Modeling of the Electrochemical Reduction of CO2 to Methanol in a Micro Flow Cell

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Abstract

Carbon dioxide levels are increasing faster than they have in hundreds of thousands of years due to fossil fuels burning [1]. The world mainly relies on these fuels as a source for the growing energy demands. A serious worldwide interest is growing towards the field of CO2 valorization as a step in transitioning away from fossil fuel economy at the same time of decreasing the CO2 spiking concentrations [2]. One attractive option is the CO2 electrochemical reduction into fuels, especially methanol as a green fuel that can be readily employed in existing energy converting systems [3], [4].
In this work, an experimental setup for the CO2 electro reduction into methanol was modeled using COMSOL Multiphysics®. The model features a simple geometry, as shown in Figure 1, for a microfluidic flow cell in which the reduction takes place. The Electrochemistry Module, namely the Tertiary Current Distribution interface and Secondary Current Distribution interface were coupled in the study to cover the whole physical phenomena occurring inside the cell. Governing equations are Nernst Planck equation and the charge conservation law, which were solved for steady state operation using COMSOL. This model considers species mass transport, charge transport and electrode kinetics. An array of electrochemical reactions for the reduction of CO2 to various products at the cathode surface was included in the model.
When validated against experimental data, the model showed good agreement with respect to the concentration of the produced methanol [5]. Figure 2 shows the methanol produced along the cathode side. The different kinetic parameters for the reactions were obtained by fitting the model to experimental data. Furthermore, the model showed that the convective flux of the methanol in the vertical direction is much larger than its diffuse flux in the horizontal direction. This remark boosted the understanding of the flow behavior inside the cell and it can be of help for the future design of an effective electrochemical cell for CO2 reduction. Figure 3 shows a cut line plot of the electrolyte potential at half the cell height. The Donnan potential shifts at the membrane boundaries are clearly visible in the figure. Figure 4 shows a 2D surface plot for the hydrogen ion concentration. It displays the increase in H+ concentration at the anode where it is produced, and its consumption at the cathode side to produce methanol.
It should be noted that this work is the first attempt to model the electrochemical reduction of CO2 to methanol; which is a step forward towards the scale up of the process

to industrial operation. The model represents an advancement in interpreting how the system works and gave better insights on the kinetics and transport inside the cell. It represents a viable tool which will be used to determine the best operating parameters to maximize the methanol production and optimize the performance of the cell.

Reference

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[5] J. Albo et al., Production of methanol from CO2 electroreduction at Cu2O and Cu2O/ZnO-based electrodes in aqueous solution, Appl. Catal. B Environ., 176–177, pp. 709–717 (2015)

Figures used in the abstract

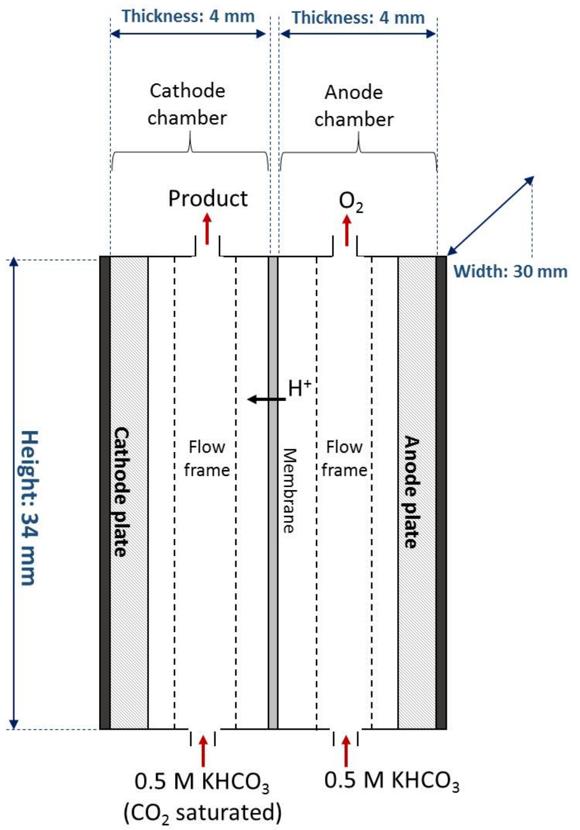

Figure 1: Flow Cell configuration.

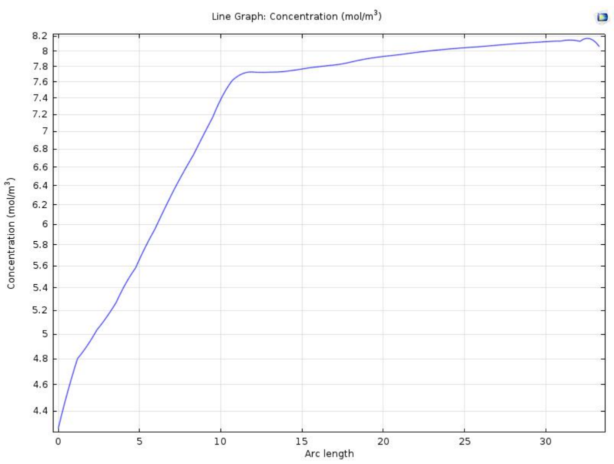

Figure 2: Methanol production along the cathode surface.

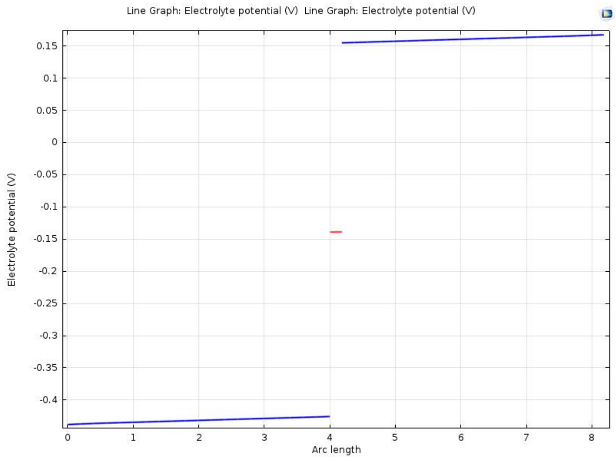

Figure 3: Electrolyte potential along a horizontal line at half-cell height.

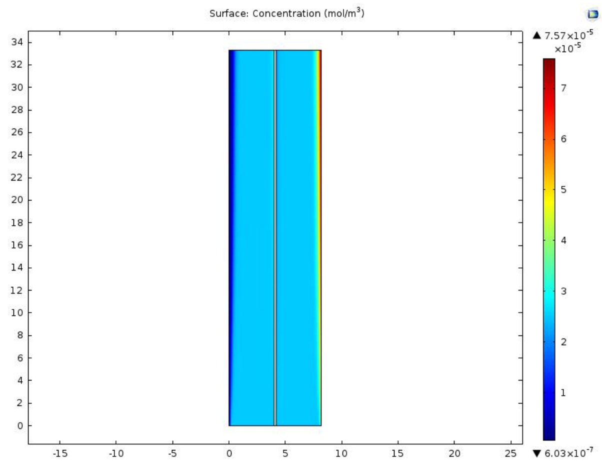

Figure 4: Hydrogen ion concentration.