

3-Dimensional Analysis of Coupled Heat and Mass Transfer in a Thermochemical Heat Storage System

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Abstract

Thermochemical heat storage technology has gained much attention recently, due to exceptional benefits, such as a high energy storage density and the ability to achieve long-term energy storage with minimal heat loss. This technology is presently undergoing laboratory research and development. Critical factors such as system design, material selection, and operating conditions are of great importance to optimize the performance of these systems. As a result, conducting numerical simulations prior to constructing physical prototypes can lead to time and cost savings. In this study, the numerical investigation of the performance of a designed prototype is presented. A parametric study has been conducted to find the influence of different parameters and operating conditions on the ad-/desorption processes and the efficiency of the system. Based on the results, increasing the water vapor pressure, enhancing thermal conductivity, and decreasing the initial water loading of zeolite through an efficient desorption process have a great influence on the efficiency of the system. An efficiency of about 70% for adsorption and desorption processes has been found. Based on the results, the geometry of the heat exchanger was modified for better heat exchange between the zeolite bed and heat transfer fluid flow.

Keywords: Thermochemical Heat Storage, Numerical Simulation, Zeolite, Thermal Analysis.

Introduction

There is a global aim to reduce the consumption of energy derived from fossil fuels due to their limited resources and environmental concerns. To accomplish this goal, it is necessary to expand the utilization of renewable energy sources. Solar energy is currently among the most widely employed sources. Nevertheless, its daily and seasonal availability remains a significant challenge, particularly in storing this cost-free energy during periods of low solar radiation. The concept of thermochemical heat storage technology has emerged as a promising solution to bridge the gap in timing between heating demand and solar energy supply. This technology offers a noteworthy advantage over alternative thermal energy storage methods, as it ensures extended energy preservation with minimal heat loss and a high energy density. Within these systems, the reversible processes of desorption and adsorption enable the storage of solar heat from summer to winter, enabling the substantial use of solar energy in residential buildings. However, it is still at an early stage of research and development compared to sensible and latent heat storage technologies, which are standard products. Thus, the supply of these heat storage systems in the private market is currently limited to a small number and there is a need for research and development in this field [1].

The CFD simulation can be used to obtain a comprehensive understanding of the complex processes in these systems and to represent them with high temporal and spatial resolution. This makes it possible to adjust the system design and reaction control in a targeted manner in order to achieve an optimum performance. Most studies for investigating heat and mass transfer phenomena in thermochemical storage systems used 1D or 2D numerical models. These are inadequate for

analyzing processes in more complex geometries used in current prototypes. In this study, a 3-dimensional numerical model is developed to simulate coupled heat and mass transfer with ad-/desorption processes in a design prototype. Based on the results of the numerical simulations, the performance of the system can be estimated for practical applications and suitable modifications can also be considered and investigated without the need for high cost and effort for experiments. The results of simulations have been used to investigate the performance of the system in terms of zeolite bed temperature, water uptake, the temperature of the oil as the heat transfer fluid (HTF), and the efficiency of the system. The simulations have been conducted considering different operating conditions to define the optimal condition and design.

Physical Model

In this study, the adsorption and desorption processes of zeolite/water pair in a closed thermochemical storage prototype have been studied numerically. In the studied system, during desorption, saturated zeolite in the reactor is dried by the hot HTF, flowing through the heat exchanger, and energy is stored in the zeolite due to the reaction between zeolite and water. As a result of this process, the water molecules are released from the zeolite in the gaseous state and will be condensed to the liquid state, in the condenser. This reduces the amount of water in the zeolite and the energy is stored as chemical energy. The process of adsorption begins with the evaporation of water vapor in the evaporator, placed at the bottom of the reactor. The water vapor flows into the reactor and is adsorbed in the pores of dry zeolite. The released energy from this reaction is extracted by the HTF flow. The geometry used for the CFD simulation is shown in Figure 1. The system consists of a heat

exchanger (HTX), a reactor, and a fixed bed with zeolite particles, where the reaction between the zeolite and water takes place. The heat exchanger has a 14-layer two-row helical-shaped tube with geometrical parameters as listed in Table 1. The computational domain including the bed filled with zeolite 13X, the HEX containing HTF and tubes is presented in Figure 2.

