hydrogen bubbles in a liquid electrolyte with respect to bubble growth, departure diameter and eventually detachment of the bubble with an interface-capturing Volume-of-Fluid (VoF) Method. The third-party framework *geoChemFoam* based on the open-source library OpenFOAM provides the solver *interTransferFoam*, being able to model bubble formation due to specie diffusion [2]. In the conference contribution, this solver is extended by a suitable contact angle model to describe the bubble detachment from the electrodes. Furthermore, a parameter variation of the contact angle is conducted regarding the corresponding departure diameter and resulting wake flow behind the bubble. The main objective of this work is the identification of dominant factors affecting bubble detachment such as contact angle, coalescence and flow rate as well as the investigation of bubble-induced mixing in the bubble wake.

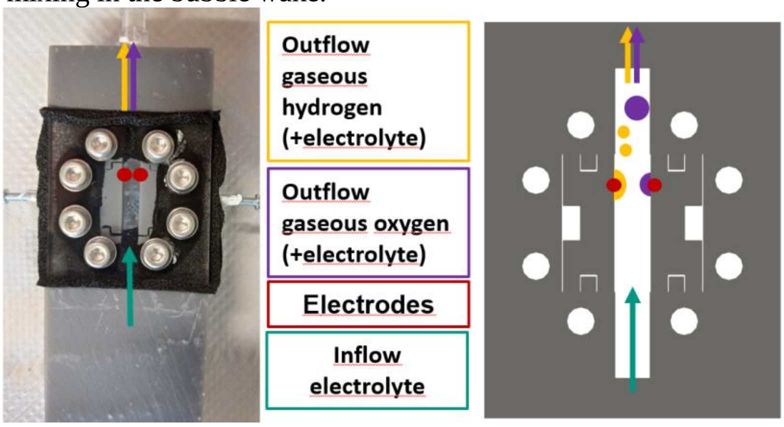

Figure 1: Manufactured and schematics of the reference electrolysis cell design [1]

References:

[1] P. Hadikhani et al. "A membrane-less electrolyzer with porous walls for high throughput and pure hydrogen production." Sustainable Energy & Fuels 5.9 (2021), 2419-2432.

[2] A. Patsoukis-Dimou & J. Maes "Volume-Of-Fluid Simulation of Gas Dissolution in Liquid: Rising Bubbles and CO2 Trapping", 14th International Conference on Computational Dynamics in Oil and Gas, Metallurgical and Process Industries (CFD2020), Oct 2020.