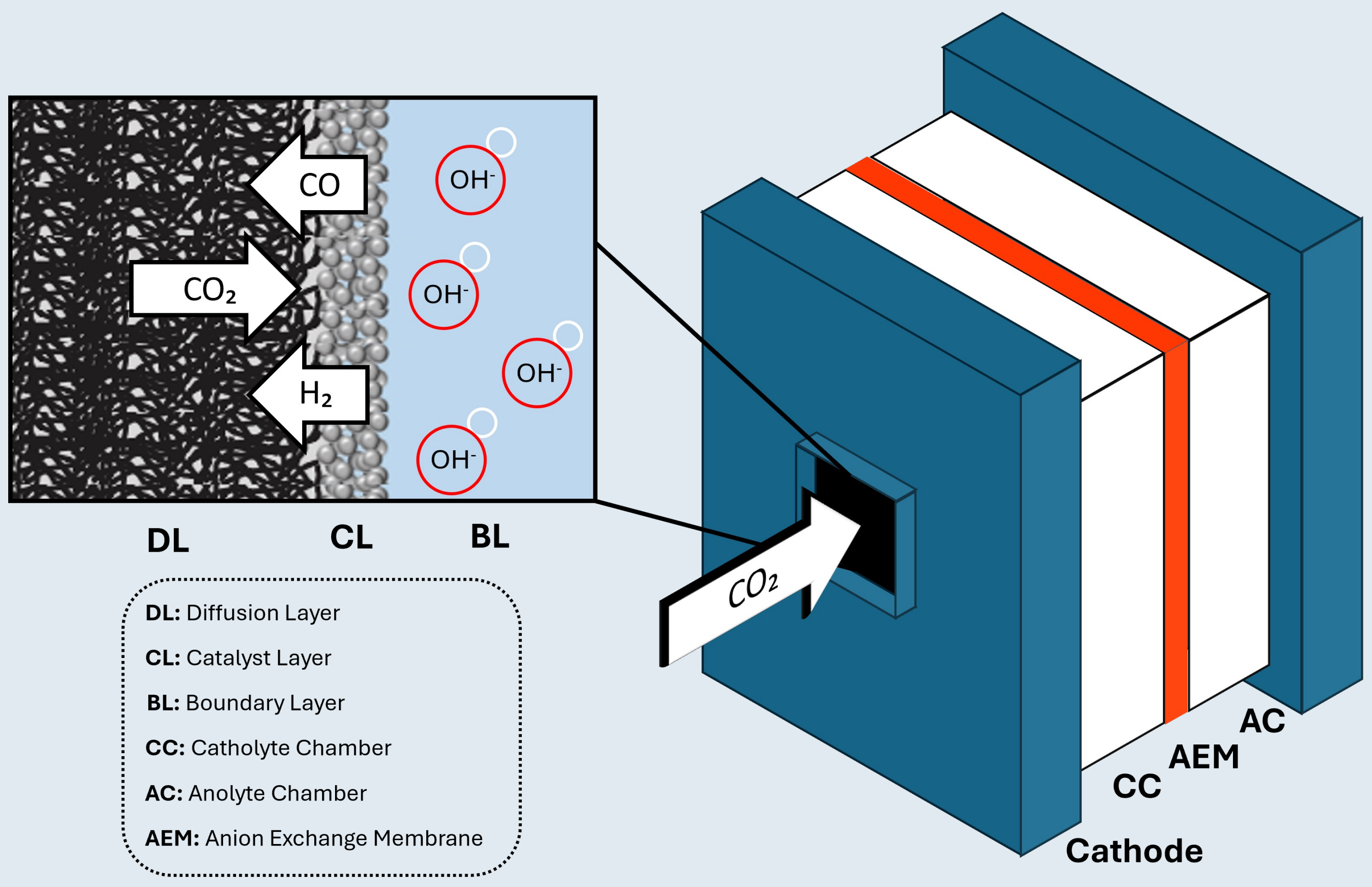

Gas Diffusion Electrode (GDE) for CO_2 Conversion in 2D Flow Cell Electrolyzer

A 2D GDE-based flow cell model is used for understanding CO_2 reduction reactions (CO_2RR) problematics and criticality. The model offers valuable results through fitted simulation that will aid optimizing experimental conditions.

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Introduction & Goals

Reactions occurring at the interfaces of **GDE-Flow Electrolyzers** needs further research to understand mechanisms and principles due to its high setup complexity.

To enhance understanding of lab-scale electrolyzer, a **2D flow cell model** has been implemented. This model will serve as a ground base for more detailed representations or variations occurring during the CO_2RR to understand and mitigate them.