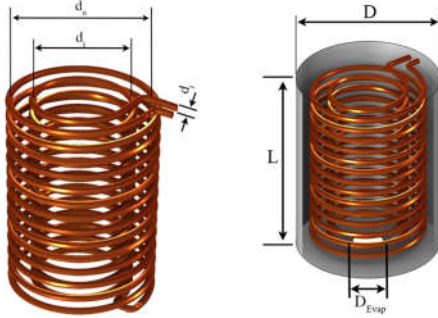


Figure 1. Geometry of the designed reactor.

Table 1: Geometric parameters of the reactor.

Name	Value	Description
L	500 mm	reactor length
D	400 mm	reactor diameter
D _{Evap}	85 mm	diameter of opening from the evaporator/condenser to the reactor
d _o	320 mm	outer coil diameter (HEX)
d _i	220 mm	inner coil diameter (HEX)
d _t	16 mm	tube diameter (HEX)
b	1 mm	tube thickness (HEX)

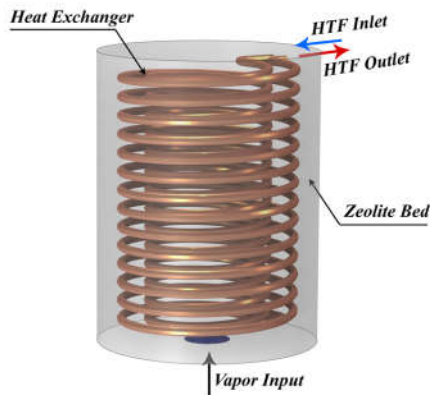


Figure 2. A schematic of the computational domain.

Governing Equations

Adsorption Kinetics

The Linear Driving Force (LDF) model can be used to calculate the adsorbed amount X based on the following formula [2]:

$$\frac{\partial X}{\partial t} = k_{LDF} [X^* - X] \quad (1)$$

where X is the amount of adsorbed water and X^* is the equilibrium adsorption capacity. K_{LDF} indicates how easily vapor flows from the surface

of the adsorbent to the inner points of the particle, and is defined as [2]:

$$K_{LDF} = \frac{15}{r_p^2} D_{ref} \exp\left(-\frac{E_a}{RT}\right) \quad (2)$$

where r_p is the radius of the zeolite particles, D_{ref} is the reference diffusivity, and E_a is the characteristic energy.

Dubinin's theory is used for calculating the equilibrium water uptake. The theoretical maximum amount of adsorbate that can be adsorbed by an adsorbent bed under certain conditions [3]:

$$X^* = X_0 \exp\left(-B \left(\frac{T}{T_{sat}} - 1\right)^n\right) \quad (3)$$

with the Dubinin-Astakhov fit coefficients B and n and the maximum adsorption capacity X_0 for the zeolite/water pair.

Mass Balance

The mass balance equation for the transport of the adsorbed gas in the porous region can be formulated as follows [4]:

$$\varepsilon_{eff} \frac{\partial T_s}{\partial t} + \frac{(1 - \varepsilon_{eff}) \rho_s \partial X}{M_w \partial t} - D_{eff} \nabla^2 c + \nabla(c \cdot u) = - \frac{(1 - \varepsilon_{eff}) \rho_s \partial X}{M_w \partial t} \quad (4)$$

where c is the water vapor concentration, D_{eff} is the effective diffusion coefficient in the porous region, ρ_s is the density of the adsorbent, M_w is the molar mass of water vapor, and ε_{eff} is the effective porosity and can be defined as follows:

$$\varepsilon_{eff} = \varepsilon_{bed} + \varepsilon_p (1 - \varepsilon_{bed}) \quad (5)$$

where ε_p the pellet porosity and ε_{bed} is the bed porosity.

Under the very low pressure conditions in this system, water vapor behaves like an ideal gas, and its density is defined based on the ideal gas law, so that the pressure P of the gas is defined as:

$$P = cRT \quad (6)$$

with the water vapor concentration c , the universal gas constant R , and the temperature T . The pressure difference causes mass transport of water vapor, resulting in viscous flow. The Darcy equation holds for low gas velocities in porous media such as adsorbents and is used to model the vapor velocity:

$$u = - \frac{\kappa}{\mu} \cdot (\nabla p - \rho_f g) \quad (7)$$

where μ is the viscosity of the gas and ρ_f is the gas density. The permeability of the porous medium κ is defined with the semi-empirical Blake-Kozeny equation [5]:

$$\kappa = \frac{d_p^2 \varepsilon_{bed}^3}{150 (1 - \varepsilon_{bed})^2} \quad (8)$$

where d_p is the diameter of the zeolite particle.

