Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Federal Department of the Environment, Transport, Energy and Communications DETEC

Swiss Federal Office of Energy SFOE
Energy Research and Cleantech Division

Interim report dated 19.12.2023

NaOH-based liquid absorption heat storage system model

NLA-StorM

Date: 20.12.2023

Location: Bern

Publisher:
Swiss Federal Office of Energy SFOE
Energy Research and Cleantech
CH-3003 Bern
www.bfe.admin.ch

Subsidy recipients:
Lucerne University of Applied Sciences and Arts
Technikumstrasse 21, 6048 Horw
www.hslu.ch

Authors:
Benjamin, Fumey, HSLU, Benjamin.fumey@hslu.ch

SFOE project coordinators:
Stephan A. Mathez, stephan.a.mathez@solarcampus.ch

SFOE contract number: SI/502700-01

The authors bear the entire responsibility for the content of this report and for the conclusions drawn therefrom.

Summary

The aim of the project is to develop a comprehensive model of a sorption heat storage system, as exemplified by the demonstrator from the SFOE-funded project SI/501605-01. The focus is on the development of a detailed mathematical model for the analysis of mass and heat transport processes in this system. The approach of this model is one-dimensional, steady-state and equilibrium-based, focusing on mass and energy balance principles. This approach allowed for a segmented, in-depth study of various system components, including the absorber/desorber, the heat transfer fluid (HTF), and the spiral tube fin.

The primary results of the model are derived from the application of mass balance equations to track sorption processes in the absorber/desorber, in particular to observe changes in sorbent mass. Energy balance equations, used in tandem, allow for a complex analysis of the heat transfer dynamics, highlighting the interplay between the sorbent, the HTF, and the spiral tube fin. A significant portion of the study is dedicated to understanding the vapor flow dynamics, specifically the movement of the vapor toward or away from the absorber/desorber, a critical factor in solving the balance equations.

The project has made progress in understanding the role of natural convection in vapor uptake. This is achieved by emphasizing the importance of dimensionless numbers in characterizing mass transfer processes. Validation of the model includes curve fitting for absorption and desorption processes, which includes deriving correlations from experimental data. The focus of the study on heat transport aspects is to gain a comprehensive understanding of each component within the balance equations and to identify necessary correlations for the calculation of heat transfer coefficients.

In parallel with the development of the mathematical descriptions, a model is built using the Modelica programming language. First, a media model is constructed to mimic the behavior of the sorbent (aqueous sodium hydroxide).

Contents

1 Introduction

A reliable dynamic model of the liquid aqueous sodium hydroxide-based sorption heat storage system, as developed in the SFOE-funded project SI/501605-01, is a prerequisite for its further development. The next steps in technology development are to combine the storage system with a compression heat pump and to implement this combined system in a field demonstrator. The sorption heat storage system allows a partial transfer of the electrical heating load (heat pump) from winter to summer, thus reducing the electrical load in winter. In our project a dynamic simulation white model of the sorption heat storage system will be built and validated against the existing (SI/501605-01) and the second-generation laboratory demonstrator (Frauenfeld system).

This model will be linked to an existing model of a compression heat pump to evaluate the combined operation. During the charging process, the compression heat pump simultaneously cools the sorption heat storage condenser and heats the desorber (closed loop). The input to the closed system is electric only. In this setting, optimal operating temperatures and dynamic operation are evaluated. In the discharge mode the mechanical heat pump and the sorption heat storage system (sorption heat pump with sorption potential storage tank) are connected in series. In this setting, the sorption storage supports the compression heat pump by providing part of the temperature rise (10K to 25K). Depending on the temperature of the heat source (ambient, ground) and the heat sink (building, domestic hot water), an optimal operating condition is expected in terms of energy density of the sorption heat storage, system size and cost, and electrical load shifting. It is also expected that some operating conditions will be more favorable than others, such as achieving high domestic hot water temperatures.

2 Procedures and methodology

The project starts with a detailed definition of the system to be modeled, focusing on the sorption heat storage demonstrator developed in the SFOE-funded project SI/501605-01. The definition of the model involves first understanding the critical components of the demonstrator and the operating principles. This leads to the understanding and analysis of data collected from extensive testing of the demonstrator.

