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Modeling of a nonlinear thermochemical energy storage by adsorption on zeolites

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HIGHLIGHTS

- Thermo-chemical energy storage by adsorption–desorption in a closed system.
- Simulation of coupled heat and mass transfers within the zeolite 13X – water pair.
- Stiff system of thousands of non-linear strongly coupled equations.
- Resolution of non-linear and coupled equations for cycles under stiff conditions.
- Resolution reflecting reality and fast enough to be applied to design of systems.

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ABSTRACT

A two-dimensional model is built to analyze the coupled heat and mass transfers occurring in the zeolite 13X – water pair within a closed storage system. The proposed model consists of nonlinear coupled differential partial equations, is robust and solved for entire cycles under extreme conditions using the Gear method. The results match observations for a large set of adsorber dimensions even under extreme solicitations. They apply to both adsorption and desorption dynamics, allow energetic predictions and can be helpful to improve design and management of storage systems for building applications.

1. Introduction

Currently, the use of adsorption cycles is widespread in the environmental, chemical and biotechnological industries. One of their many applications, the thermochemical energy storage by adsorption, matches the requirements of building applications, i.e. temperature range and reversibility. The selected storage system is a closed system integrating the zeolite–water pair. The theoretical energy density of zeolites, which are microporous minerals from the aluminosilicates family, stands around 180 kWh/m^3, i.e. twice the water density used in sensible heat storage. The zeolite–water pair has excellent adsorption and regeneration capacities, low toxicity, low price and long term stability, which makes this pair a perfect candidate for low temperature energy storage dedicated to real estate [1,2]. The zeolite–water pair appears in many studies about refrigeration [3,4] and energy storage [2,5].

The modeling of such storage systems is essential for both their design and management and requires a good understanding of the nonlinear and strongly coupled physical phenomena occurring in them. Before 2000, numerous predictive tools were available in the literature [6,7]. Most of them were one-dimensional models, only suitable under restricted operating conditions and could be classified either as uniform-temperature models [8,9] or as uniform-pressure models [6,10] considering only heat transfer and neglecting mass transfer in the adsorbent. However, hydrodynamics and thermal aspects occurring during the adsorption of

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Nomenclature

Latin letters

A	volume fraction of adsorbate in the bed
B	volume fraction of adsorbent in the bed
E_n	activation energy, K
J	Jacobian
K	permeability of the adsorbent, m^2
L	bed length, m
M	molar mass, kg mol^{-1}
M	mass-matrix
NTU	number of transfer units of heat exchanges
Pe	Peclet number
R	gas constant, J mol^{-1} K^{-1}
R	second member
R_1, R_2	inner and outer radii of the metal tube, m
R_3	radius of the adsorbent bed, m
T	temperature, K
Z	vector of variables
a	thermal diffusivity of the fluid, m^2 s^{-1}
c	specific heat, J kg^{-1} K^{-1}
d	diameter
h	time step
i, k	temporal indexes
nr	number of radial meshes
nz	number of longitudinal meshes
p	pressure, Pa
q	amount of water within the adsorbent bed, kg m^{-3}
r	radial coordinate
t	time, s
u	gas velocity in the adsorbent, m s^{-1}
v	velocity of the heat transfer fluid, m s^{-1}
z	longitudinal coordinate

Greek letters

ΔE	energy variation stored or released within the adsorbent bed between two instants, kWh m^{-3}
ΔH	heat of adsorption, J kg^{-1}
ΔT	temperature variation, K
Ω	volume, m^3
β	parameter dependant on the current order
ε	porosity
λ	thermal conductivity, W m^{-1} K^{-1}
μ	viscosity, Pa s
ρ	density, kg m^{-3}
ψ	function of previous states
τ	dimensionless time

Subscripts or exponents

a	adsorbed phase
b	adsorbent bed
cond	condenser
e	equilibrium
evap	evaporator
f	fluid
g	gaseous phase
in	inlet
m	metal tube
p	adsorbent particle
s	adsorbent solid
0	initial
Σ	of the adsorbent–adsorbate pair

fixed bed have been indicated to play a key role [11]. To take these aspects into account, many numerical studies considered coupled heat and mass transfers in the last decades: numerous one-dimensional studies which only consider either the longitudinal or the radial dimension [12–14], some two-dimensional studies [3,15,16] and even a three-dimensional one [17]. These models include nonlinear and strongly coupled equations. In the studied problem, very low pressures (p << 200 mPa) are encountered during the phase of adsorption and make the time integration of the equations associated with the coupled transfers fails. Until now, this problem using the same design and operating conditions has not been solved for an entire cycle but only for desorption [12]. Other authors overcome this numerical difficulty by modeling an adsorber set up in a way to avoid very low pressure: omission of the radial diffusion due to compact equipment design [3,17], the cylindrical adsorbent beds heated or cooled by an external fluid which allows obtaining as lowest pressure approximately 1000 Pa.

In this work, a model of thermochemical energy storage in a system adapted to the problems of energy management in buildings is provided and could help to improve the yield of such processes. This two-dimensional model of coupled heat and mass transfers correctly reproduces, in a reasonable time (5 min), the behavior of the studied adsorber over several cycles in the worst conditions in terms of dimensions and solicitations, overcoming the numerical difficulty of the resolution for the adsorption characterized by very low pressures.

In the first part, we will describe the storage system and the physical model of transfers occurring within it. Then, we will detail the numerical method used to solve the resulting model. Finally, the application of the numerical method to a thermochemical energy storage by adsorption will be presented and discussed.

2. Description of the storage system and physical model of transfers

The studied thermochemical energy storage system is shown in Fig. 1a. It is a standard closed system integrating the zeolite–water pair.

2.1. Description and functioning of the storage system

The storage system is composed of an adsorber, an alternative system able to provide an heat transfer fluid at different temperatures (hot or cold), an evaporator and a condenser connected to the adsorber using four valves (valves 1 and 2 connected to the condenser and 3 and 4 to the evaporator).

At the beginning of the process, the four valves are closed and the adsorbent bed is saturated with steam, in thermodynamic equilibrium with its environment. The sorption cycle, shown in Fig. 1b, works similarly to an ordinary thermal cycle. It is composed of two half-cycles: the charge and the discharge of the thermal energy from the storage system. The isosteric heating and the desorption allow thermochemical energy storage within the adsorber whereas the isosteric cooling and adsorption phases lead to the thermal energy release when it is required.

During isosteric heating, the hot heat transfer fluid flows from the alternative system to the adsorber, heating the adsorbent bed.