Heat Transfer

Three different regions are considered: the adsorbent bed, the heat transfer fluid, and the heat transfer tube. The energy equation for the porous zeolite can be written as follows [4]:

$$(\rho C_p)_{eff} \frac{\partial T_s}{\partial t} + \rho_f C_{p,f} u \cdot \nabla T_s - k_{eff} \nabla^2 + \frac{h_i A_i}{V_s} (T_s - T_t) + Q_{ambient} = Q_s \quad (9)$$

where ρ_f and $C_{p,f}$ are the density and heat capacity of water vapor, and $(\rho C_p)_{eff}$ is the effective volumetric heat capacity and is given by:

$$(\rho C_p)_{eff} = \varepsilon_t \rho_f C_f + (1 - \varepsilon_{eff}) \rho_s C_s + (1 - \varepsilon_{eff}) \rho_s C_l X \quad (10)$$

Q_s is the heat generated by the adsorption of water vapor in zeolite particles and is calculated as:

$$Q_s = (1 - \varepsilon_{eff}) \rho_s \frac{\partial X}{\partial t} |\Delta H| \quad (11)$$

where ΔH is the enthalpy of the reaction. The heat transfer diffusion equation can be considered for the heat transfer in a heat transfer tube [4]:

$$\rho_t C_{p,t} \frac{\partial T_t}{\partial t} - k_t \nabla^2 T_t + \frac{h_i A_i}{V_t} (T_t - T_f) + \frac{h_o A_o}{V_t} (T_t - T_s) = 0 \quad (12)$$

where k_t , $C_{p,t}$ and ρ_t are the thermal conductivity, heat capacity and density of the tube, respectively. The equation for heat transfer in the HTF region can be written as follows [4]:

$$\rho_{htf} C_{p,HTF} \frac{\partial T_{HTF}}{\partial t} - \rho_t C_{p,t} \nabla T_{HTF} - k_{htf} \nabla^2 T_{HTF} + \frac{2}{r_t} h (T_{HTF} - T_s) = 0 \quad (13)$$

Definition of Initial and Boundary Conditions

Three physical areas were used as the basis for calculation. One of them is the volume filled with adsorbent particles. The reaction between zeolite and the water takes place in this area. The zeolite bed is assumed to be a single porous block with the same porosity, specific heat capacity, heat transfer coefficient, and density as the packing of zeolite beds. This assumption can significantly increase the simulation speed. The second region is for the heat transfer fluid, where the equations for mass, momentum and heat transfer are solved. The heat transfer tube has a thickness of 1 mm, which is modelled with the "thin layer", and a heat transfer coefficient is considered at this boundary. The surfaces of the heat exchanger and the reactor walls in contact with the adsorbent are considered as boundaries without mass flux.

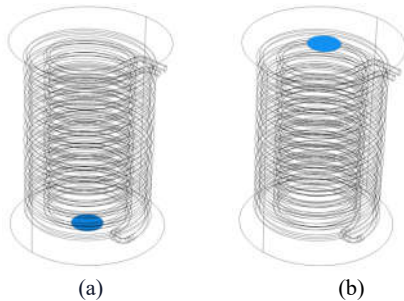


Figure 3. Constant concentration and water vapor pressure boundary conditions at (a) the evaporator and (b) the condenser interface.

At the bottom of the simulation region, where the evaporator is located during the adsorption process, a heat flux of zero in the normal direction and a constant water vapor concentration is assumed, and the same also at the top of the simulation region where the condenser is located for modelling desorption process, as presented in Figure 3.

