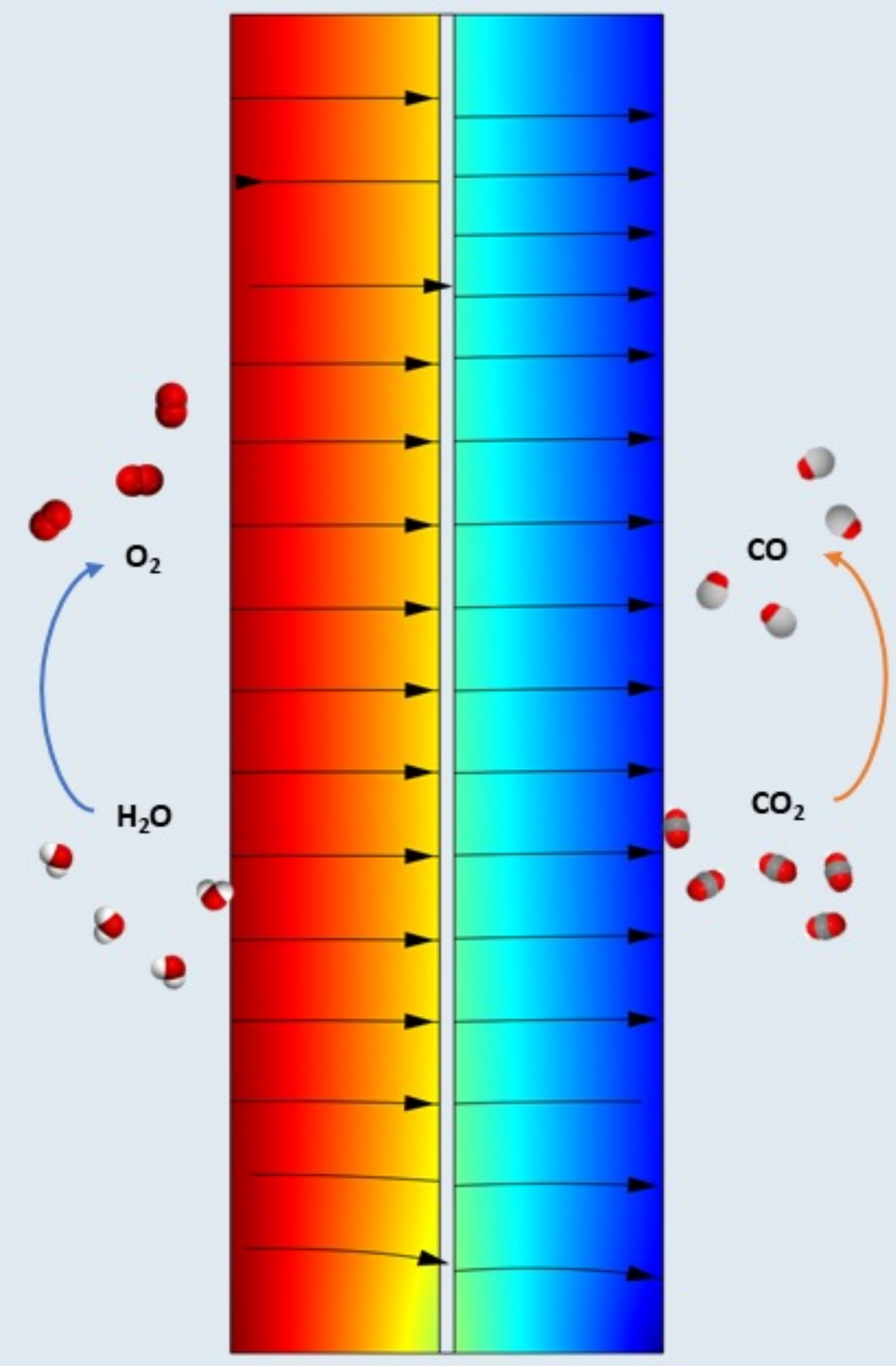


2D Model of the Artificial Leaf

Development of a comprehensive COMSOL® modeling for the Solar-Driven CO_2 electroreduction to added-value product, toward the climate change mitigation.

M. Agliuzza[1], C.F. Pirri[1,2], A. Sacco[2]

1. Applied Science and Technology Department, Polytechnic University of Turin, Turin, Italy.

2. Center for Sustainable Future Technologies @Polito, Italian Institute of Technology, Turin, Italy.

Introduction

Electrochemistry is the most promising process for decarbonization, since it allows the conversion of CO_2 into added-value products in an up-scalable and sustainable technology. In this work, a 2D model of the reactor is developed, which successfully replicates the experimental data for the conversion of CO_2 into CO: it can predict the performance of the device, along with chemical conditions at the electrode surfaces [1].