Based on this information, a sophisticated mathematical model is developed to analyze the mass and heat transport processes in the sorption storage system. The foundation of this model is a one-dimensional, steady-state, equilibrium-based approach that integrates mass and energy balance principles. This methodology is broken down into discrete segments for a detailed examination of the system components, which include the absorber/desorber, heat transfer fluid (HTF), and spiral tube fin.

The model uses mass balance equations to monitor the sorption processes within the absorber/desorber, tracking the mass change of the sorbent. Simultaneously, energy balance equations are used to quantify the complex heat transfer dynamics, focusing on the interactions between the sorbent, the HTF, and the spiral tube fin. A significant portion of the study is devoted to analyzing the vapor flow dynamics, particularly the rate at which the vapor moves toward or away from the absorber/desorber, a crucial aspect in solving the balance equations.

In addition, the modeling addresses the role of natural convection in vapor uptake and emphasizes the importance of dimensionless quantities such as Rayleigh, Grashof, Schmidt, and Sherwood, which are essential in characterizing mass transfer processes. Key to the validation of the model is curve fitting for absorption and desorption processes, which involves fitting curves to experimental data to derive correlations.

The work on the heat transport aspects aims at a thorough understanding of each component of the balance equations and to identify the necessary correlations for the calculation of heat transfer coefficients.

This comprehensive understanding of heat and mass transport is essential for accurate analysis and prediction of the system behavior and thus contributes significantly to the field of sorption storage systems.

In parallel with the analytical work to understand and model the sorption heat storage system, Modelica model development is underway with Dymola. This parallel initiative focuses on creating a simulation environment that reflects the results of the analytical model. The Modelica model, specifically tailored to the sodium hydroxide media, is being constructed based on correlations derived from key research papers [1] [2].

Our efforts in 1D modeling within Modelica have been primarily directed at implementing the experimental correlations of various properties (e.g., medium density, viscosity, enthalpy, etc.) as a function of concentration and temperature. We are currently engaged in modeling the NaOH-H2O medium in Modelica, which is an innovative endeavor within our scope. After successfully modeling this medium, our immediate next step is to create a single lamella modeled as a single cell. After that, we plan to integrate different cells developed in the previous step to model the absorption/desorption tubes.

3 Activities and results

The project has achieved both qualitative and quantitative results that have significantly advanced our understanding of the sorption heat storage system.

Results from the initial step of understanding the data are outlined by Figure 2, which shows the transport of vapor from evaporator to absorber over the entire length of the heat and mass exchanger and varying operating conditions. This required analyzing the data stemming from concentration and temperature changes between inlet and outlet flow rates of all moving fluids. This is a key initial finding required to further understand the heat and mass transfer dynamics. This step has presented a challenge in the form of missing or faulty data. These gaps can be bridged by conducting additional experiments to supplement the incomplete data sets.

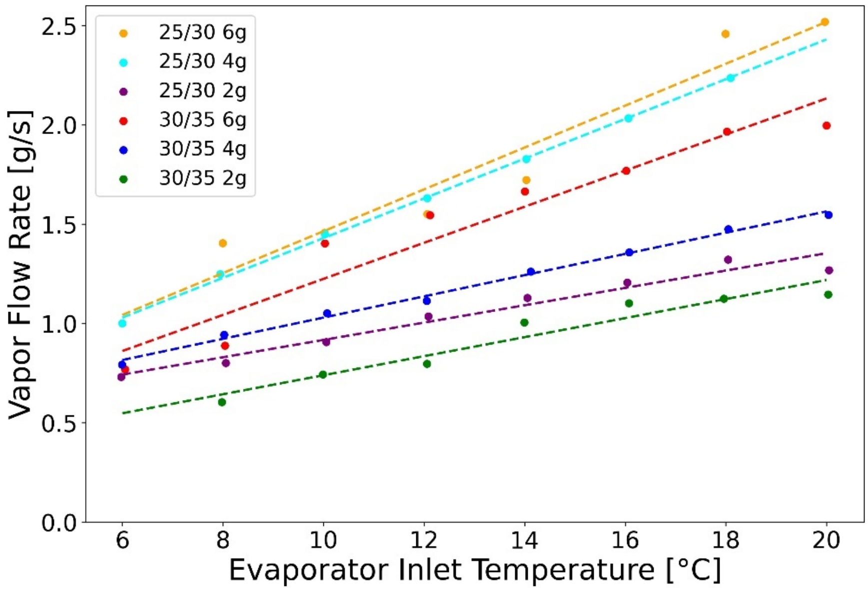

Figure 1 Vapor flow rate vs evaporator inlet temperature during absorption. Legend indicates absorber inlet and outlet temperatures along with mass flow rate of NaOH per tube per minute. Linear trendlines are indicated with dotted lines.

