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Modelling the performance of a photocatalytic electrochemical cell for CO_2 utilization

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Photocatalytic electrochemical cells (PEC) for CO_2 reduction are a promising photoelectrochemical technology to help reduce greenhouse gas emissions and produce carbon-based fuels and chemicals. However, there is still a lack of understanding of the complex interactions between fluid dynamics, electrochemistry and semi-conductor photocatalysis and their effects on the device performance, including solar-to-fuel efficiency [1].

Accordingly, in this work, a numerical model for a PEC for CO_2 utilization and fuel production is developed using COMSOL Multiphysics and validated with published experimental data. The model couples computational fluid dynamics with electrochemical kinetics and semiconductor photocatalysis accounting for the complex interactions inside the PEC driven by light absorption operating at the Shockyley-Queisser limit. Fig. 1 illustrates the PEC configuration, which consists of a microfluidic channel with two electrodes on the opposite walls. During operation, only anode is illuminated by the incident light. The initial modelling results show that the photoelectrochemical reaction is effected by both overpotential in semiconductor and activation loss at the interface of photocatalyst/electrolyte. Moreover, the process of charge generation and transfer within the PEC is classified and internal irreversible losses in the PEC have been categorized. Based on these findings, a comprehensive understanding of the PEC system is provided.

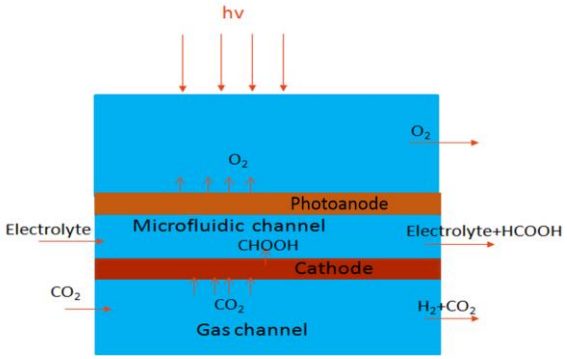

Figure 1. Schematic of the PEC geometry

References

[1] Jan Ronge, Tom Bosserez, David Martel et.al. Chem. Soc. Rev., 2014, 43, 7963.