In addition, the integration with photovoltaics as electrical source is implemented: the model simulates the electrochemical cell integrated with a module of Dye-Sensitized Solar Cells (*Artificial Leaf*) [2], such that the performance of the device as a function of the solar irradiance can be inspected as well.

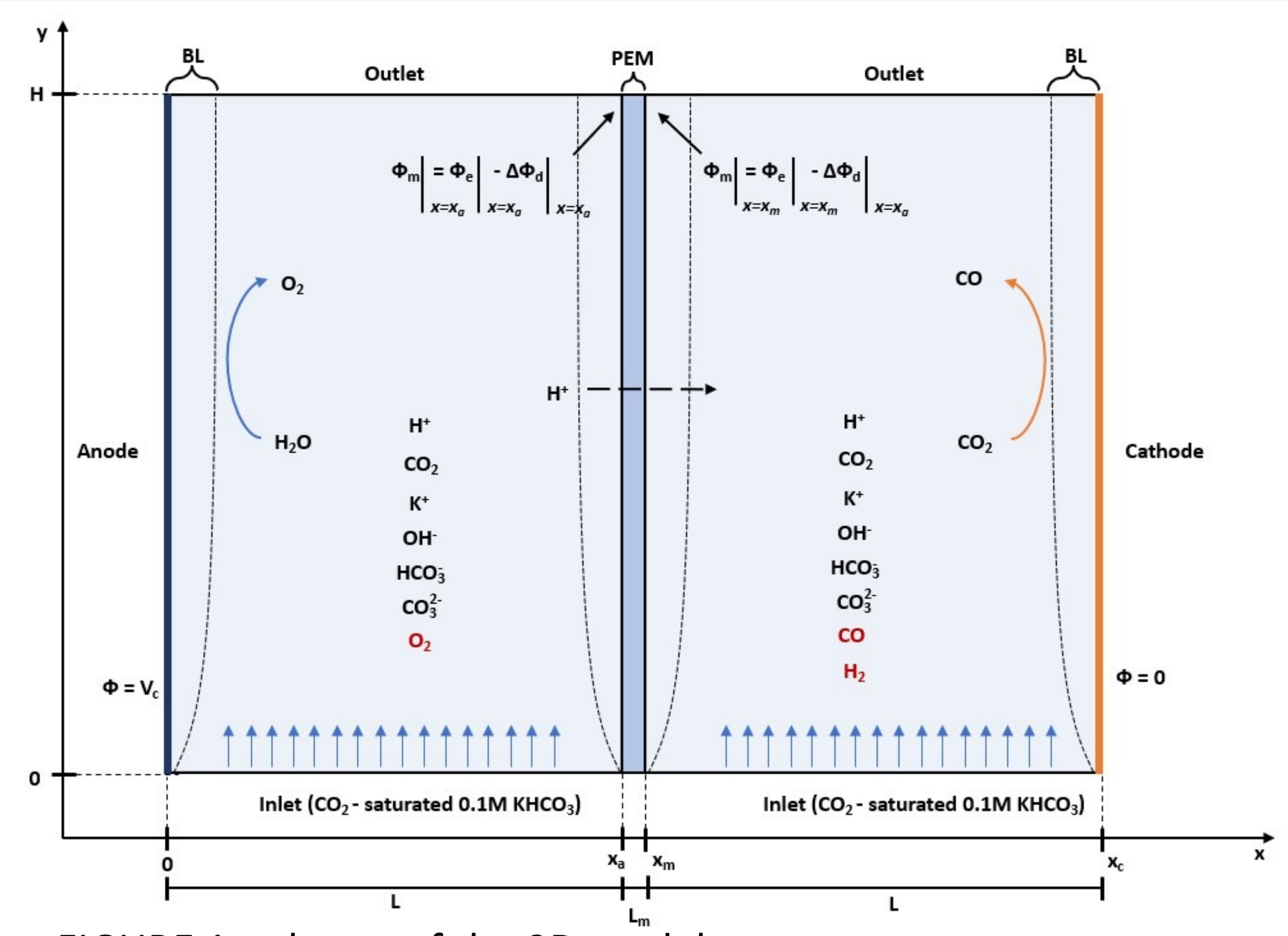
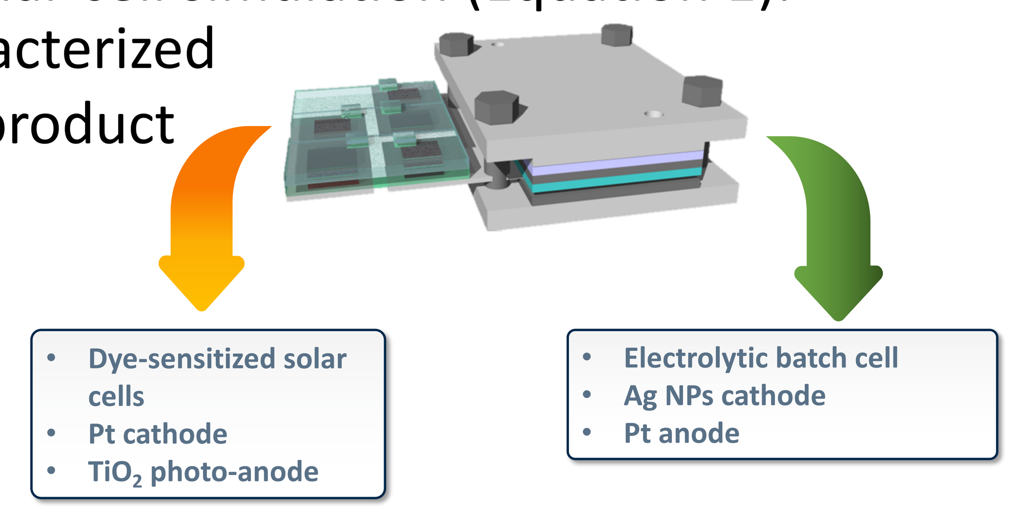