Using Modelica, we have the freedom to develop custom components and models tailored to the unique requirements of our specific system. This ensures that our simulations accurately represent real-world behaviour. The component-based modelling approach is inherently modular. This means we can break down sorption heat storage system into its individual components, such as absorption spiral fins, heat exchangers, vapor transport. By representing each component separately, we can build a holistic understanding of the system's behaviour. This holistic understanding is illustrated by Figure XX that shows a schematic of the discretized, 1D, steady state model of absorber/desorber. The same is then applied to the condenser/evaporator side.

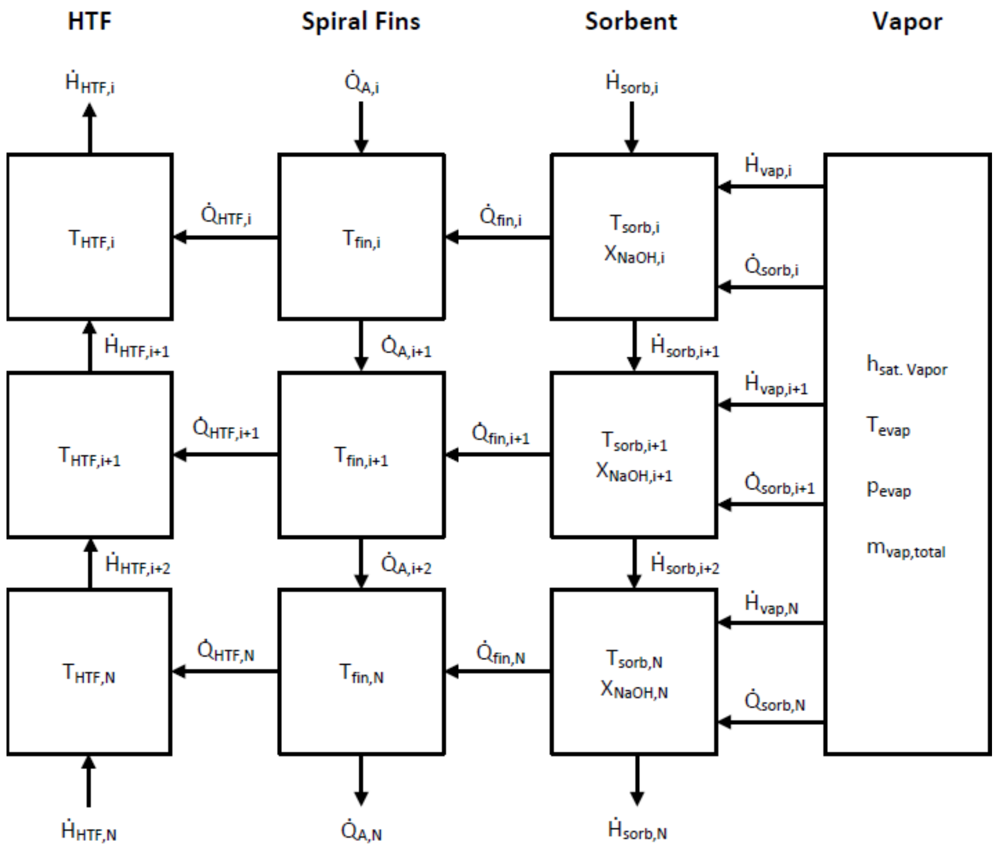

Figure 2 Schematic of discretized, 1D, steady state model of absorber/desorber.

The associated balance equations that go along with this schematic are summarized below. The equations are written as they apply to the absorption process. For the desorption process certain parameters take on a negative value.

