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Dynamic Optimization of an Adsorption Heat Storage to satisfy the Heat Demand of a House

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ABSTRACT

This study presents the modeling and operation optimization of an adsorption heat storage to improve the supply of renewable heat to a house. The system configuration is an open system with water being carried by an air flow and adsorbed on zeolite 13X beads in a packed bed. A numerical model is developed based on mass and energy balances, using a Langmuir adsorption isotherm and a Linear Driving Force (LDF) mass transfer equation. The model is implemented in Pyomo and solved with the NLP solver IPOPT. A sensitivity analysis on the discretization parameters is performed to choose a good compromise between accuracy and computational time. The chosen model is then validated against experimental data from the literature, with a mean absolute percentage error less than 5%. The dynamic optimization of the operation of the system to satisfy a heat demand is then performed. The trajectory for the inlet fluid velocity is optimized in several heat demand scenarios. The results show that this numerical framework is able to follow realistic heat demands for a house even in the case of large peaks corresponding to domestic hot water production, with quadratic errors between the demand and supplied power less than 1%.

Keywords: Adsorption, Energy Storage, Modelling and Simulations, Optimization, Pyomo

INTRODUCTION

Heat production through renewable energy such as solar energy is a key driver of the energy transition. Due to the intermittency of solar irradiation, an energy storage solution is required to achieve a continuous heat delivery. Thermal energy storage technologies are developed based on three different principles: sensible, latent and thermochemical heat storage. The later includes adsorption heat storage based on the exothermic adsorption of a molecule on a porous structure. In this case, the heat is stored as an adsorption potential allowing long storage duration without heat losses. Moreover, this type of storage has a high energy density, up to 10 times larger than a sensible storage and 2 to 3 times larger than a latent storage [1]. Adding salts to the porous structure increases the thermal effects due to the exothermicity of the hydration reaction. However, such thermochemical systems suffer from poor cycling capacity [1] and are thus excluded from this study.

Adsorption heat storage is still under development and research efforts are required in several areas: adsorbent materials, adsorbate choice, storage structure, process optimization [2]. Some prototypes, such as in [3], have been built to assess the adsorption storage feasibility. However, it was not tested in realistic house heating demand scenarios and the operating conditions were not adjusted accordingly. The energy density of experimental prototypes is often much lower than the theoretical energy density of the adsorbent/adsorbate couple [4], highlighting the need for research on system design and operation. In particular, Lefebvre et al. emphasized the need to adjust the operating parameters in order to reach high energy density values [1].

Optimizing a system's design or operation requires a reliable and accurate model that faithfully represents its behavior. Numerous studies have developed a numerical model for an adsorption heat storage from detailed CFD models to simplified 1D models, such as in [5]. However, the models built might not be compatible with optimization studies, where a good trade-off between accuracy and computational time is essential.

Most optimization studies on adsorption heat storage focus on the design of the system ([6], [7]). Zamengo

et al., used a multi-objective methodology to assist the design of a packed bed thermochemical storage [6]. Optimal values for the adsorbent porosity and thickness are determined while maximizing heat storage density, storage rate and exergy efficiency. The conclusion suggests that modular thin beds are more efficient. Anilkumar et al. developed a 3D dynamic mathematical model using analytical equations and applied a multi-objective algorithm to design an efficient adsorption system [7]. Dimensions for the reactor tubes and the fins added to enhance heat transfer are obtained and realistic systems are simulated based on the recommendations. Those studies did not consider the optimization of the operation of the system.

Wang et al. studied the configuration planning of an adsorption heat storage for different applications in a house [8]. Charging and discharging steps are considered and decision variables include the inlet parameters: inlet air temperature, flow rate and humidity. However, constant values are obtained for each heating scenario.

In this study, a physical 1D numerical model for an adsorption heat storage is developed and validated with experimental data from [3]. The dynamic model is implemented in an optimization framework. Trajectories for the inlet conditions (air velocity) are determined in order to satisfy a heating demand from a house. The dynamic behavior of the system is further analyzed.

