



# One-dimensional model of a closed low-pressure adsorber for thermal energy storage



M. Schaefer<sup>a,\*</sup>, A. Thess<sup>a,b</sup>

<sup>a</sup> Institute of Energy Storage, University of Stuttgart, Pfaffenwaldring 31, 70569 Stuttgart, Germany

<sup>b</sup> Institute of Engineering Thermodynamics, German Aerospace Center (DLR), Pfaffenwaldring 38-40, 70569 Stuttgart, Germany

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## ABSTRACT

The energy transition from fossil to renewable energy requires the development and integration of efficient energy storages. For thermal energy storage, concepts based on adsorption are promising. One key challenge is to overcome limitations of the storage performance by the heat and mass transfer. Against this background, a closed low-pressure adsorber with zeolite 13X honeycomb adsorbent is studied numerically to identify the limiting factors. The focus of the study is on the adsorption process with the heat extraction limited to the end of the zeolite honeycomb arrangement. A detailed model which takes effects of rarefied gas flow (e.g. slip) as well as cooling effects by the inflowing vapour into account is derived. The model is applied to study the mass transport, heat transport and adsorption over a broad range of relevant geometry and process parameters. The simulations demonstrate that the adsorption process is not limited by the mass transport and isobaric conditions can be assumed in most of the studied cases. In addition, special effects of rarefied gas flow are found to be negligible. Regarding the heat transport, the convective cooling by the vapour is found only to be significant for a very short initial time period. Further analysis show that the process is mainly limited by the heat transport. Only for short channels and wide channel diameters the process becomes limited by the adsorption.

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## 1. Introduction

### 1.1. Motivation and subject matter

The energy transition from fossil to renewable energy requires the development and integration of efficient energy storages. Energy storages are required for both electrical and thermal energy. For thermal energy storage (TES) the thermochemical energy storages (TCES) offer several specific advantages. The main advantages are: high energy density, high efficiency, negligible long-term losses and the possibility to utilize the TCES as a heat pump or transformer [1]. A broad definition of TCES also includes TES based on adsorption. One key challenge is to overcome limitations of the storage performance (e.g. discharging power and temperature) by the heat and mass transfer [2]. Against this background, a closed low-pressure adsorber system with zeolite is studied numerically to identify the limiting factors. Closed low-pressure adsorber systems are of particular interest for seasonal storage of solar energy [3] as well as for domestic heat pump systems [4] but are also studied for industrial application [5].

The scheme and storage principle of the examined closed adsorption system is shown in Fig. 1. The system consists of the two main vessels: adsorber and water vessel. In accordance with applied research in the field (e.g. [6,7]), zeolite 13X and water are assumed as working materials. Both vessels are connected vacuum-tight via a pipe and are initially evacuated. During the

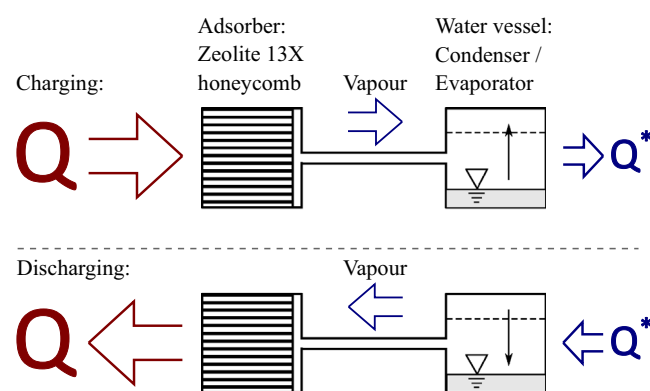


Fig. 1. Scheme and storage principle of the closed adsorption system.

\* Corresponding author.

E-mail address: [schaefer@ies.uni-stuttgart.de](mailto:schaefer@ies.uni-stuttgart.de) (M. Schaefer).

