

## Development of a Simulation Model for Adsorption-based Hydrogen Storage

## **Description**

Efficient hydrogen storage remains one of the key challenges for wide-spread adoption of hydrogen both in stationary energy systems and mobility. In addition to compressed gaseous and liquid hydrogen storage, material-based storage is gaining increased attention.

One promising concept is to store hydrogen adsorbed to the surface of microporous materials such as zeolites, metal-organic frameworks or carbon-based materials through van der Waals forces. Several of these materials are already widely produced, and could thus lead to a cost advantage. Furthermore, the storage pressures are significantly lower compared to compressed gaseous storage, while the required temperatures are above those of liquid hydrogen. However, the technology still has some disadvantages regarding reversible operation, thermal management and kinetics.

The goal of the thesis is to implement a 0D simulation model with the reaction kinetics in MATLAB Simulink and perform a parameter study via simulation to determine the impacts of operating conditions (temperature, pressure, cooling/heating power) and different materials on the storage capacity, thermodynamic efficiency and filling speed.

## Work Packages

- Literature research on different adsorption-materials and possible applications, and selection of promising material candidates (1 month)
- Development of adsorption-storage model incorporating the reaction kinetics and model validation with literature/experimental data (2 months)
- Parameter simulation of different operating conditions/materials (1,5 months)
- Post-processing and result interpretation (0,5 months)
- Written thesis (1 months)



Source: Yang, D., et al., "Numerical simulation of the hydrogen charging process in an adsorption storage tank," IJHE, 2024.

- Start: immediately
- Duration: approx. 6 months
- Paid Master Thesis
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