The electrochemical CO₂ reduction process using solar energy: multi-scale simulation, technoeconomic analysis, and pilot plant

The electrochemical CO_2 reduction has received significant attention regarding carbon capture and utilization technology. However, since its difficulties in developing efficient catalyst/reactor device and economic infeasibility, skeptical points for the industrial application of large-scale production technology also exist. To overcome the obstacles, 1) organic oxidation reaction instead of O_2 evolution reaction is applied to pair reaction, 2) high current density, high faraday efficiency, and long-term stability catalyst/reactor device should be designed, and 3) process design and demonstration with actual pilot plant is essential for commercializing.

In this talk, we present how (1)–(3) problems are solved in terms of process systems engineering. First, we developed the auto-flowsheet generator for techno-economic analysis. Second, multi-scale simulation [density function theory (DFT) – kinetic Monte Carlo (KMC) – computational fluid dynamics (CFD)] is developed. Finally, we present pilot plant for electrochemical CO_2 reduction process which has been constructed in KIST and how we find optimal operating conditions using machine learning algorithm.