Mass Balances:

Heat transfer fluid mass balance:

$$\frac{dm_{A,HTF,i}}{dt} = \dot{m}_{A,HTF,i} - m_{A,HTF,i+1}$$

The mass balance for the sorbent that flows along the spiral tubed fins absorbing water vapor:

$$\frac{dm_{sorb,i}}{dt} = \dot{m}_{sorb,i} - \dot{m}_{sorb,i+1} + \dot{m}_{vapor,i}$$

Sorbent NaOH mass species balance:

$$\frac{dm_{\text{Na},i}}{dt} = \dot{m}_{sorb,i} \cdot X_{\text{NaOH},i} - \dot{m}_{sorb,i+1} \cdot X_{\text{NaOH},i+1}$$

Sorbent water species mass balance:

$$\frac{dm_{\mathrm{H_2O},i}}{dt} = \dot{m}_{sorb,i} \cdot X_{\mathrm{H_2O},i} - \dot{m}_{sorb,i+1} \cdot X_{\mathrm{H_2O},i+1} + \dot{m}_{vapor,i}$$

Energy Balances:

Energy balance for the heat transfer fluid:

$$\frac{dU_{HTF,i}}{dt} = \dot{H}_{HTF,i+1} - \dot{H}_{HTF,i} + \dot{Q}_{HTF,i}$$

Energy balance for spiral finned tubed transferring heat in axial and radial directions.

$$\frac{dU_{fin,i}}{dt} = \dot{Q}_{A,i} - \dot{Q}_{A,i+1} + \dot{Q}_{fin,i} - \dot{Q}_{HTF,i}$$

Energy balance for the sorbent:

$$\frac{dU_{sorb,i}}{dt} = \dot{H}_{sorb,i} - \dot{H}_{sorb,i+1} + \dot{H}_{vap,i} + \dot{Q}_{sorb,i} - \dot{Q}_{fin,i}$$

A key factor in this balance equation is the variation in internal energy due to the sorption process. Elaborating on the left side of the previous equation produces the following:

$$\frac{dU_{sorb,i}}{dt} = u\frac{dm}{dt} + m\left[\frac{\partial u}{\partial X}\frac{\partial X}{\partial t} + \frac{\partial u}{\partial T}\frac{\partial T}{\partial t}\right]$$

We can see that the overall internal energy is affected by several factors: it changes with the total mass of the sorbent, the mass fraction of NaOH, and the temperature, all varying over time.

Each of these balance equations is then solved. The necessary relationships between sorbent enthalpy as function of temperature and NaOH mass fraction are sourced from [1]. Each heat transfer term ca be solved using the heat transfer equation in the form of:

$$\dot{Q} = h \cdot A \cdot \Delta T$$

The necessary heat transfer coefficients (h) are then obtained by applying various Nusselt correlations from literature that consider the characteristic of the fluid and the geometry of the heat and mass exchanger. Identifying suitable correlations that match the unique geometry of the spiral finned tube and its flow regime has been challenging. A significant aspect of the vapor absorption process is the natural convection within the sorbent, which has been complex to replicate with existing correlation models. Another significant challenge has come in modeling the configuration of the fluid as it traverses the length of the spiral tube fin. This aspect is crucial since the surface area of contact between the vapor and the sorbent directly affects the rate of vapor absorption. Similarly, the contact area between the sorbent and the spiral finned tube is vital for heat transfer.

4 Evaluation of results to date

Quantitatively, the mathematical model developed has provided insightful data on mass and heat transport dynamics within the system. Through the application of mass balance equations, we've quantitatively tracked the changes in sorbent mass within the absorber/desorber.

The curve fitting for absorption and desorption processes has led to valuable findings, particularly in deriving correlations from experimental data, which have been key in validating the model. This can be quantitatively shown by Figure 3, which shows the curves that were fitted to data extracted from the data analysis. The mean error of this absorption curve relative to testing data is only 2% over the entire data. This process has not only provided quantitative data but also qualitative insights into the nature of the system's responses to varying conditions.

