WP5 TASK 5.3

# Industrial-scale CO2 electrolysis


## ABSTRACT

Carbon capture and utilization (CCU) is a viable approach to convert atmospheric $CO_2$ into various valuable end products such as fuels, chemicals, and construction materials. In the context of CCU, this research focuses on the conversion of $CO_2$ to elemental carbon via molten carbonate electrolysis. New reactor designs were studied to enable upscaling to industrial process including the effect of industrial power supplies on the specific energy consumption and product quality.


## MOTIVATION

To increase the applicability of molten carbonate electrolysis new reactor designs are required. Advances and challenges related to stacking of single molten carbonate electrolysis cells into stacks in the similar manner as in case of water electrolysis needs to be studied. Further, replacing batch process with a continuous process might be a promising pathway towards industrial scale process.

## RESULTS

The electrodeposition process of carbon in molten lithium carbonate electrolysis and the associated gas-liquid flow hydrodynamics characteristics were investigated using computational fluid dynamics (CFD) for the first time. The high-temperature (750 ◦C) process is challenging for conducting measurements, making CFD a valuable tool for providing insights into the novel coaxial-type cell design. The CFD simulation addresses the electric field distribution, oxygen gas evolution, and electrodeposition of carbon. The effect of gas bubble sizes (1, 0.8, and 0.6 mm) on the CO2 -electrolysis process was examined at different electrical current densities (0.15 ±0.01 A cm–2). The CFD results reveal that gas holdup increases by decreasing the bubble size and that the bubble size significantly impacts the current density distribution by affecting the two-phase flow dynamics.

The results also indicated that the current density distribution is not as uniform as anticipated with the coaxial setup. This uneven distribution causes the carbon deposition on the cathode surface to become uneven. Also, as of now, the numerical investigation only considers the main reactions of the carbon deposition by only considering the carbon and oxygen formation. Experimental work (in HYGCEL WP5.2) revealed that the presence of metallic impurities affects the carbon morphology.

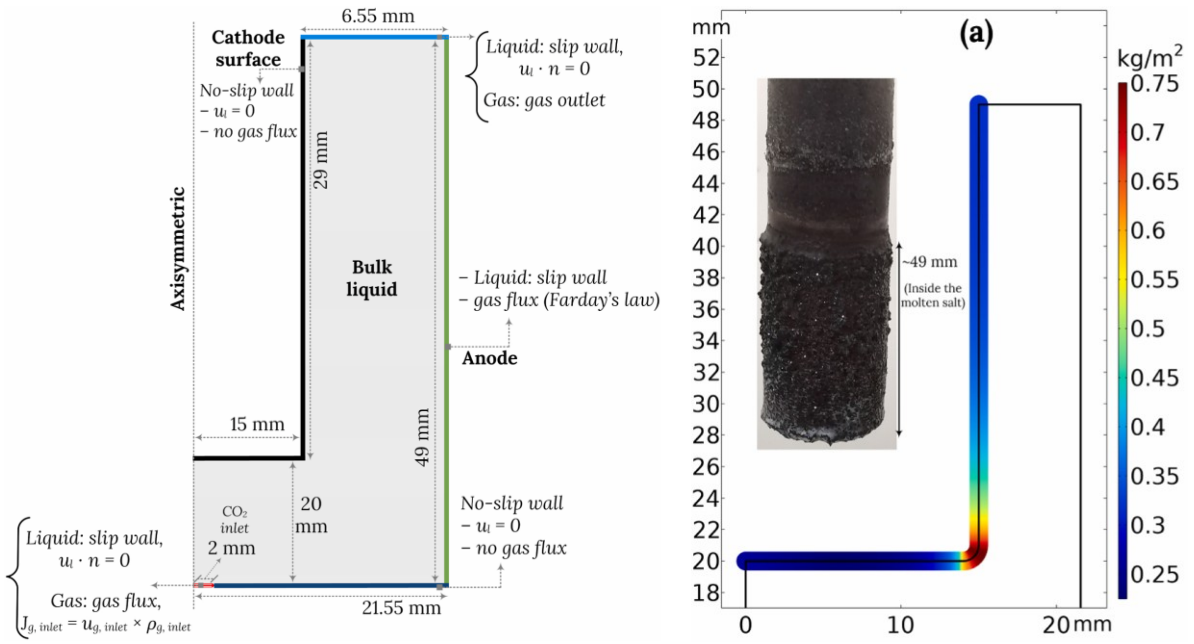


**Figure 1. Left figure: Schematic illustration of the boundary conditions of the CFD analysis. Right figure: carbon deposition on the cathode surface obtained via CFD simulation and a photograph of the cathode from the experiment.**

The current study successfully employed computational fluid dynamics to investigate the hydrodynamics characteristics and electrodeposition process of carbon in a molten lithium carbonate electrolysis cell. The study aimed to provide further insights into the high-temperature process occurring in the co-axial reactor, where currently no practically viable solutions exist for process monitoring. The challenges of model validation were addressed, and attempts were made to assess the validation quantitatively and qualitatively. The results indicate that gas bubble size plays a critical role in the liquid electrolyte hydrodynamics and charge transfer mechanism, affecting the current density distribution at the cathode. Moreover, due to the design of the cell, the electric field distribution is stronger at the corners of the cathode, resulting in relatively larger carbon deposition in those regions. The numerical study presented in this work has demonstrated the potential applications of CFD in high-temperature molten salt processes.

Study showed that the current ripples generated by power electronics do not have very significant effect on the product quality and current waveform control is not effective on the carbon morphology control. Current ripples were found to cause additional power consumption as already known in case of water electrolysis.

## APPLICATIONS and IMPACT

Molten carbonate electrolysis is still not in commercial phase. The key aspect in the molten carbonate electrolysis profitability is the purity of end product in addition to the specific energy consumption of the process. Corrosion heavily affects the carbon quality, and it is challenging to reach low-cost stack structure to elevate system voltage in order to limit the current requirement and power supply cost.

## MAIN CONTACT

Tero Joronen, TAU, tero.joronen@tuni.fi

## AUTHORS

Tero Joronen, Jyrki Mäkelä, Miika Sorvali, TAU

Vesa Ruuskanen, Tuomas Koiranen, Emma Laasonen, Anafi Aini, Jero Ahola, LUT