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The coupling between numerical simulation and experimental approach for understanding and optimizing electrochemical devices

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The use of computational tools to study complex processes has received interest in recent decades, due to the increase in computing power, the development of new tools suitable for different simulation scales and low-cost compared to physical experiments. A wide range of research and engineering systems can be studied using Finite Element Analysis, such aerospace analysis, weather simulation, heat exchangers, chemical reactors, etc. As well as fluid dynamics, electrochemical systems can be described by partial differential equations and particular boundary conditions that allow a wide understanding of fundamental aspects of these kind of reactors. Generally, thermodynamics and kinetic parameters can be obtained in the literature or performing simple experiments, including their nonlinear dependences. The literature also can be useful for the validation of the models, allowing the performing of a large set of simulations considering different conditions. For the understanding and optimization of the systems, the data is analyzed using multivariate approach, for the identification of the key parameters, which can be optimized to reach the maximum performance of the reactor. In previous works, it was studied the electrolyte behavior of alkaline water electrolysis, considering the interfacial pH changes due to the reaction stoichiometry, showing that the interfacial pH conditions (near electrode) differ too much from the bulk when current are flowing, only in one of the electrodes, anode in alkaline and cathode in acid medium. This model was used as base for the description of the electrochemical behavior of the spectroelectrochemical cell, showing the non-uniform current distribution at the thin electrolyte layer. It was studied the impact of the bubble presence on the electrolyte convection and in the performance of electrolyzers, considering the impact of the void fraction on the conductivity and the electrode activity, due to the blocking of active sites by gas phase. Actually, we are focusing in the coupling of electrochemistry under high-energy conditions, for example a microwave-assisted

electrochemical reactor was simulated, coupling the equations of electrochemical, heat/mass transfer and electromagnetism by solving the shared variables simultaneously. The results shows that there is a hot-spot caused by antenna effect over the electrode surface, which was observed experimentally and affects the whole electrochemistry, material and solvent proprieties, etc. According to the model, the spot temperature depends on the cell size, electrode size and position, electrolyte conductivity and microwave power. As these works shows, numerical simulations can be very useful for experimentalist, showing unmensurable data, predicting results, everything before performing the first experiment.

Keywords: Electrolysis, Finite Element Method, Numerical Analysis

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