The remaining parts of the paper are organized as follows: first, the adsorption heat storage is described. Then, the numerical model is presented along with a sensitivity analysis on the discretization parameters and the validation of the model. After that, the optimization problem is formulated and the results from case studies are explained. Finally, a discussion presents the limitations and future work before a conclusion on this study.

SYSTEM DESCRIPTION

This study considers the supply of renewable heat from solar collectors to a house. An adsorption storage is added to tackle the intermittency of solar energy and reduce the need of a back-up heat production. The storage is the main focus of this work. The system considered is an open system, using air as a carrier and water as the adsorbate. This choice keeps the complexity of the system and the investment cost lower than other configurations. The adsorbent is zeolite 13X in a packed bed.

The two modes of operation are schematized in Figure 1. When excess solar heat is available, it can be used to desorb water from the zeolite, and thus charge the heat storage. This step requires high temperatures, in the range of [120;180]°C which can be achieved with suitable solar collector technologies such as evacuated tube collectors. The choice of the collectors and the detailed analysis of the desorption step is outside the scope of this study. Once the storage is charged, i.e. all the water has been removed, it can be kept in this state for extended periods without any heat losses. When heat is needed in the house but cannot be directly supplied by the solar collectors, humid air is sent to the adsorption storage. This air can be the interior air of the house or the outside air if its humidity and temperature allow for a sufficient temperature lift. The water contained in the air is adsorbed on the zeolite, releasing heat which is collected and carried by the dried air flow. The heat can then be used for space heating or domestic hot water production in the house.

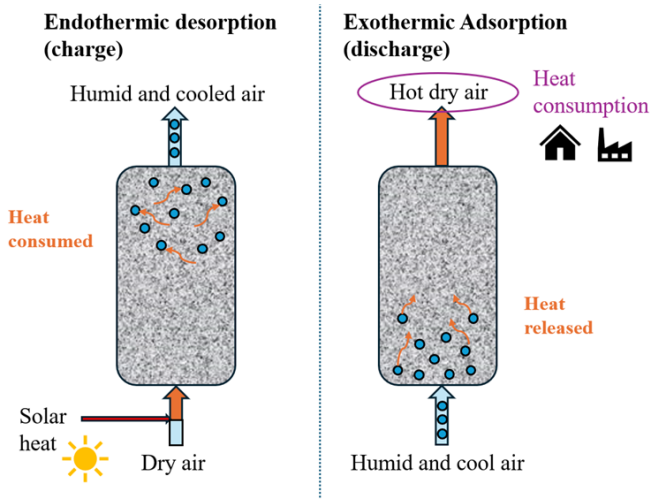

Figure 1. Schematic of the adsorption heat storage utilization in a house

NUMERICAL MODEL

Model equations

The model of the adsorption heat storage is a 1D model considering only spatial variations along the height of the packed bed. Since the system is open, a constant pressure equal to the atmospheric pressure is considered. There are 7 variables in the model, described in the nomenclature, each depending on the spatial coordinate z and time t, which are omitted for improved readability: $\rho_w, \rho_{da}, \bar{q_w}, q_{eq}, \rho, T, u$.

The model is based on mass and energy balances:

- Mass balance on the dry air, assuming a constant dry air flow

$$\frac{\partial(u\rho_{da})}{\partial z} = 0 \quad (1)$$

- Mass balance on water, neglecting axial dispersion

$$\frac{\partial \rho_w}{\partial t} = -\frac{\partial(u\rho_w)}{\partial z} - \frac{\rho_b}{\varepsilon_b}\frac{\partial \bar{q_w}}{\partial t} \quad (2)$$

