Modeling multi-physical transport for CO_2 electroreduction

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Multi-physical transport processes on multiple scales are occurring in electrochemical devices and components for CO_2 electroreduction [1]. These coupled transport processes determine the local environment in the catalyst layer and subsequently also the reaction rates at the catalytic sites.

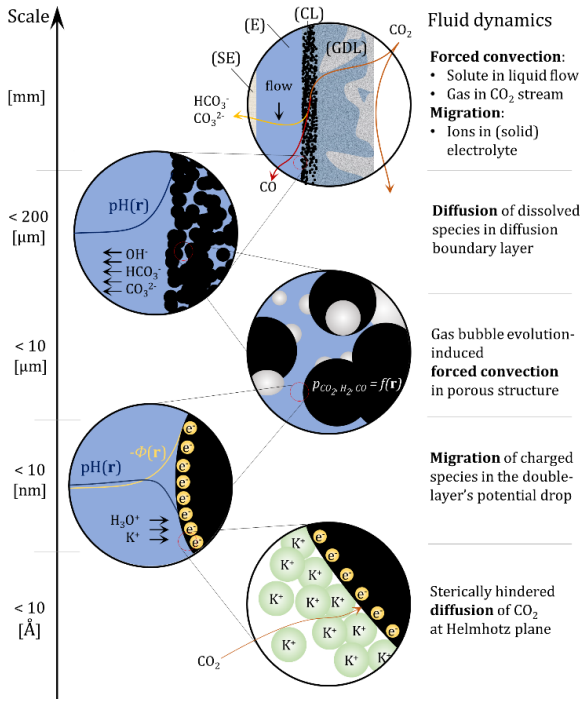

Figure 1. Illustration of the multi-scale transport phenomena inside the cathode compartment during a CO_2reduction reaction [1]

Experiments are typically unable to provide locally resolved information within a working cell, therefore making it difficult to provide diagnostic insight that can improve understanding and lead to optimized design and operation. I will review how coupled multi-physics modelling approaches on multiple scales can provide locally resolved insights, starting from the double layer [2], the pore-scale [3,4], all the way to the volume-averaged continuum-scale.

[1] I. Stephens et al., Journal of Physics: Energy, **2022**, *4*, 042003.
[2] J. Gu, S. Liu, W. Ni, W. Ren, S. Haussener, X. Hu, Nature Catalysis, **2022**, *5*, 268-276.
[3] S. Suter. S. Haussener, Energy Environmental Science, **2019**, *5*, 1668-1678.
[4] E. Johnson, E. Boutin, S. Liu, S. Haussener, EES Catalysis, **2023**, 10.1039/D3EY00122A.