<u>Multi-scale design guidelines for photo-electrochemical fuel processing reactors</u>

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Abstract

Solar radiation is the most abundant energy source available but it is distributed and intermittent, thereby necessitating its storage via conversion to a fuel (e.g. hydrogen or carbohydrates) for practical use. Solar photoelectrochemical (PEC) approaches provide viable routes for the direct synthesis of solar fuels. Practical PEC reactor concepts have to provide the functionality of radiation absorption, charge generation and separation, selective electrochemical reaction, and ion conduction.

I will describe the modeling efforts in our laboratory supporting the design of cost-competitive PEC reactors. Cost competitive approaches to PEC reactors include the utilization of i) concentrated irradiation[1,2], ii) utilizing photoelectrodes synthesized by less controllable, cheap and fast processing routes, or iii) targeting chemical reactions producing more valuable fuels such as hydrocarbons[3]. Modeling these approaches to solar fuel processing requires focusing on different scales in the PEC reactor and component models, and incorporating different transport phenomena in the model. Utilization of concentrated radiation requires implementation of the locally resolved energy conservation equation in order to understand how thermal management can be used to ensure a high performant operation in a PEC device potentially at elevated temperatures. Utilization of morphologically complex multi-component photoelectrodes required to incorporate the exact morphology of the photoelectrode which we achieved by the utilization of advanced 3D imaging techniques and the subsequent use of the digitalized structure in direct numerical simulations (Monte Carlo and finite volume methodologies). And finally, utilization of electrodes selective towards the reduction of CO_2 requires the incorporation of complex kinetic data.

Advanced multi-scale computational models of PEC reactors proof to be a valuable tool for the design and optimization of these reactor and provide unprecedented insight into the relevant phenomena.

References

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Short biography

Sophia Haussener is an Assistant Professor heading the Laboratory of Renewable Energy Science and Engineering at the Ecole Polytechnique Fédérale de Lausanne (EPFL). Her current research is focused on providing design guidelines for thermal, thermochemical, and photoelectrochemical energy conversion reactors through multi-physics modeling. Her research interests include: thermal sciences, fluid dynamics, charge transfer, electro-magnetism, and thermo/electro/photochemistry in complex multi-phase media on multiple scales. She received her MSc (2007) and PhD (2010) in Mechanical Engineering from ETH Zurich. Between 2011 and 2012, she was a postdoctoral researcher at the Joint Center of Artificial Photosynthesis (JCAP) and the Energy Environmental Technology Division of the Lawrence Berkeley National Laboratory (LBNL). She has published over 50 articles in peer-reviewed journals and conference proceedings, and 2 books. She has been awarded the ETH medal (2011), the Dimitris N. Chorafas Foundation award (2011), the ABB Forschungspreis (2012), and the Prix Zonta (2015). She is a deputy leader in the Swiss Competence Center for Energy Research (SCCER) on energy storage, serves as an Associate Editor for the Journal of Renewable and Sustainable Energy, and acts as a Member of the Scientific Advisory Council of the Helmholtz Zentrum.