- Mixture composition

$$\rho = \rho_w + \rho_{da} \quad (3)$$

- Energy balance on the whole system, assuming a

homogeneous temperature between the solid and the fluid

$$\left[\rho C_{v_f}\frac{\varepsilon_b}{1-\varepsilon_b}+\rho_s(1-\varepsilon_s)C_{p_s}+\rho_s(1-\varepsilon_s)\bar{q_w}C_{p_w}\right]\frac{\partial T}{\partial t}=C_{p_f}\frac{\varepsilon_b}{1-\varepsilon_b}\frac{\partial(u\rho T)}{\partial z}-\frac{\Delta H_{ads}\rho_s(1-\varepsilon_s)}{M_w}\frac{\partial\bar{q_w}}{\partial t} \quad (4)$$

- Langmuir isotherm

$$q_{eq}=\frac{Kq_mP_w}{1+KP_w} \quad (5)$$

$$K=K_0\exp\left(-\frac{\Delta H_{ads}}{RT}\right) \quad (6)$$

-Linear Driving Force (LDF)

$$\frac{\partial\bar{q_w}}{\partial t}=K_{LDF}(q_{eq}-\bar{q_w}) \quad (7)$$

-Ideal gas law for the fluid phase

$$\rho=\frac{PM}{RT} \quad (8)$$

The model uses a simple adsorption isotherm, Langmuir, with parameters values as follows: $K_0 = 4.06\text{e}-12\ Pa^{-1}$ and $q_m = 0.228\ kg_w/kg_s$. The LDF model is used to describe the mass transfer in the adsorbent. The lumped parameter K_{LDF} takes into account the external diffusion and internal diffusion in the particle and adsorption on the zeolite crystal. A constant K_{LDF} value of $0.0025\ s^{-1}$ was chosen based on the average value computed with the equations detailed in [5].

Initial conditions for the temperature, water concentration in fluid and adsorbed water concentration along the height of the column are required. Inlet conditions for the fluid temperature, water concentration and velocity are also fixed.

Resolution method

The model was implemented in the Pyomo framework [9]. Pyomo.dae was used to discretize the partial differential equations. The finite difference method was chosen for both time and space discretization, using a fully implicit Backward Euler scheme (first order, constant step). The discretized equations system forms a NonLinear Programming (NLP) problem solved with the IPOPT solver [10]. For a simulation, the number of variables matches the number of constraints, and a dummy objective is added for the resolution.

The model comprises a large number of variables and nonlinear equations and has to represent a steep adsorption front travelling through the storage tank. This makes the problem stiff and difficult to solve. An initialisation strategy was therefore developed as shown in Figure 2. The model was first solved one time step at a time, reducing drastically the complexity of the problem. The results at the end of a time step are used as initial conditions for the next, replacing the implicit scheme for time discretization by an explicit formulation. The results for every time steps are then used together to initialize the simulation over the complete time horizon. The results from the complete simulation are then used to initialize the dynamic optimization, which will be described later in the article.

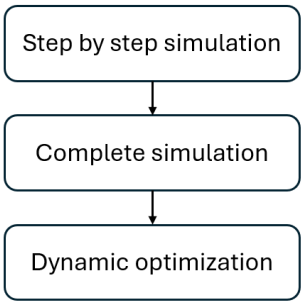

Figure 2. Initialisation strategy

Sensitivity on discretization

A sensitivity analysis on the discretization both in time and space was performed, considering zero degree of freedom, i.e. in a simulation configuration. The inlet conditions are fixed to constant values: $u_{in} = 0.3\ m/s, T_{in} = 293\ K, \rho_{w_{in}} = 0.012\ kg_w/m_f^3$ from [3]. Initially, the storage is at 298K and does not contain water.

Figure 3 presents the temperature profiles obtained at the outlet of the column during adsorption simulations with three different time steps: 50s, 100s and 200s and a fixed spatial discretization of 20 points. The temperature quickly rises due to the exothermic adsorption and stays at a high temperature during several hours. Once the column is saturated and adsorption can no longer take place, the temperature decreases back to the inlet temperature. The profiles obtained with the three discretization time steps are following similar trends, reaching the same adsorption temperature, with only small differences during the transitions. A finer discretization allows to represent steeper transitions at the beginning and at the end of the adsorption phenomenon. Given the small differences between the results, a time step of 100s was chosen, as a good compromise between accuracy and computational time due to the number of variables.