FIGURE 1. scheme of the 2D model

Methodology

Model: 2D geometry of a batch cell reactor for CO_2 reduction. Cathode and Anode electrodes (Ag nanoparticles and Pt foil, respectively) are modeled through their kinetic parameters in the Butler-Volmer equations, in the Tertiary Current Distribution physics. Secondary Current Distribution is used for the ion-exchange membrane, and the single diode equation for the solar cell simulation (Equation 1).

Experiment: *Artificial Leaf* characterized with chronoamperometry and product analysis



$$I = I_{ph} - I_0\left[exp\left(\frac{V+IR_s}{nV_t}\right)-1\right]-\frac{V+IR_s}{R_{sh}}$$

EQUATION 1: single-diode model

Results

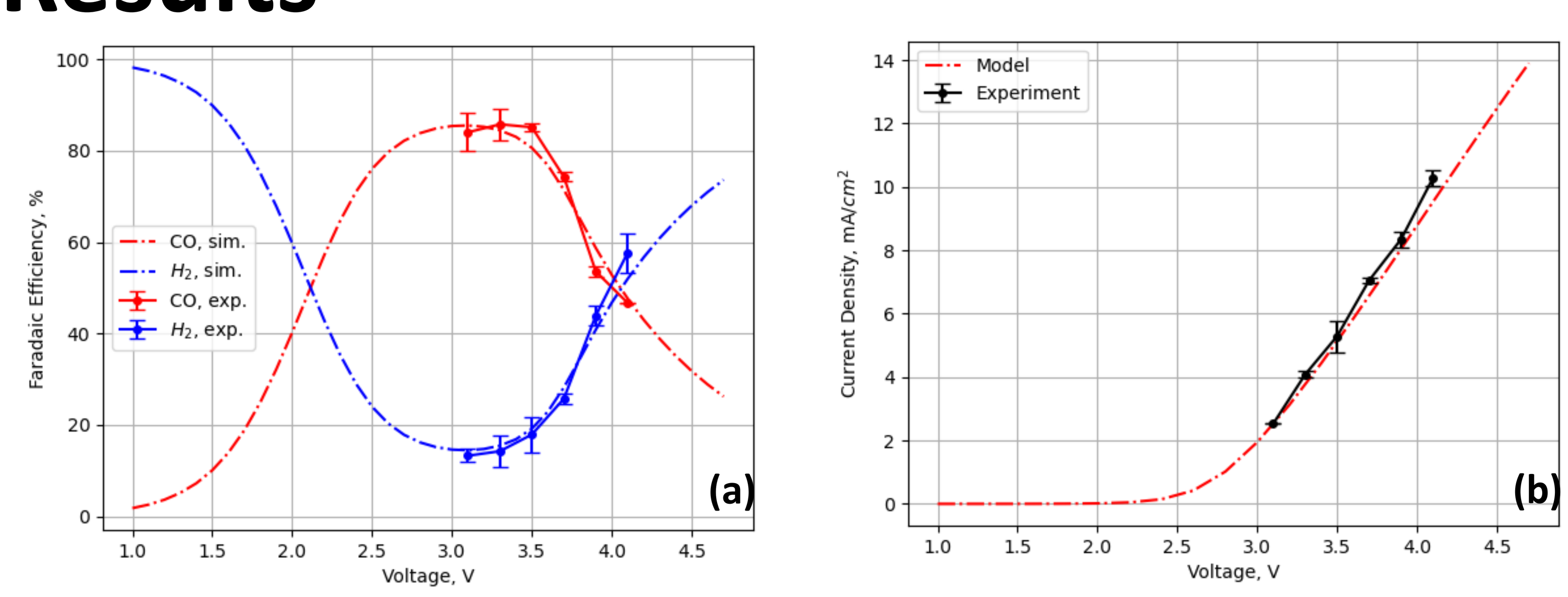


FIGURE 2. Model validation with experimental FEs and Current Density

Model validation through experimental results:

