# SIMULATION MODEL FOR ADSORPTION BASED HYDROGEN STORAGE

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## Introduction

With the necessity of mitigating climate change, the energy system, currently based on fossil fuels, needs to be decarbonized. A promising candidate for an alternative, carbon neutral energy carrier is hydrogen, as it combines a high gravimetric energy density with the possibility of climate neutral production and utilization. One of the key aspects for transitioning to a sustainable hydrogen society is the storage of hydrogen with high volumetric energy density. Combining less safety risks than compressed hydrogen with higher volumetric storage densities than compressed and liquid hydrogen storage, makes adsorption storage a promising concept.

Ideally, a storage vessel provides a high volumetric energy density and a large total storage capacity. Hydrogen uptake and release should be feasible close to ambient conditions with respect to temperature and pressure, to minimize the energy needed for desorption, but also providing enough binding energy to contain the hydrogen. Additionally, the cooling and heating power needed for hydrogen ad- and desorption should ideally be small enough to realize cost efficient operation. The adsorption material should be readily available, sustainably sourced and energy-efficiently produced, with the material being non-toxic, having a long lifetime (low degradation) and being recyclable after the end of life.

The current adsorption storage technology still has shortcomings regarding several of these desired properties. Main challenges of state-of-the-art adsorption storage materials are ambient temperature operation and storage capacity.

## Objectives

To tackle these challenges the characteristic operation parameters are to be identified and their interrelations determined. With the impact that each parameter has on the system identified, the properties of the storage system can be tuned to enhance specific aspects e.g. operating temperature, storage capacity, and mass flow amongst others.

## Methods

A MATLAB Simulink 0D thermodynamic simulation model of hydrogen adsorption on a carbon material with different operation modes was implemented. The simulation is based on the Dubinin-Astakhov model and real experimental data of ad- and desorption measurements, taken from literature [1]. The utilisation of a simulation model omits the need for extensive experimental series making it possible to investigate the whole parameter space. Measurements can then be evaluated and/or supported with simulations and process parameters can be optimised. Finally, results of experiments can be compared, and, the simulation can estimate further measurement outcomes.

## Preliminary Results

The simulation model was used to conduct parameter studies on temperature, pressure and heat transfer to investigate various operating conditions and their impact on storage capacity and the extent of cooling and heating required for operation.

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In Figure 1, three different parameters, namely stored mass (a), system temperature (b) and system pressure (c) are shown for a predefined measurement procedure. Traversing the simulated measurement from left to right, four different stages can be seen (I-IV).

First (I), 1.90 kg of hydrogen is almost isothermally adsorbed up to a predefined maximum system pressure of 4.0 bar. As can be seen by the slight increase in temperature the heat resulting from the adsorption process cannot be fully cooled away with the chosen heat transfer factor [2]. Second (II), the storage system is switched to isothermal desorption until reaching 2.8 bar system pressure and 1.35 kg hydrogen stored. Similarly to stage one, the temperature reduction, due to desorption, cannot be fully counterbalanced by the heating. In the third stage (III), hydrogen is desorbed by heating (temperature programmed desorption) up to a maximum temperature of 293 K, until the system reaches ambient pressure. In stage four (IV) the simulated measurement has reached its final state where the desorption has stopped at a system pressure of 1 bar and 0.20 kg of hydrogen remaining.

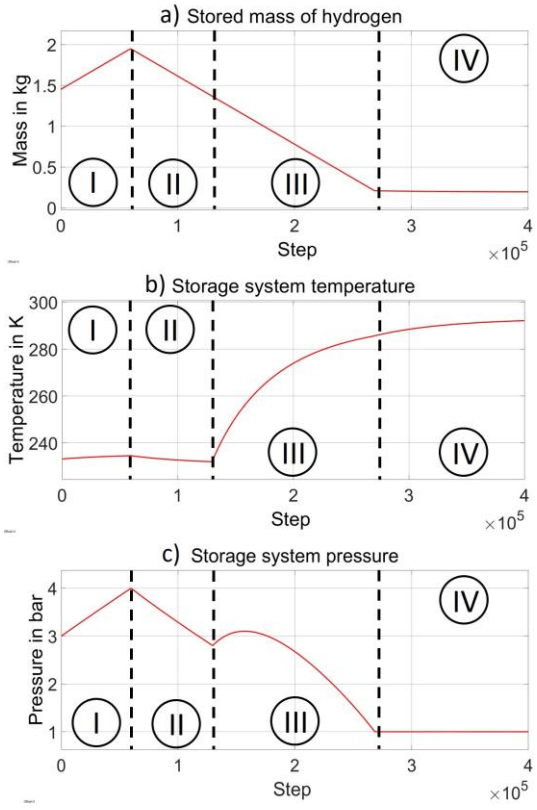


*Figure 1: Stored mass (a), temperature (b) and system pressure (c) during simulation of a measurement procedure consisting of four distinct stages: isothermal adsorption (I), isothermal desorption (II), temperature programmed desorption (III) and final condition at the end of the simulation (IV).*

## Outlook

In the next step, different predefined measurement procedures will be implemented in the simulation model and their results will be compared to measurement data from real-world experiments. With the simulation model being validated, it has the potential of predicting measurement outcomes for various operation modes.

## References

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