Numerical Model

The coupled heat and mass transfer equations are solved in parallel in COMSOL® Multiphysics 6.1 software. The available interfaces of 'heat-transfer-in-porous-media' and 'transport-of-diluted-species-in-porous-media' are used for programming the equations. The linear driving force (LDF) model is utilized for modelling the adsorption rate and solving the adsorbed amount, which is modelled using the available module 'Domain-ODEs-and-DAEs'. The flow in the heat exchanger has been modelled using a 'laminar-flow' interface. The vapor flowing from the evaporator or into the condenser is considered as an ideal gas and its velocity is modeled with the Darcy equation. The formula for gas velocity in three directions has been entered in the mass transport equation. User-defined functions are written for programming the reaction kinetics and thermophysical properties. The computational grid is generated by discretizing the domains in extremely small elements, aiming to get high precision of the numerical results. It is important here to intensify the mesh at the points where higher gradients are to be expected. The meshes and the time step dependence of the computation have been investigated to verify the accuracy of the simulations. The optimization has been performed by progressively reducing time steps and mesh size, taking the final values where further decreasing the time steps and mesh size did not significantly change the results. The mesh used contains 1,098,787 tetrahedral elements as shown in Figure 4.

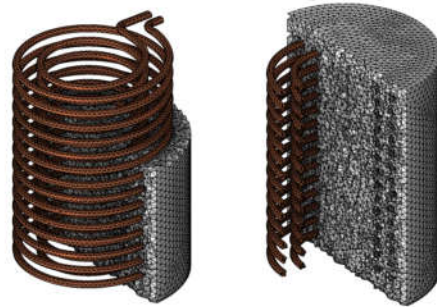


Figure 4. Computational mesh.

The simulation has been validated using the results from previous experiments to confirm the accuracy of the numerical study. The results of the validation of the developed model with experiments by Wu et al. [6] for the desorption process are presented in Figure 5. As can be seen, the results from the

numerical model developed here agree well with the experiments.

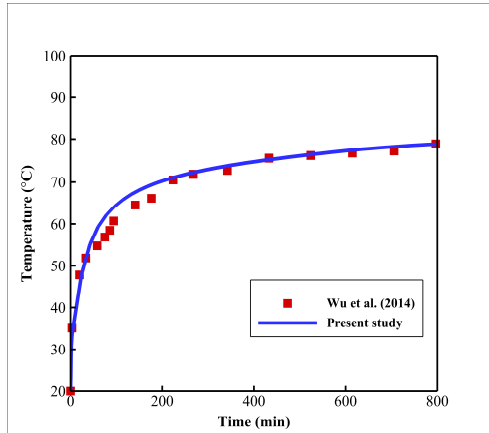


Figure 5. Validation of the model with the experiments conducted by Wu et al [6].

The thermophysical properties of water vapor, tubes, zeolite, and other operating parameters used in this work are given in Table 2.

Table 2. The thermophysical properties and operating parameters [4].

Name	Value	Description
d_p	2 mm	particle diameter
ϵ_{eff}	0.635	porosity
ΔH	3300 kJ/kg	iso-steric adsorption heat
E_a	10000 J/mol	activation energy surface diffusion
k_s	0.125 W/(m · K)	zeolite thermal conductivity
ρ_{bulk}	680 kg/m ³	zeolite bulk density
$C_{p,s}$	837 J/(kg · K)	specific heat of zeolite
D_{ref}	5.8e-9 m ² /s	reference Diffusivity
X_0	0.261	maximum adsorption capacity of zeolite
B	5.36	Dubinin-Astakhov fit coefficients
n	1.73	
$C_{p,HTF}$	1930 J/(kg · K)	HTF specific heat
K_{HTF}	0.115W/(m · K)	HTF thermal conductivity
ρ_{HTF}	914 kg/m ³	HTF density

Results

This section presents the results of numerical investigations. The results are discussed in terms of water adsorption and temperature variations.