Figure 4 presents the results of adsorption simulations with various numbers of spatial discretization points and a time step of 100s. There are some discrepancies between the profiles. First, the adsorption temperature reached varies by 2°C between 10 and 100 discretization points. Besides, the steepness of the temperature profiles at the beginning and at the end of the adsorption phase is reduced when the number of discretization points is reduced. This can lead to an inaccurate estimation of the adsorption duration. In particular, 10 discretization points does not allow to represent the curvature at the end of the adsorption phase, while all the other plots are superimposed in this zone of the graph.

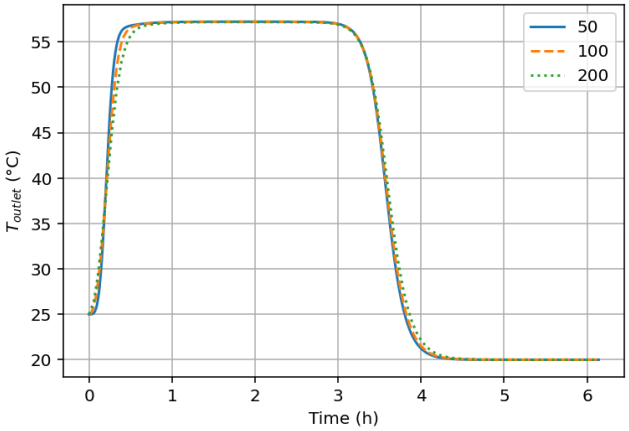

Figure 3. Sensitivity analysis on the time step duration

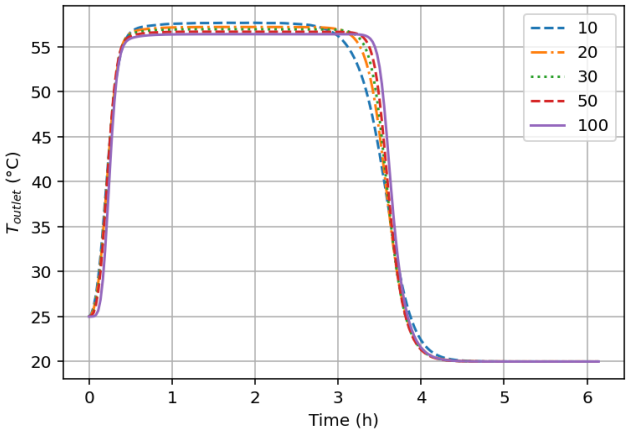

Figure 4. Sensitivity analysis on the number of spatial discretization points

Increasing the number of discretization points thus improves the accuracy of the model resolution but at the cost of a larger problem which will be more difficult to use in optimization studies. Table 1 presents the number of variables for each discretization tested. Since most variables depends on the spatial coordinate z, the number of variables increases greatly with the number of discretization points. In order to keep the complexity of the problem as low as possible for optimization while keeping a good accuracy, 20 points were chosen.

Table 1: Number of variables in the problem for each spatial discretization

Number of discretization points	Number of variables
10	33267
20	64317
30	95367
50	157467
100	312717

Validation

The model with the chosen discretization of 20 points in the spatial dimension and a time step of 100s was validated against experimental data from the work of Tatsidjodoung et al. [3]. The configuration from their prototype was reproduced in the model for all design and operation parameters, as well as initial and inlet conditions. The cylindrical bed considered has a volume of 144L for a height of 20cm. In the experimental bench, air diffusers ensure a uniform distribution of the flow over the entire section of the bed, justifying the use of a 1D model despite the large diameter of 72cm.
The experiment chosen for the validation is their "test 12" where an adsorption step is performed for two adsorption beds in series. The results at the outlet of the first bed (M1 in [3]) are considered for the validation because of the availability of the corresponding data.