## Nomenclature

### Symbols

$A$	cross-section area (m <sup>2</sup> )
$c$	specific heat capacity at constant volume (J/kg K)
$c_p$	specific heat capacity at constant pressure (J/kg K)
$d_i$	inner/channel diameter of zeolite cut-out (m)
$d_{mp}$	mean macro pore diameter of zeolite (m)
$d_o$	outer diameter of zeolite cut-out (m)
$D_{eff}$	effective diffusivity of water uptake in zeolite (m <sup>2</sup> /s)
$D_{Kn}$	Knudsen diffusivity of vapour in zeolite (m <sup>2</sup> /s)
$e$	specific internal energy (J/kg)
$E$	char. energy in Dubinin-Astakhov equation (J/kg)
$G_p$	Poiseuille coefficient (–)
$h$	specific enthalpy (J/kg)
$\Delta h_a$	heat of adsorption (J/kg)
$\Delta h_e$	heat of evaporation (J/kg)
$k_a$	adsorption kinetics parameter (s <sup>–1</sup> )
$Kn$	Knudsen number (–)
$l_{mol}$	mean free path of vapour molecules (m)
$L$	channel length of zeolite cut-out (m)
$\dot{m}$	infinitesimal mass flow rate (kg/s)
$n$	heterogeneity parameter in Dub.-Ast. eq. (–)
$p$	vapour pressure (Pa mbar)
$\dot{q}$	heat flux (W/m <sup>2</sup> )
$Q$	heat input/output of adsorber (W)
$Q^*$	heat input/output of water vessel (W)
$r$	radial coordinate of zeolite cut-out (m)
$R_s$	specific gas constant of vapour (J/kg K)
$s$	fitting parameter of dynamic viscosity (–)
$t$	time (s)
$\tilde{t}$	non-dimensional time $\tilde{t} := t/t_{tot}$ (–)
$t_{tot}$	total process duration (s)
$t_{p,99}$	relative time for $p(L, \tilde{t}) = 0.99 p(0)$ (s)
$T$	temperature (K, °C)
$T_{htx}$	temperature of heat exchanger (K)
$u$	mean vapour velocity in zeolite channel (m/s)
$u_{slip}$	slip velocity of vapour at channel wall (m/s)

$\nu$	specific volume (m <sup>3</sup> /kg)
$dV$	infinitesimal control volume (m <sup>3</sup> )
$X$	water uptake of zeolite (kg/kg)
$X_{eq}$	adsorption equilibrium of zeolite (kg/kg)
$z$	axial coordinate of zeolite cut-out (m)

### Greek symbols

$\alpha_1, \alpha_2$	fitting parameters of specific heat of adsorbate
$\beta$	coefficient of thermal expansion of adsorbate (K <sup>–1</sup> )
$\gamma$	diameter ratio of zeolite cut-out (m/m)
$\delta$	local rarefaction parameter (–)
$\varepsilon$	inner porosity of zeolite (m <sup>3</sup> /m <sup>3</sup> )
$\lambda$	heat conductivity (W/m K)
$\lambda_{eff}$	effective heat conductivity (W/m K)
$\mu$	dynamic viscosity (Pa s)
$\rho$	density (kg/m <sup>3</sup> )
$\tau$	mean tortuosity of zeolite (–)

### Subscripts

0	initial state
a	adsorbate, adsorption
c	channel
in	inlet of adsorber
max	maximum
min	minimum
ref	reference state
s	saturation state
v	vapour
wvl	water vessel
z	zeolite

### Abbreviations

TCES	thermochemical energy storage
TES	thermal energy storage

charging process the adsorbed water in the zeolite is desorbed by a high-temperature heat input  $Q$ . At the same time the arising vapour is being condensed in the water vessel while releasing the heat of condensation  $Q^*$  at a low-temperature level. Over the storing period the two vessels are simply separated by a valve. During the discharging process the charging process is reversed by evaporating the water in the water vessel by a low-temperature heat input  $Q^*$ . The vapour is then adsorbed by the zeolite while releasing the heat of adsorption  $Q$  at a high-temperature level. With the focus on seasonal storage of solar energy, typical operating temperatures of the water vessel are in the range of  $T_{wvl} \approx 5 \dots 25$  °C. Hence, the vapour pressure in the water vessel is in the range of  $p_{wvl} \approx 8 \dots 32$  mbar, defining the in- and outlet pressure of the adsorber.

Most publications regarding modelling and simulation of closed low-pressure adsorbers assume a packed-bed adsorber filled with spherical adsorbent particles [8,9] or adsorbers with coated heat exchanger tubes [4]. In contrast, an adsorber with structured zeolite honeycombs is examined in this study to analyse possible limitations of the storage performance by the heat and mass transfer. The particular advantage of this adsorber system is its geometric simplicity which allows a straightforward derivation of the conceptual mathematical model. The manufacturing process of zeolite honeycombs for TES application has been presented in [10]. Fig. 2 shows different manufactured zeolite honeycombs with variation of the channel width and web thickness. Typical channel

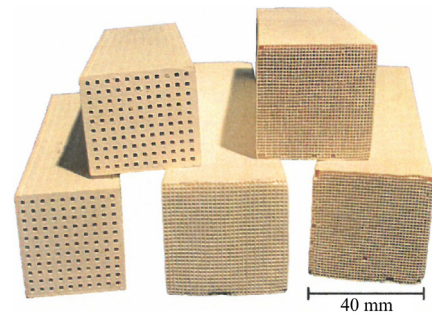


Fig. 2. Different zeolite honeycombs with variation of the channel diameter and web thickness, courtesy of Benjamino R. Formisano.

widths vary around 1 mm with a web thickness in the range of 0.2 ... 2 mm.

### 1.2. Literature review

Many of the publications regarding honeycomb adsorbents focus on the manufacturing process and the experimental examination, e.g. [11–13]. The field of application often covers catalysis or gas sep-

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