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Electrochemical CO_2 reduction is a promising carbon dioxide utilization technology that can enable sustainable carbon cycling, converting CO_2 into valuable chemical products. Electrochemical cells dedicated to CO_2 conversion can employ gas diffusion electrodes (GDEs), that allow for significantly higher current densities with respect to the ones obtained by traditional planar electrodes.

GDEs design is not trivial, since various complex factors can contribute to determine the cell performance. The latter depends in fact on electrodes material and geometry (e.g. thickness, porosity), applied voltage and current, applied pressure, electrolyte and gas composition. These quantities and their effects on cell operations can readily be considered in simulation frameworks, that represent a powerful tool to optimize the cell design and upscaling the technology, that should achieve high reaction rates, energy efficiency, and long-term stability to be profitably implemented in industrial environment.

In this work, a one-dimensional model for the simulation of a GDE for CO_2 reduction is presented. The model includes the hydrophobic catalyst layer (CL), the diffusion layer (DL) and the microporous layer. Species are generated according to the applied current and transported via multicomponent diffusion, Darcy flow, and capillary-driven electrolyte motion in the CL. Gas pressure is determined by solving the gas-phase mass balance with Darcy's law, where permeability and porosity depend on local saturation, coupling gas and liquid transport. The gas feed is humidified carbon dioxide (97.5 % CO_2, 2.5 % H_2O). Gas pressure was fixed at the DL/gas-feed interface, and a no-flux condition was imposed at the CL/electrolyte interface. The capillary pressure is related to saturation and to the contact angle through a Leverett J-function closure equation for hydrophobic porous media.

COMSOL Multiphysics is employed to perform numerical time-dependent simulations to observe the operations of a GDE, focusing on the effect of the applied back pressure (BP, namely an overpressure on the gas feed side) on pore saturation. To simulate the experimentally observed loss of hydrophobicity, the contact angle was assumed to decrease linearly during the simulation, mimicking electrowetting. Four different values of BP are tested, showing that, for the GDE properties considered, an increase of 30 mbar in BP results in a delayed flooding, depending on the loss of hydrohpobicity due to electrowetting. $\theta_{crit} \sim 92° BP = 0 \text{ mBar} 90 \text{ °} BP = 20 \text{ mBar}$. An increase of BP will in fact consequently increase also the gas pressure in the domain, causing a higher capillary pressure contrasting the flooding phenomenon.

The presented model can be used to train a reduced-order surrogate model representing the cathodic solid-liquid interface in a computationally efficient yet representative way. This step is necessary to effectively implement a full cell model, either in 2-D or 3-D configurations, and is crucial to envision an effective usage of multiphysical models in scaling up GDEs technologies, thus making this solution industrially viable. In perspective, these models can

serve as generators of synthetic data to train optimal control algorithms, sensitive to specific operating conditions and microstructure parameters.