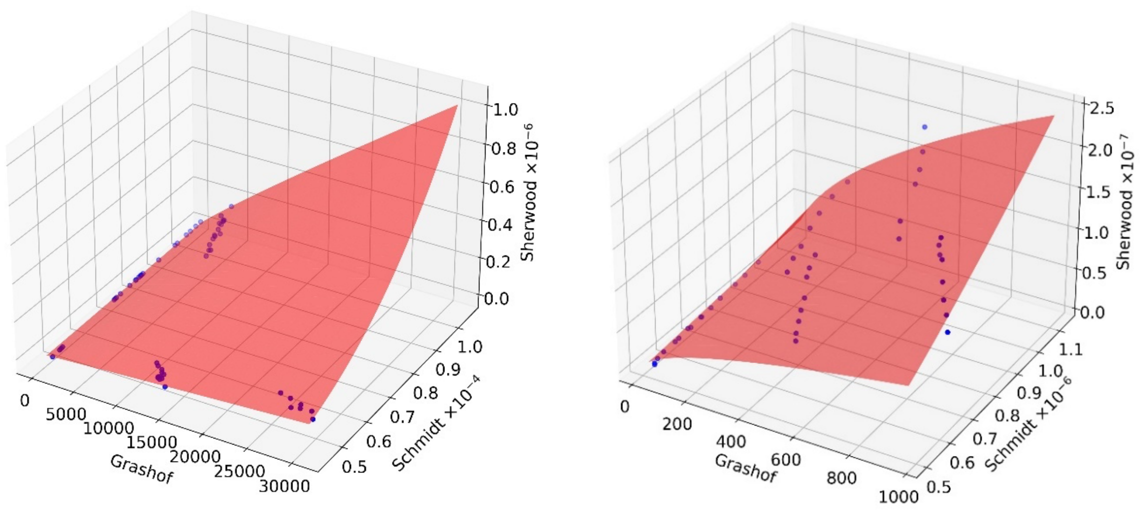

Figure 3 Dimensionless numbers from with fitted plane. Desorption left, Absorption right.

Correlations in the following form can now be used to analyze absorption and desorption data that was not included in the operational tests. More detailed evaluation will be possible when the Modelica model is completed.

5 Next steps

Going forward, focus will be on finishing the Modelica model with the accompanying mathematical descriptions. To this end, the sequential modeling process will be followed: starting with a single fin conceptualized as a solitary cell after the successful modeling of the medium. The subsequent phase will involve integrating cells from prior stages to model the absorption/desorption tubes upon successful implementation of the fin.

In the forthcoming months, additional testing is scheduled to fill the gaps in the existing operational data. This will not only allow us to complete missing information but also to corroborate the accuracy of the model by experimenting with new operational parameters for the demonstrator and evaluating the outcomes.

To ensure the model's continuous refinement, an iterative process will be implemented. This will involve regularly revisiting the model with new data, adjusting and enhancing the simulation to reflect the latest understanding and experimental findings. Through this cyclical process of testing, validation, and modification, the model will be progressively honed to better mimic the real-world behavior of the system. Feedback loops will be established between the testing phase and the modeling phase, ensuring that each informs and improves the other, ultimately leading to a robust and reliable model.

In the final phase of our modeling work, the refined sorption component model will be applied to evaluate broader system. We aim to develop a storage model that examines the performance of our heat storage system with a compression heat pump across various scenarios. This model will help us understand the potential for shifting the electrical load from winter to summer by using renewable energy to charge the sorption heat storage. During summer, the system would store heat through a heat pump powered by renewable sources like solar PV. Then, in winter, the stored heat would assist the heat pump, improving its efficiency and acting like a virtual electrical battery. This concept not only promises to enhance the system's coefficient of performance but also aligns with sustainable energy management practices.

6 National and international cooperation

International:

We are in continuous exchange with international partners within the framework of the IEA SHC/ES Task 67/40 funded by the SFOE project Participation in IEA SHC/ES Task 67/40 (SI/502705-01).

National:

In collaboration with the company Matica, we are developing sorption heat storage towards a commercially available product. This is done within the framework of the SFOE funded demonstration project SorpStor Frauenfeld (SI/502688-01), the Innosuisse flagship project swissSTES and further supported by the Swiss Climate Foundation.

7 Publications

No publication has been made yet. A scientific publication is planned for the first half of 2024, presenting the model and first results in conjunction with a heat pump.

8 References

[1] J. Olsson, A. Jernqvist, and G. Aly, "Thermophysical properties of aqueous NaOH-water solutions at high concentrations," *International Journal of Thermophysics,* vol. 18, no. 3, pp. 779-793, 1997, doi: 10.1007/bf02575133.
[2] A. Alexandrov, "The Equations for Thermophysical Properties of Aqueous Solutions of Sodium Hydroxide," *Proceedings of the 14th International Conference on the Properties of Water and Steam,* 01/01 2005.