The temperature profiles at the outlet of the bed are plotted in Figure 5. The shapes of the profiles are similar, even in the transition regions when temperature stabilizes at the beginning and the end of the adsorption phase. This ensures that the model predicts an accurate adsorption duration. The region when the temperature starts to decrease, after about 3 hours of heat supply, is not well reproduced by the model. There seems to be a break in the experimental curve at 3.5 hours without physical justification. Therefore, this part of the curve cannot invalidate the numerical model. The overall mean absolute percentage error between the two curves is 4.46% with an adjusted value of ΔH_{ads} equal to -56398 J/mol in the model, which lies in the range of experimental measurements of [45-75] kJ/mol [11]. The error below 5% ensures the validation of the model.

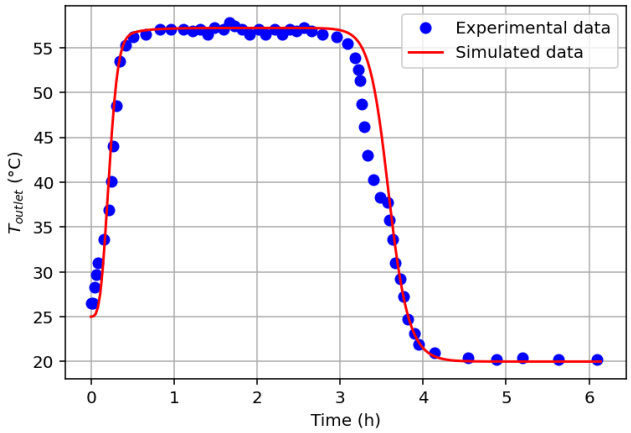

Figure 5. Comparison of the experimental [3] and simulated outlet temperature profiles

