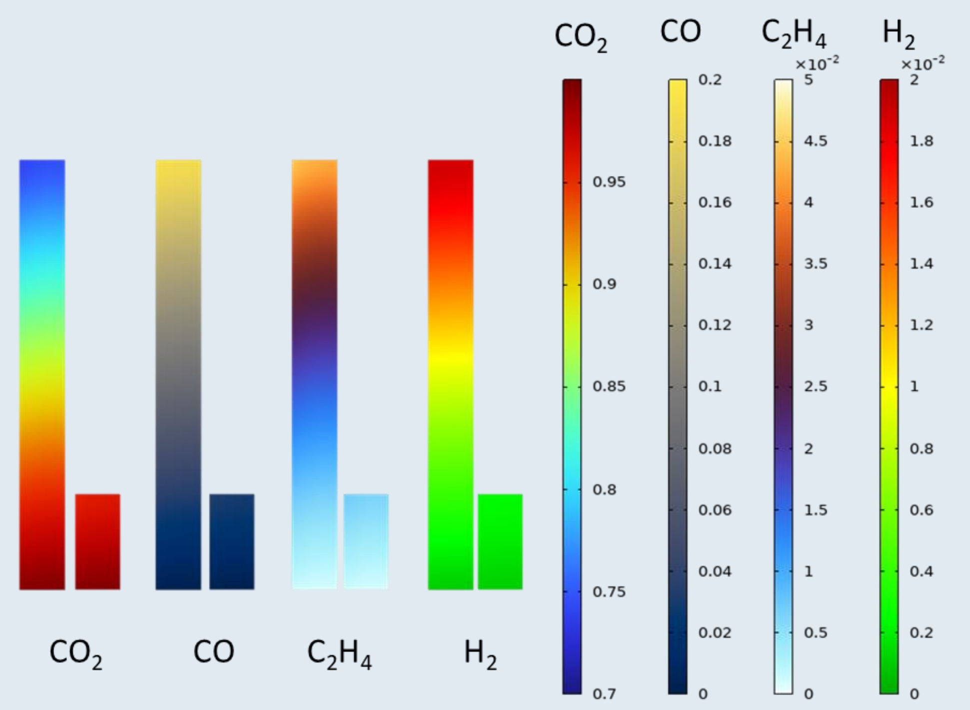

Shown mass fractions in gas channel (3mm wide)

Optimizing electrochemical conversion of CO_2 to C2 products

Multiphysics Simulations of electrochemical reduction of CO_2 to enhance the performance.

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Abstract

The low-temperature electrochemical conversion of CO_2 to ethylene offers significant potential for reducing the chemical industry's reliance on fossil fuels. Despite recent advancements, the key performance indicators—activity, selectivity, and durability—are insufficient for industrial implementation

To optimize the electrochemical cell and operating conditions, a multi-physics computational model is developed at the cell-level to understand the impact of different geometrical features, material properties, and operating variables. Initially, a steady-state isothermal 1D model based on existing literature [1] is developed, assuming a liquid-free gas diffusion layer (GDL). Gas and liquid flow, transport of 14 species (multi-species diffusion), and 13 reactions (heterogeneous and homogeneous) are modeled in the different (porous or open channel) regions.

This model is then extended to 2D to capture spatial variations and study the impact of material properties and operating conditions on performance. Different parameter variations have been investigated, including gas feed composition, catalyst loading, catalyst active area, GDL porosity.

