

Theoretical Bachelor Thesis, Research Internship

Simulation of Direct Air Capture with pH-Swing Absorption

Description

CO₂ removal via Direct Air Capture (DAC) can play a crucial role in mitigating the climate crisis (IPCC, 2022). Amongst various emerging technologies, our research focuses on absorption-based methods with electrochemical regeneration (AEC), where research demand meets promising predictions of energy and cost factors (Rosen, 2024).

The proposed thesis contributes to this matter by simulating DAC with pH-Swing, a technique that utilizes the well-known dependency of CO₂ solubility on pH (Figure 1). Hereby various chemical approaches and process topologies follow the same underlying principle (Seo, 2023), as illustrated in Figure 2.



Figure 1: pH-Dependency of CO₂ solubility can easily be observed in our daily life. Pictures from Spektrum (2019) and DAZ (2022).

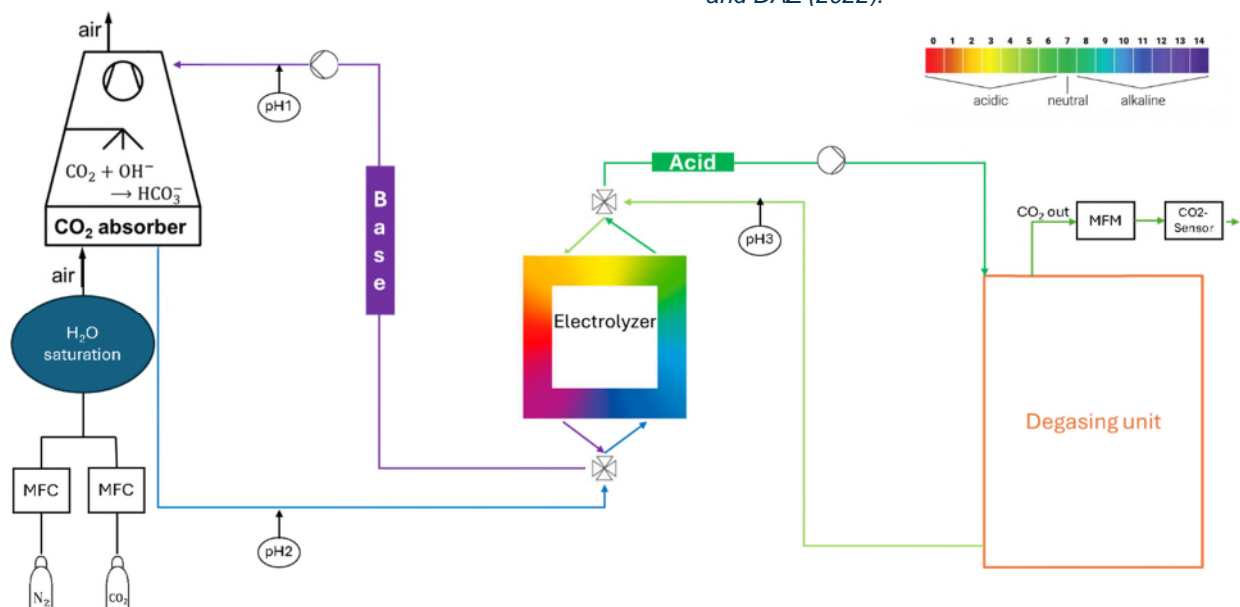


Figure 2: Schematic illustration of an electrochemical carbon capture system. The pH-dependent solubility of carbonate species is utilized to capture and release CO₂.

First aim of the study is to adapt and implement preexisting surrogate models for electrolysis, absorption and desorption into a suitable software framework and investigate how different process parameters influence an idealized AEC system. Further steps include comparing different process topologies regarding their minimum thermodynamic energy demand and a stepwise increase of the model depth of the electrolyzer. The obtained results will pose a decision basis for the design of a laboratory-scale AEC test stand and a future scale-up.

Prerequisites

- Physical Chemistry and thermodynamics, in particular Vapor-Liquid equilibria, Free Energy and activity modeling
- Intermediate Programming skills (e.g. Python, Matlab, Aspen or else)
- No fear of mathematics (linear algebra, algebraic and differential equation solving)
- Experience in electrochemistry is beneficial but not required

Our offer

- Thorough Onboarding and Support throughout the thesis
- Excellent supervision in a communicative and pleasant work group
- Valuable contribution to sustainable research

Start

immediate

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