OPTIMIZATION

Formulation of the optimization problem

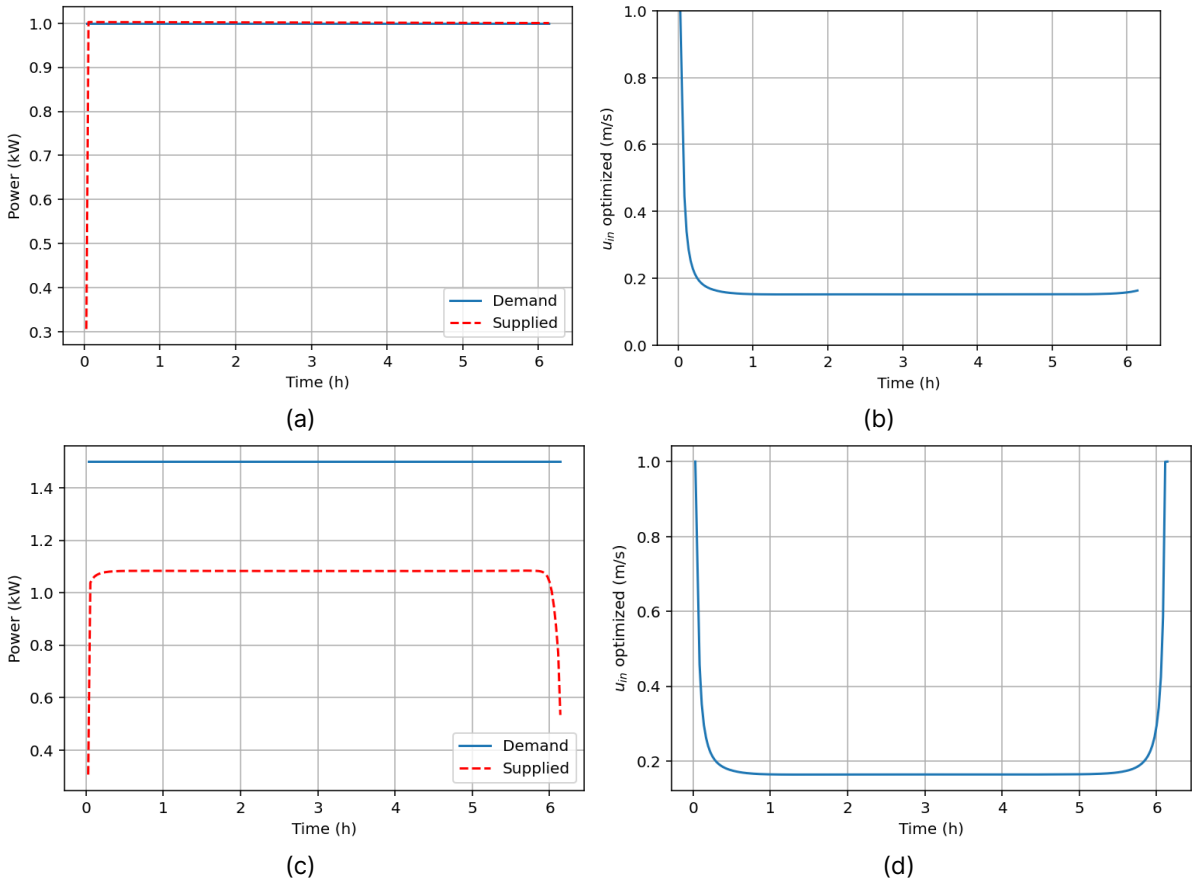

Figure 6: Various power demand scenarios and the obtained power supplied and the optimal velocity profiles – constant heat demand

The validated numerical model described previously is then used to perform dynamic optimization of the operation of the heat storage. The design of the system is fixed. The dimensions used are the same as in the validation part, taken from the experimental bench in [3].
The objective function is to minimize the squared difference between the heat power demand and the heat power supplied by the storage at each time step (quadratic error):

$$\min_{u_{in}(t_i)} \sum_{t_0}^{t_f} \left(\dot{Q}_{demand}(t_i) - \dot{Q}_{supplied}(t_i) \right)^2 \qquad (8)$$

The optimization variables are the inlet velocity $u_{in}(t_i)$ at each time step. The velocity is bounded in the interval [0;1] m/s, to ensure that it is lower than the fluidization velocity. The other inlet conditions, namely the temperature and water concentration, remain fixed to the previously mentioned values because in an open system there are generally imposed by the ambient conditions. The only controllable variable is thus the velocity, through the manipulation of the fan.

Results

To assess the capability of the storage system to satisfy the heat demand of a house, several demand scenarios have been created. These scenarios are realistic heat demands of a room. The heat demand of a whole house is larger and would require several modules of the studied adsorption heat storage. To simplify, only one module is studied here.

Figure 6 shows the results for two distinct scenarios considering a constant heat demand, corresponding to the heating during the night or the middle of the day, when no big change occurs in the demand. Figure 6 (a) shows a heat demand of 1kW, that is almost perfectly matched by the heat supplied, with an objective value (sum of squared errors) of 0.91. The only discrepancy is at the beginning, because the adsorption heat delivery at the outlet of the column is not instantaneous. The corresponding optimal inlet velocity profile is shown in Figure 6 (b). At the initial time, the velocity is as high as possible to start the heat delivery as soon as possible and reduce the difference between the heat demand and the heat supply in the first minutes. Once the heat delivery has started, the velocity goes quickly to its constant value ensuring the required power.