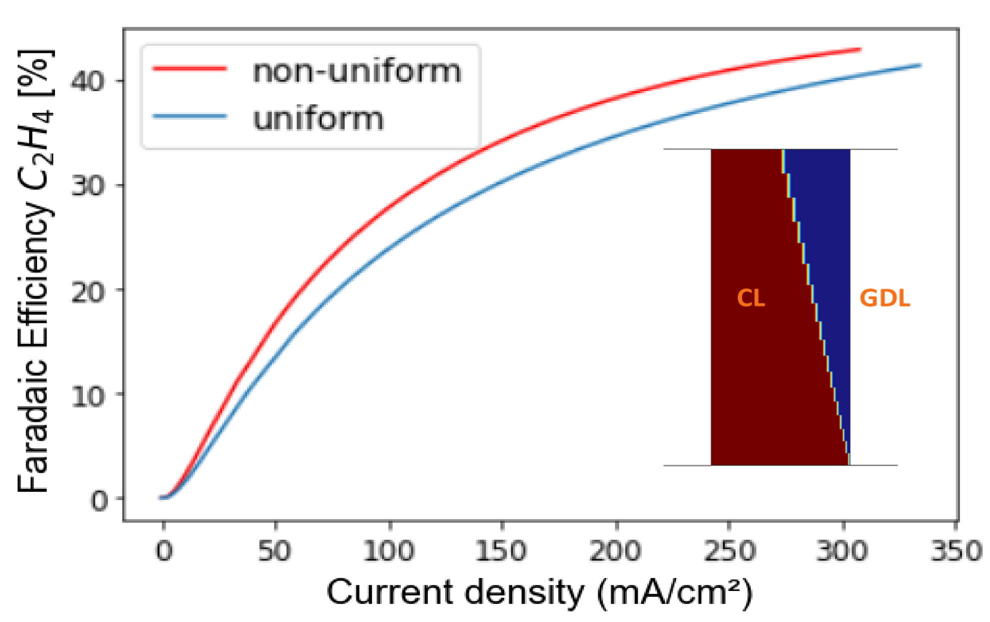


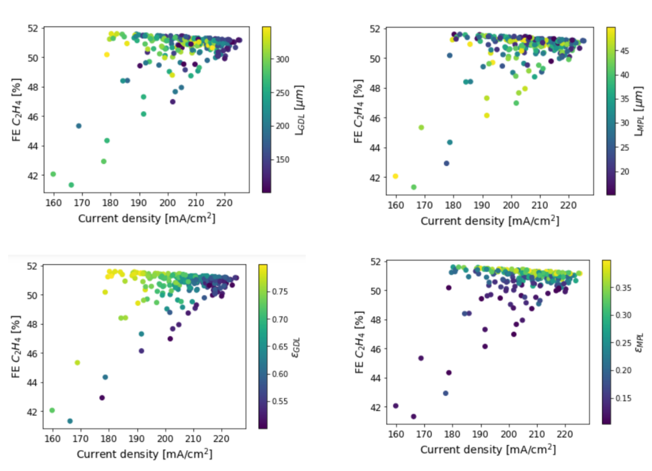
FIGURE 1: Effect of non-uniform catalyst loading on the performance of the electrolyzer. Blue part shows the absence of catalyst material on the substrate.

Methodology

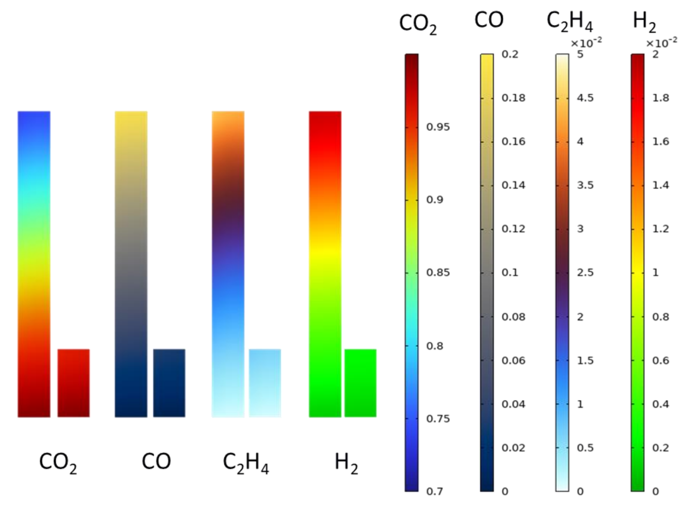
A Multiphysics model coupling tertiary current distribution, transport of concentrated gases and fluid flow in free and porous medium is developed to simulate the electrochemical reduction of carbon dioxide to useful compounds. The reactions are modelled using the Butler Volmer kinetics. The produced gases are average over the width of the catalyst layer and introduced then to the transport of concentrated gases domain as a flux boundary condition. Results are compared to experimental measurements from the literature (FIGURE 2).