Adsorption Process

A reference case (Case_{ref,Ad}) was considered for the adsorption process. For this case, an initial temperature, T_i , of 20 °C and initial water vapor pressure, P_i , of 10 Pa was assumed in the reactor. The pressure in the evaporator was assumed to be 1230

Pa. The initial concentration, c_i , can be defined as P_i/RT_i and for this case, an initial water loading capacity, X_i of about 0.14 is calculated, based on Eq(3). A volumetric flow rate of 2 lit/min and an inlet temperature of 20 °C is assumed for the oil flow. Moreover, for all simulations, a heat transfer coefficient of 5.4 W/(m² · K) is assumed for the outer walls of the reactor. The results of the simulation are shown in Figure 6, which shows the variation of temperature and water uptake at 50, 100, 200, and 400 minutes. It can be observed that the temperature around the heat exchanger is lower considering the cooling effect of the HTF, and the water uptake increases in these areas. This can be explained by a better heat transfer between the cold HTF and the bed in these areas, so that the temperature of the bed decreases significantly. Based on the Dubinin-Astakhov equation, the decrease of the temperature in the adsorption bed leads to an increase of the adsorption capacity of the zeolite, so that a higher amount of water can be adsorbed. On the other hand, increased heat generation and better heat transfer in the areas around the heat exchanger leads to the achievement of higher outlet temperatures for the HTF, which is important in heat storage systems. This also demonstrates the importance of optimizing the heat exchanger design in these systems so that heat transfer between HTF and the adsorption bed is effective and uniform throughout the bed.

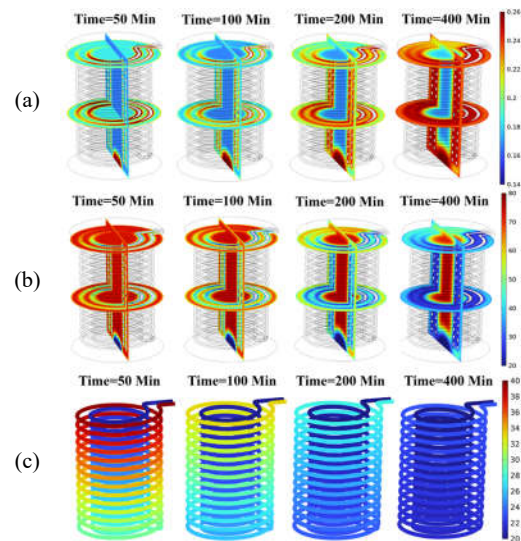


Figure 6. Variation of (a) water uptake and (b) bed temperature (c) HTF temperature at 50, 100, 200, and 400 min for Case_{ref,Ad}

From the temperature and water uptake contours, it is evident that the heat generated in the middle region of the reactor cannot be properly removed by the HTF, primarily due to the low thermal conductivity of the zeolite. Using different types of fins, perforated plates from metals and improving the geometry of the heat exchanger can improve the performance of the system.

As can be further observed in this figure, initially due to the sudden increase in the partial pressure of water vapor, the equilibrium loading increases, leading in turn to increasing water adsorption. As a result, the heat produced at the beginning of the process is much higher, Eq.(11), leading to higher temperature increase at the beginning of the adsorption process. Gradually and with the saturation of zeolite, the average temperature of the bed is getting closer to the oil inlet temperature.

Desorption Process

During desorption, energy is stored in the zeolite due to the thermochemical reaction between zeolite and water. For simulations, the pressure in the condenser is assumed to be 1200 Pa. An initial temperature, T_i , of 20 °C and initial water vapor pressure, P_i , of 1200 Pa was assumed in the reactor. The initial concentration, c_i , can be defined as P_i/RT_i and for this case, an initial water loading capacity, X_i of about 0.256 is calculated, based on Eq.(3). A volumetric flow rate of 2 lit/min and inlet temperature of 180 °C is assumed for HTF. The temperature and loading of the bed and the average temperature of the HTF region for the 50, 100, 200, and 400-minute periods are shown in Figure 7.

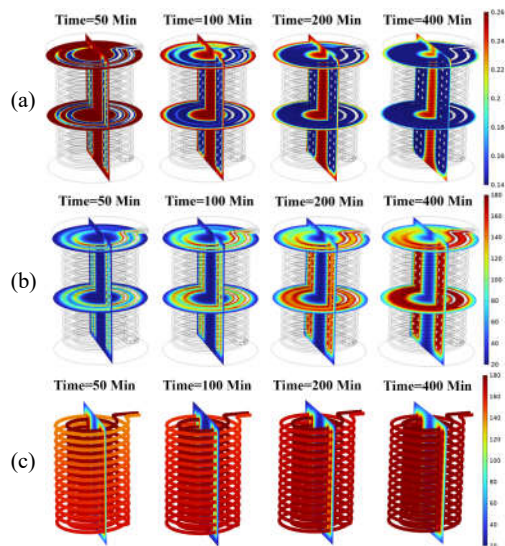


Figure 7. Variation of (a) water loading and (b) zeolite bed temperature (c) HTF oil temperature at 50, 100, 200, and 400 min for Case_{ref, Des}.