The main problem in GDE-Flow Electrolyzer is the **electro-flooding** of the GDE-pores, which prevents CO_2 passage and thus, to perform CO_2RR. A careful cell simulation design will allow us to predict and prevent unexpected results, guide the experimental optimization and guarantying the efficiency and selectivity towards selected products (CO). Software's outputs will be verified and tuned by comparing them to the results of a corresponding experimental ones that **simulates real scenarios**.

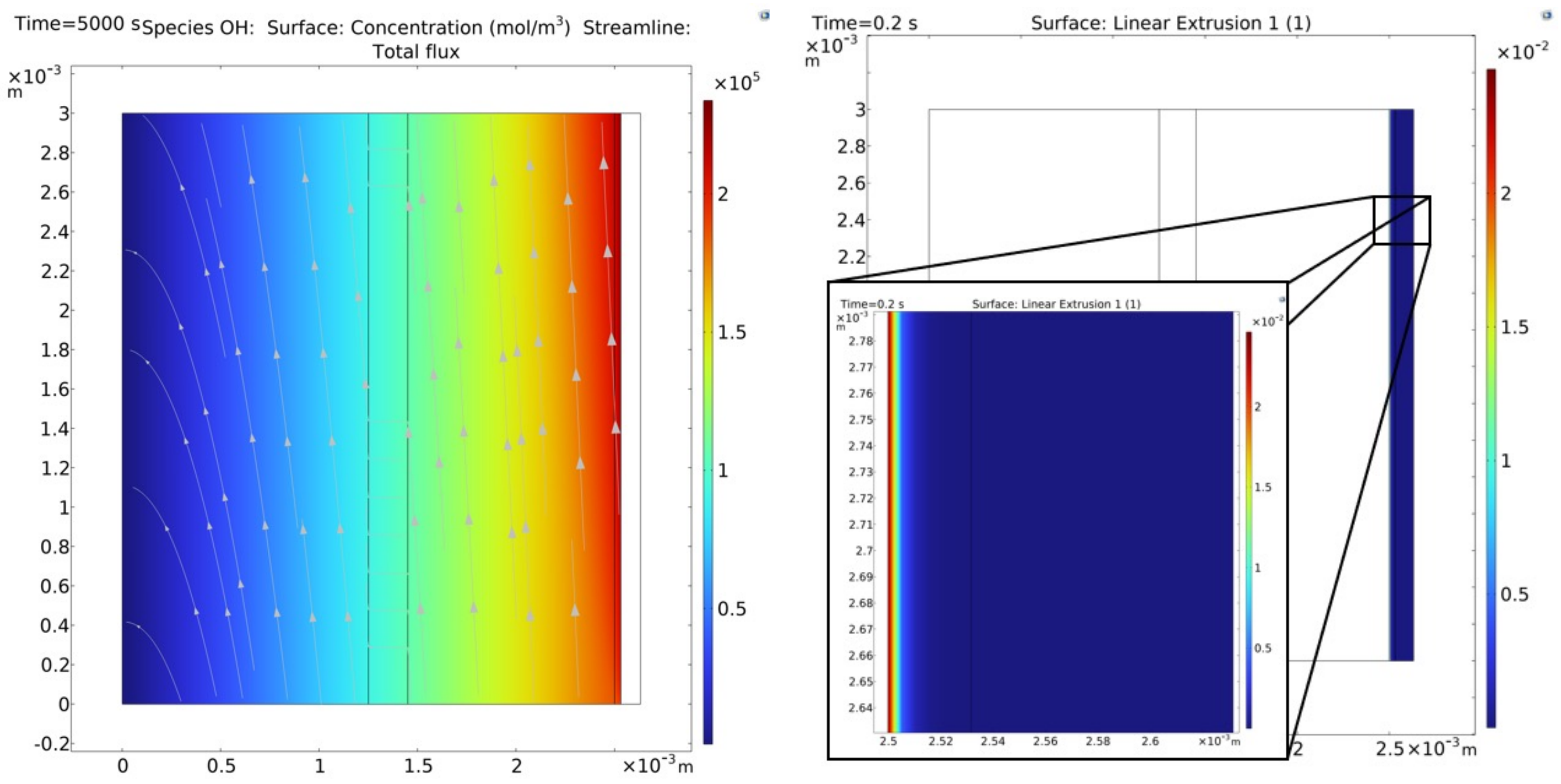

FIGURE 1. Left: Distribution of OH^- over the modeled cell. Right: Highlighted region of the GDE-pore CO_2 saturation.