Results

Model allows quick scanning of GDL and MPL properties.



There are inhomogeneities in the long electrolyzer



Shown mass fractions in gas channel (3mm wide)

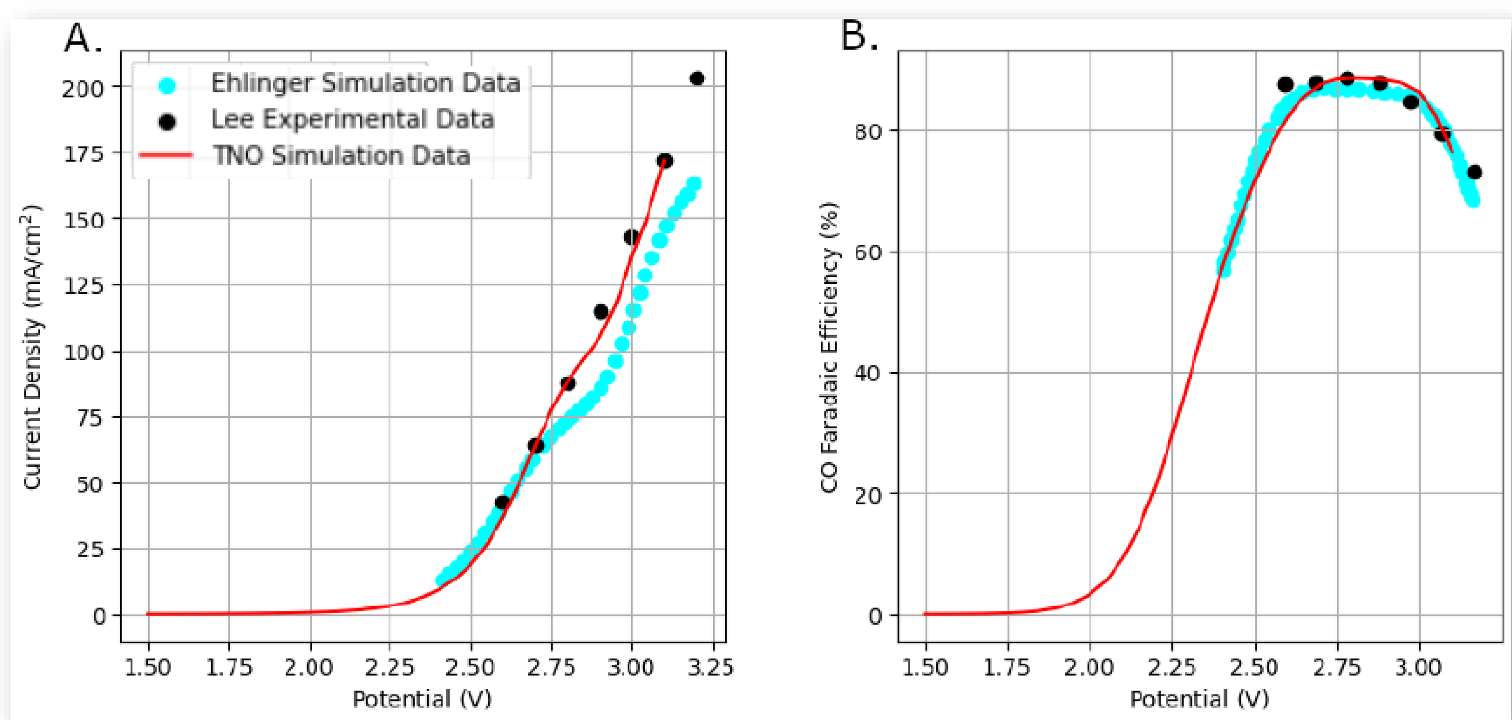


FIGURE 2: Comparison of our numerical model with experimental and simulation data from literature (Data from: Ehlinger, Victoria M., et al *ChemElectroChem* 11.7 (2024): e202300566.)

REFERENCES

[1] Weng et al. Energy and Environmental Science 13, 3592 (2020)

[2] Ehlinger, Victoria M., et al ChemElectroChem 11.7 (2024)

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