The zeolite is initially saturated. When the desorption process starts and the HTF passes through the zeolite bed with a high temperature of 180°C, the temperature of the bed rises and the water is released from the bed, flowing into the condenser. Over time, the temperature within the reactor gradually reaches the same level as that of the HTF, causing the zeolite to dry out. The amount of water desorbed is a function of temperature, pressure and particle diameter of the adsorbent. As depicted in the figure, the central region of the

reactor exhibits a minimal temperature variation, attributed to the low thermal conductivity of zeolite.

Effects of Operating Conditions

In order to determine operating conditions for the optimal performance of the system, various functional parameters were considered and simulations were performed. One factor affecting the adsorption process is the water vapor pressure entering the reactor from the evaporator. To determine the extent to which the performance of the storage system is affected by this parameter, different evaporator temperatures (T_{Ev}) of 5, 10, 15, 20, and 30 °C are taken into consideration. The initial equilibrium loading of the zeolite (X_i) is also an important parameter and has a great influence on the amount of heat released during the adsorption process. To investigate the effects of this parameter, the simulations have been conducted considering an initial loading of 0.08 and 0.14. For all conducted simulations, an oil volumetric flow rate of 2 lit/min and an initial temperature of 20 °C are assumed. As discussed in the previous section, the cooling effect of the HTF in the center of the reactor is limited due to the low thermal conductivity of the zeolite, which may have a negative effect on the adsorption and desorption processes. To investigate this, several values have been considered for d_o , d_i and D_{Evap} , and the influence on the performance of the system was studied. Based on the results with a decreased value of 180 mm for d_i and 80 mm for D_{Evap} , the best performance has been achieved. This case is considered as a modified design (MD) to get better heat transfer in the middle of the reactor, leading to higher efficiency. The result of the simulation shows better heat transfer within the bed and more effective cooling by HTF. The results of the study in terms of zeolite bed temperature are presented in Figure 8 and the changes of water uptake with time is presented in Figure 9. Based on the results, it becomes evident that a lower initial X leads to a more efficient adsorption process, resulting in greater released energy and an increased potential for reaching higher temperatures. A lower equilibrium loading at the beginning leads to a higher capacity for water adsorption at the same temperature and pressure, which directly affects the heat released during the adsorption process. The higher temperature in the evaporator means higher pressure amount of incoming water vapor, leading to a rise in the average amount of adsorbed water. It leads to an increase in the temperature of the bed and water uptake, which can be explained by the reaction kinetics. Since, the capacity of adsorption augments by reducing the temperature of the adsorbent and raising pressure of the incoming water vapor. A higher evaporator pressure leads to a larger adsorption potential, which in turn increases the water vapor adsorption rate.

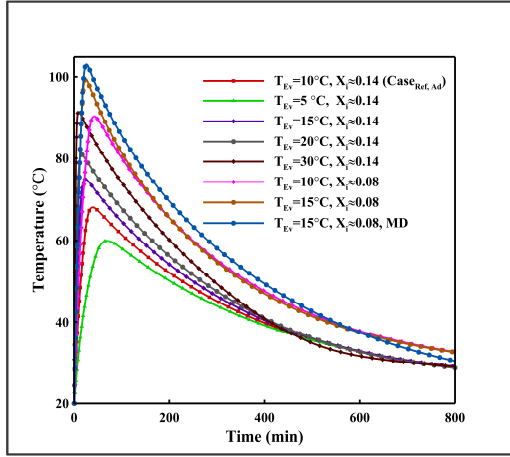


Figure 8. The influence of the evaporator temperature, and initial loading on the average bed temperature during adsorption process.