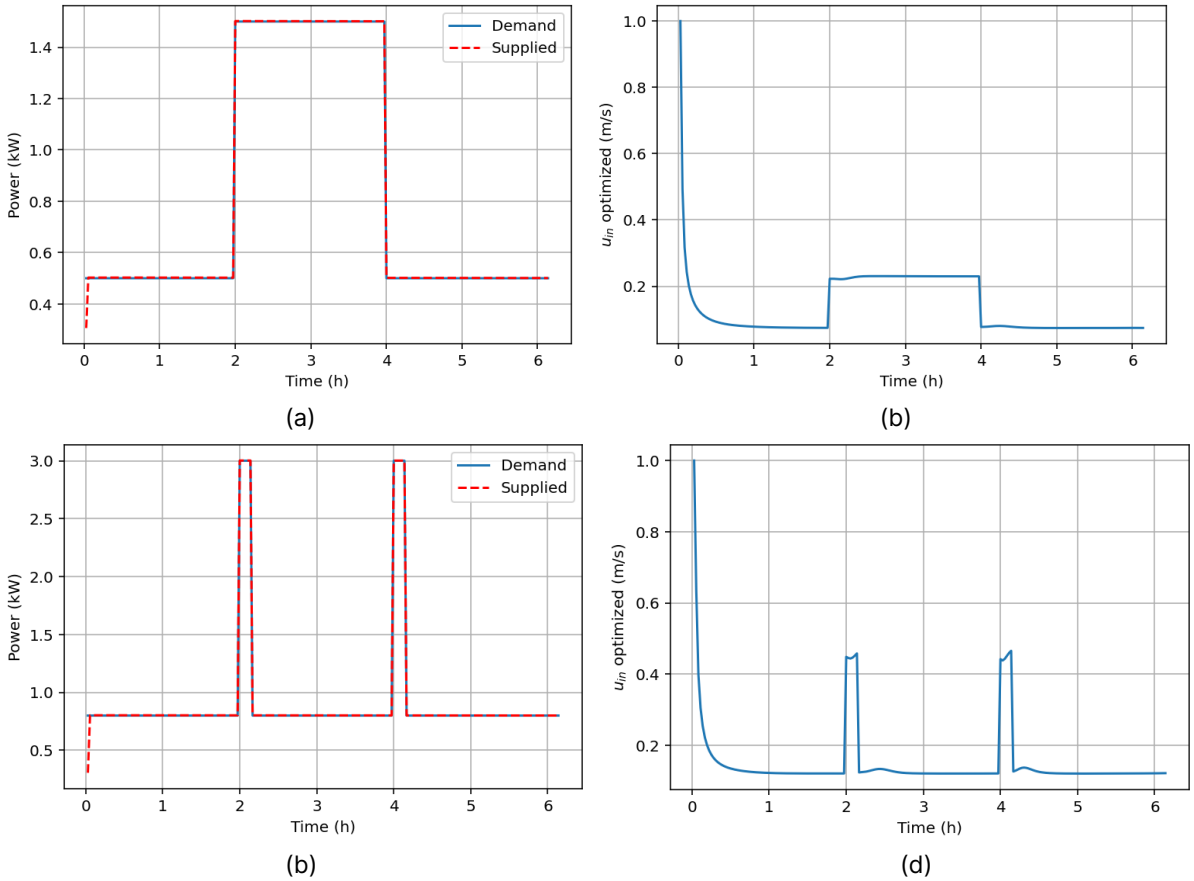

Figure 7: Various power demand scenarios and the obtained power supplied and the optimal velocity profiles – variable heat demand

In Figure 6 (c), a similar scenario with a greater heat demand of 1.5kW is shown. In this case, the adsorption storage is not able to satisfy the heat demand, the heat supplied is lower than the demand and the objective is still high with a value of 42.8. Indeed, the capacity of the storage is exceeded, the zeolite cannot adsorb more water and saturates. The optimal solution is here to use the adsorption storage for preheating over the whole time period. A back-up heater will then be necessary to satisfy the heat demand. The optimal inlet velocity for this scenario is shown in Figure 6 (d). As previously, the velocity is high at the very beginning, to start the heat delivery as quickly as possible. It then stabilizes to a value ensuring a stable heat delivery over the whole time horizon. Towards the end of the time period, the storage tank is nearly saturated and not much heat can still be extracted. The velocity increases again to try to match the heat demand, but the supplied power still decreases. This case shows the capacity of the methodology to adjust the inlet velocity to satisfy a heat demand. When the heat demand is too high and the system will not be able to satisfy it over the whole time horizon, the methodology adjusts the inlet velocity to supply the maximum power during the whole time period. In another approach, the volume of the heat storage unit could be optimized to ensure that the heat demand can always be satisfied.

Additional scenarios with variable heat demands were also tested and are shown in Figure 7.

