OC2.7 Modeling CO_2 electrochemical reduction in porous cathodes for liquid-phase electrolyzers

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The CO_2 electrochemical reduction (CO_2R) powered by green energy is crucial for "defossilizing" the production of fuels and added-value chemicals, aligning with the UN and EU Sustainable Development Goals.[1] Since the early 2000s, numerous studies have employed finite element (FEM) and finite difference (FDM) modeling to simulate the performance of CO_2R electrolyzers with different configurations, electrolytes, and electrode types.[2] These experimentally validated models enhanced process understanding and device optimization over time.

This work aims to advance CO_2R technology by developing representative models for the parametric analysis and optimization of zinc porous cathode electrolyzers. Simulations consider steady-state operations with various temperatures, inlet pressures, and flow rates of liquid CO_2, including different configurations of the electrolyzer components (cathodic porosity, fiber diameter, pore length, fiber cross-sectional geometry, electrode thickness, and electrolytic chamber dimensions).[3] Validated with experimental data from state-of-the-art literature,[4,5] the models were implemented using mesh-based software designed for multiphysics phenomena simulation, considering species transport in aqueous solutions, flow in the Reynolds regime, and secondary current distribution.[6] This methodology significantly improved CO production, achieving a record partial current density of 263.6 mA/cm² at -1.1 V vs. RHE,[3] a 486% increase over the reference case.[4] The results underscore the remarkable potential of computational modeling in guiding the manufacture of electrolytic structures. Optimized CO_2R conditions demonstrate the possibility of producing green fuels economically interestingly when integrated with renewable energy sources such as photovoltaic electricity.

Acknowledgements: This work received funding from FCT (Fundação para a Ciência e a Tecnologia, I.P.) under the projects LA/P/0037/2020, UIDP/50025/2020 and UIDB/50025/2020 of the Associate Laboratory Institute of Nanostructures, Nanomodelling and Nanofabrication—i3N, and by the project CO2RED, DOI 10.54499/PTDC/EQU-EPQ/2195/2021. The work was also supported by the European project SYNERGY (H2020-WIDESPREAD-2020-5, CSA, Grant No. 952169), M-ECO2 – Industrial cluster for advanced biofuel production, Ref. C644930471-00000041, co-financed by PRR – Recovery and Resilience Plan of the European Union (Next Generation EU), and by the European Union via the project X-STREAM (Horizon EU, ERC-2023-COG, Grant No. 101124803).

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