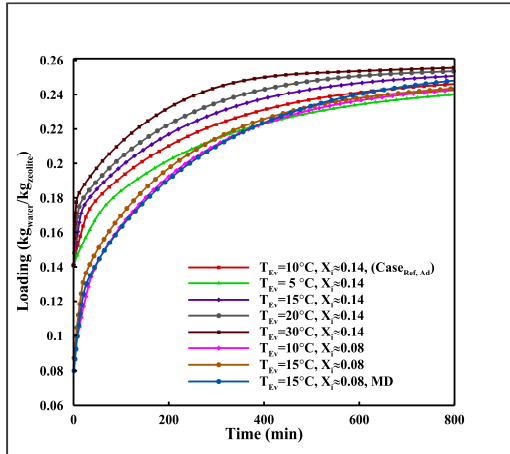


Figure 9. The influence of the evaporator temperature, and initial loading on water uptake during adsorption.

For the desorption process, two parameters of the temperature of inlet hot oil ($T_{in,HTF}$) and condenser pressure, P_c , have been taken into consideration. The simulation results in terms of bed temperature and zeolite loading are presented in Figure 10.

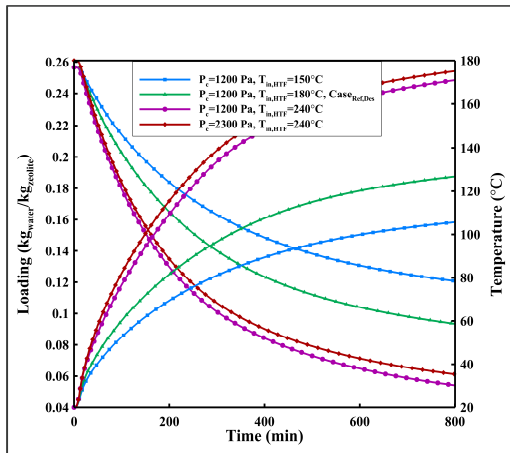


Figure 10. The influence of condenser pressure and inlet oil temperature during desorption process

Based on the results, providing higher temperature for the oil cycle leads to lower water loading in zeolite, resulting in better performance, which also means higher amounts of adsorption enthalpy can be expected at the following adsorption process. Also, at higher condenser pressure, the transfer of the water vapor released as a result of the desorption process, would be more difficult, so lower pressure is desired.

Thermal Energy Analysis

The thermal analysis has been conducted for both adsorption and desorption processes considering a reference temperature of 20 °C. The oil cycle provides the heat needed for the desorption process (Q_{HTF}). This heat can be considered as the sum of sensible heat, evaporation enthalpy, stored heat, and heat loss to the environment (Q_{lost}). Sensible heat (Q_{Sens}) is the share used to heat the zeolite bed to reach the temperature of the oil circuit. After the desorption process, this heat is lost to the ambient air. The stored heat is composed of evaporation enthalpy and binding enthalpy ($Q_{s,Des}$). The evaporation enthalpy is the energy used to convert the water in the zeolite pores to the gaseous state, and the binding enthalpy is the share forcing the water molecules in the zeolite to desorb. Desorption efficiency can be defined as follows [7]:

$$\eta_{Des} = \frac{Q_{s,Des}}{\int_0^t \dot{m} C_{p,HTF} (T_{HTF,in} - T_{HTF,out}) dt} \quad (14)$$

where \dot{m} is the mass flow of HTF, $C_{p,HTF}$ is the specific heat capacity of the heat transfer fluid, and $C_{p,s}$ is the specific heat of the zeolite bed. $T_{HTF,in}$ and $T_{HTF,out}$ are the inlet and outlet temperatures of the heat transfer fluid.

During the adsorption process, heat is generated by the thermochemical reaction and the adsorption enthalpy is released. The released heat is the sum of the binding enthalpy and condensation enthalpy. The enthalpy of binding is the energy released during the adsorption process and theoretically stores the same amount during the desorption process, and the enthalpy of condensation is the heat released when the adsorbed water molecules begin to form a quasi-liquid phase in the micropores. Some of the heat released is transferred to the oil cycle (Q_{HTF}). The sensible heat (Q_{Sens}) is the heat used to warm the bed from room temperature to the temperature of the water circuit. The rest is the heat loss from the reactor wall to the environment (Q_{lost}). The adsorption efficiency can be defined as follows:

$$\eta_{Ad} = \frac{\int_0^t \dot{m} C_{p,HTF} (T_{HTF,out} - T_{HTF,in}) dt}{Q_{s,Ad}} \quad (15)$$

where $Q_{s,Ad}$ is the heat released during adsorption process. The thermal analysis for different cases considering different boundary and operating conditions was performed considering a process duration of 800 min for adsorption and desorption processes. The results for adsorption and desorption cases are presented in Table 3 and Table 4,

respectively. As expected, higher water vapor pressure leads to higher energy release during the adsorption process. The results of the thermal analysis show the great influence of the initial loading on the heat released again in the adsorption process. Thus, effective desorption can improve the performance of the system so that the zeolite has more capacity to adsorb water vapor and release energy. Moreover, based on the results, higher water vapor pressure leads to higher energy release during the adsorption process. The temperature of the inlet oil flow has a great influence on the efficiency and time of the desorption process, and due to achieving lower loading value, it will increase the efficiency of the subsequent adsorption process.

Table 3. The results of the thermal analysis for different cases in adsorption process.

Operating Conditions	Q_{HTF}	$Q_{s,Ad}$	Q_{Sens}	Q_{lost}	η
	[Wh]	[Wh]	[Wh]	[Wh]	
$T_{Ev}=10^{\circ}C$, $X_i \approx 0.14$	3,595	5,188	424	1,169	69.3
$T_{Ev}=5^{\circ}C$, $X_i \approx 0.14$	3,354	4,870	429	1,087	68.9
$T_{Ev}=15^{\circ}C$, $X_i \approx 0.14$	3,789	5,448	423	1,235	69.5
$T_{Ev}=20^{\circ}C$, $X_i \approx 0.14$	3,924	5,625	420	1,285	69.7
$T_{Ev}=30^{\circ}C$, $X_i \approx 0.14$	4,085	5,837	433	1,320	70.0
$T_{Ev}=15^{\circ}C$, $X_i \approx 0.08$	5,804	7,772	210	1,759	75.0
$T_{Ev}=15^{\circ}C$, $X_i \approx 0.08$, MD	6,460	8,387	188	1,739	77.3

Table 4. The results of the thermal analysis for different cases in desorption process.

Operating Conditions	Q_{HTF}	$Q_{s,Des}$	Q_{Sens}	Q_{lost}	η
	[Wh]	[Wh]	[Wh]	[Wh]	
$P_c=1200$ Pa, $T_{in,HTF}=150^{\circ}C$	9,014	6,667	975	1,372	74
$P_c=1200$ Pa, $T_{in,HTF}=180^{\circ}C$	10,672	8,009	960	1,704	75
$P_c=1200$ Pa, $T_{in,HTF}=240^{\circ}C$	13,231	9,943	826	2,462	75.2
$P_c=2300$ Pa, $T_{in,HTF}=200^{\circ}C$	10,831	8,456	570	2,505	78.1
$P_c=2300$ Pa, $T_{in,HTF}=240^{\circ}C$	12,352	9,816	439	2,575	79.5

Conclusion and Outlook

A numerical model was developed to describe the superimposed energy and mass transfer with ad-/desorption reactions in a designed thermal energy storage reactor and to study the thermal analysis of the system. Based on the results, improving the geometry of the heat exchanger is helpful to achieve effective and uniform heat transfer throughout the bed. The current simulation identified the zones with poor heat and mass transfer in the center of the adsorption bed, which can be further modified. Moreover, the low thermal conductivity of the zeolite was a limiting factor to

reach high efficiency. Therefore, the use of various methods to increase the thermal conductivity is advised. This can be achieved by introducing surfaces and fins with high thermal conductivity at different locations in the packed bed. The simulations have also shown that the initial loading of the zeolite at the beginning of the adsorption process has a great influence on the heat released and the efficiency of the system. Thus, longer and more efficient desorption through higher inlet temperature for the oil flow can favor the subsequent adsorption phase. Although the process of adsorption and desorption was considered long enough, at the end of the process some of the energy remains in the bed as sensible heat, which is later lost to the environment. This energy can be used to preheat the reactor in the next cycle or as a heat source for the evaporator. Based on the results from the parametric study, with the right parameters the efficiency (η) of about 70% can be achieved for both adsorption and desorption processes.

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