- Faradaic Efficiencies of CO production and Hydrogen evolution reaction (Figure 2a)
- Current density curve (Figure 2b)

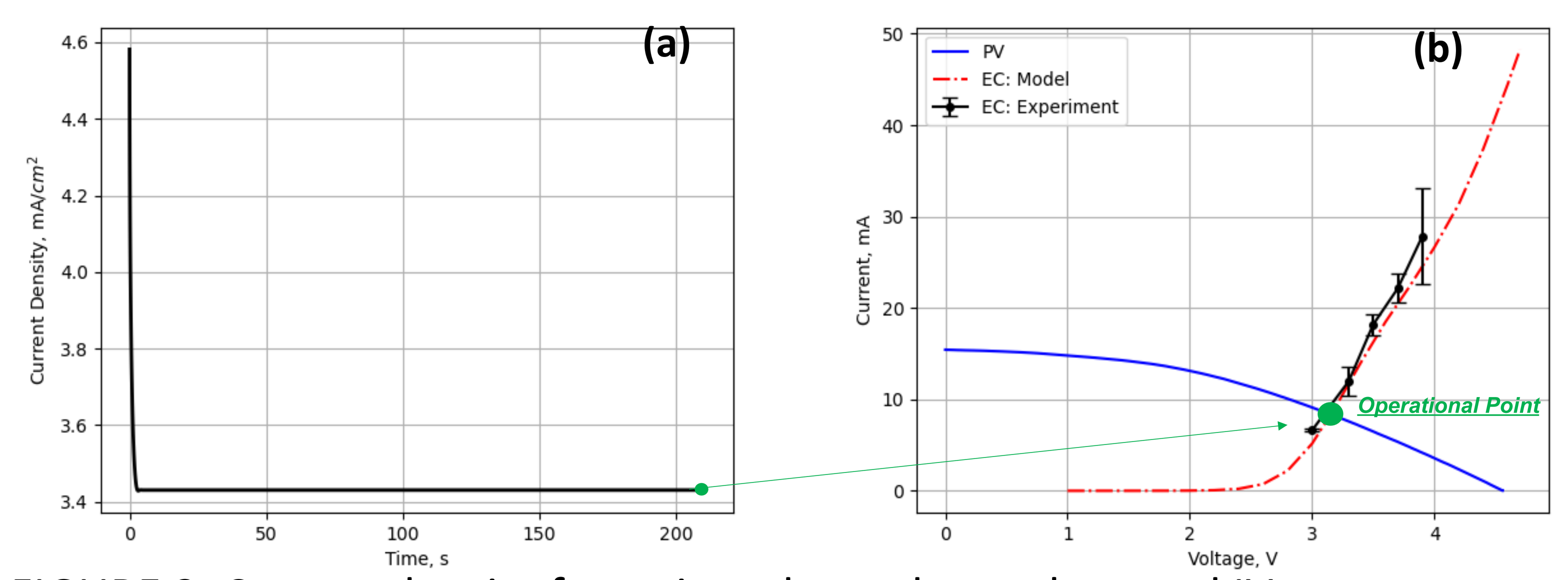


FIGURE 3. Current density from time-dependent solver, and IV superimposition of the PV and EC

Simulation of the *Artificial Leaf:*

- Time-dependent simulation with the single-diode model integration to predict the operational point (Figure 3a)
- Overlap of the experimental PV and EC curves (Figure 3b)

REFERENCES

1. M. Agliuzza et al., A comprehensive modeling for the CO2 electroreduction to CO, Journal of Physics: Energy, 6 015004. (2024).
2. A. Sacco et al., An Integrated Device for the Solar-Driven Electrochemical Conversion of CO2 to CO, ACS Sustainable Chemistry & Engineering, 8 (20), 7563-7568. (2020).

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