Figure 7 (a) shows a small baseline heat demand of 0.5kW and a larger power of 2 kW for 2 hours. This could be the heat demand of a room with a peak during the hours 6-8pm when people come back home and need more thermal comfort. In this case, the adsorption storage is able to track the heat demand efficiently, with an objective value of 0.06, adjusting the value of the inlet velocity as shown in Figure 7 (b).

Finally, a scenario representing domestic hot water needs has been tested. A baseline heat demand of 0.8kW is chosen and two peaks at 3kW, each lasting 10 minutes, are added. Again, the storage system is able to track the variable heat demand and adjust the fluid velocity, with an objective value of 0.06. Satisfying the real power of domestic hot water production in a house would again require several modules of storage operating in parallel.

Discussion

The design of the system was fixed in this study, following the prototype dimensions from [3], who tested two adsorption beds in series. Several beds are required to satisfy the heat demand of a whole house. However, this study focused on the dynamic behavior rather than the sizing of the system. Thus, heat demands for a single room were tested according to the size of the adsorption heat storage modelled. Future work should focus on the optimization of the design of the system according to the real heat demand of a house.

This study shows the capability of an adsorption heat storage to follow a heat demand of a house. The dynamic behavior is even able to track fast changes, such as the ones required for domestic hot water production. However, the velocity required to achieve those fast changes is high, leading to high operational costs due to the electricity consumption of the fan. In this study, the water concentration at the inlet is fixed because it is not controllable in most open configuration adsorption systems. Nevertheless, adding a humidifier to increase the inlet humidity of the air flow could help reach higher supplied power values without using as much electricity. Moreover, this added degree of freedom could help achieve a more efficient operation of the storage through dynamic optimization.

Another approach would be to change the system for a closed configuration allowing more control over the inlet variables.

CONCLUSION

In this work, a numerical model for a packed bed adsorption heat storage was developed. The model is based on mass and energy balances and uses a Langmuir isotherm to describe the adsorption phenomenon and a LDF model for the mass transfer.

A sensitivity analysis was conducted to choose the discretization parameters offering a good compromise between accuracy and model complexity. A time step of 100s and 20 spatial discretization points were chosen. The model was then validated against experimental data from the literature. The value of ΔH_{ads} in the model was adjusted within the range of experimental data to the value of - 56398 J/mol, in order to reduce the modeling error to less than 5%. Dynamic optimization was then performed on the chosen design. Optimal trajectories for the inlet velocity were computed in order to match a heating demand of part of a house. The methodology was able to track constant and variable heat demands with sums of quadratic errors less than 1%. When the heat demand is too high to be satisfied, the methodology plans the optimal pre-heating.

The results confirmed the potential of the dynamic optimization methodology for the future operation of a real adsorption heat storage unit. Future work will focus on the optimization of added degrees of freedom, such as the inlet humidity, as well as the simultaneous optimization of the design and operation of the system.

NOMENCLATURE

Symbol	Description	Unit
ε	Porosity	[-]
ρ_i	Species mass concentration in fluid	$[kg_i/m_f^3]$
ρ	Density	$[kg/m^3]$
ΔH_{ads}	Heat of adsorption	$[J/mol]$
C_p	Specific heat capacity at constant pressure	$[J/(kg.K)]$
C_v	Specific heat capacity at constant volume	$[J/(kg.K)]$
K	Langmuir equilibrium constant	$[Pa^{-1}]$
K_{LDF}	Linear Driving Force constant	$[s^{-1}]$
M	Molar mass	$[g/mol]$
$\bar{q_w}$	Average mass concentration of water in the adsorbed phase	$[kg_w/kg_s]$
q_{eq}	Mass concentration of water in the adsorbed phase in equilibrium with the fluid phase	$[kg_w/kg_s]$
$\dot{Q}$	Heating power	$[W]$
R	Ideal gas constant	$[J/(mol.K)]$
P	Pressure	$[Pa]$
T	Temperature	$[K]$
u	Interstitial velocity	$[m/s]$
Subscripts	**Description**	
b	Bed	
da	Dry air	
s	Solid	
w	Water	

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