Methodology

The model is split in two components:

- **2D Flow Cell:** Considers electrodes separated by an ion-exchange membrane with a laminar flow electrolyte; GDE saturation is extruded from the 1D model.
- **Cathode with GDE:** Electrolyte imbibition and evaporation are simulated as a function of the boundary pressure, and the wettability and permeability of the different domains (weak form Richard's equation and Leverett model).

Results

The results are presented in terms of CO and H_2 faradaic efficiencies (FE), namely the ratio between the flux of species produced and the current density when applying a fixed potential difference (Figure 1A).

$$\mathrm{FE} = \frac{V\, C_x\, z\, F}{A\, V_M\, j}$$

V = Flux rate, C_x = Conc. CO or H_2, z = Number electrons, F = Faraday constant, A = Area, V_M = Molar volume, j= Current.

The FE and overall cell performance is determined by the GDE properties: the model simplifies the optimization of the cell architecture. Figure 2B shows saturation for different wettability.

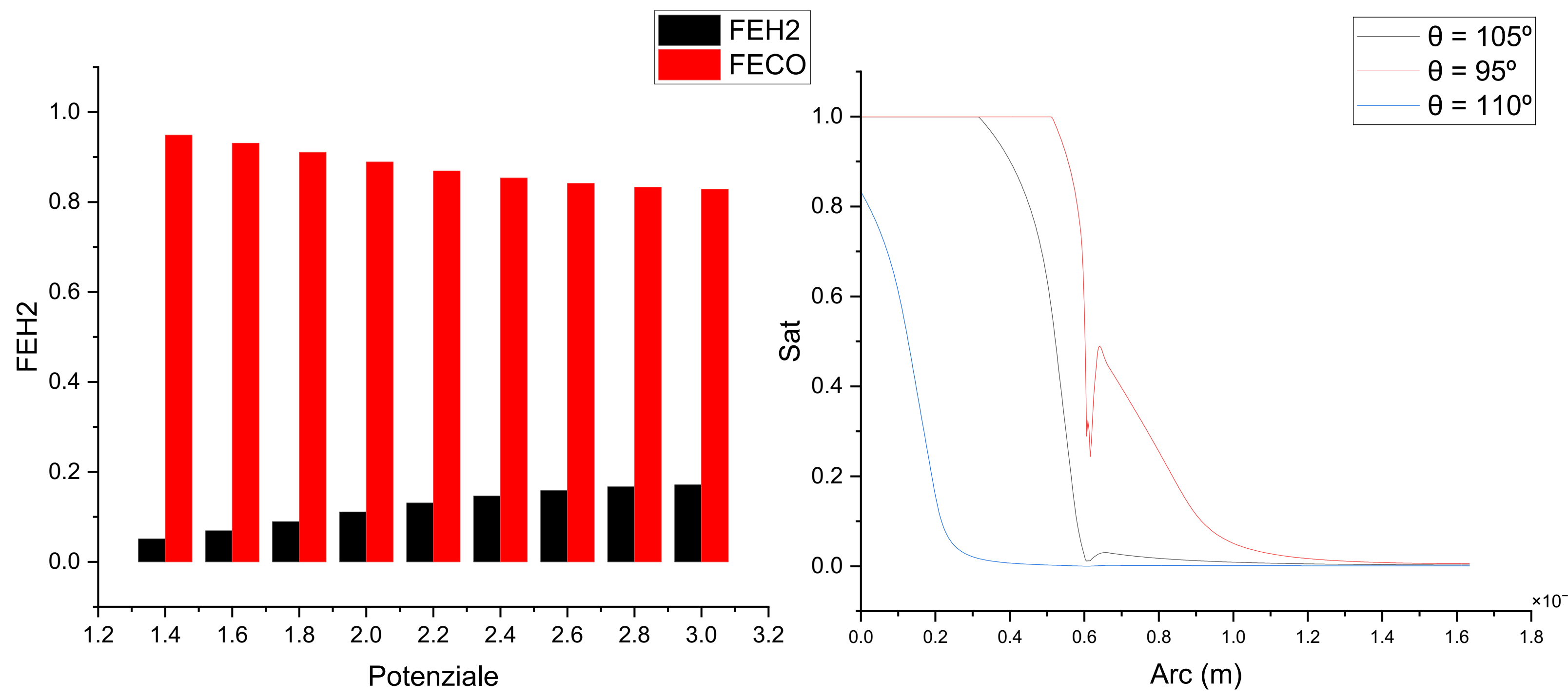

FIGURE 2. Left: FE of CO and H_2 at different potentials. Right: Pore saturation through the GDE with different water contact angle inputs.

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