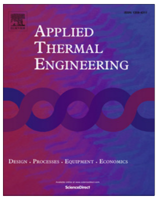
Applied Thermal Engineering 110 (2017) 601–615

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng



Research Paper

Modelling and experimental study of low temperature energy storage reactor using cementitious material

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HIGHLIGHTS

- Numerical study of a thermochemical reactor using a cementitious material for TES.
- Development and test of an original prototype based on this original material.
- Comparison of the experimental and numerical results.
- Energy balance of the experimental setup (charging and discharging phases).

ARTICLE INFO

Article history:
Received 31 May 2016
Revised 23 August 2016
Accepted 24 August 2016
Available online 25 August 2016

Keywords:
Thermochemical storage
Ettringite
Hydration-dehydration
Modelling
Reactor prototype

ABSTRACT

Renewable energy storage is now essential to enhance the energy performance of buildings and to reduce their environmental impact. Most adsorbent materials are capable of storing heat, in a large range of temperature. Ettringite, the main product of the hydration of sulfoaluminate binders, has the advantage of high energy storage density at low temperature, around 60 °C. The objective of this study is, first, to predict the behaviour of the ettringite based material in a thermochemical reactor during the heat storage process, by heat storage modelling, and then to perform experimental validation by tests on a prototype. A model based on the energy and mass balance in the cementitious material was developed and simulated in MatLab software, and was able to predict the spatiotemporal behaviour of the storage system. This helped to build a thermochemical reactor prototype for heat storage tests in both the charging and discharging phases. Thus experimental tests validated the numerical model and served as proof of concept.

1. Introduction

The use of renewable energy in the building sector can considerably reduce its environmental and socio-economic impacts. The excess solar energy in summer could be stored and then released later in autumn or winter, in order to decrease the phase shift between solar radiation and thermal energy needs. Many heat storage materials can be used in the building sector in order to avoid the phase shift between solar radiation and thermal energy demand. Thermal energy storage in general, and phase change materials (PCMs) in particular, have been a main topic in research for the last 20 years [1], but they usually allow to reduce short phase shifts. Another way of reaching this goal of seasonal thermal heat storage could be to explore thermochemical storage, and to use a particular shape of cementitious materials. Indeed, ettringite, a common hydrated phase found in cement-based materials, has the advantage of high energy storage density at low temperature (60 °C) compared to existing adsorbent materials such as zeolites [2,3]. This component is found in small quantities in Portland cement paste (around 10%), while high ettringite content (40–80%) can be reached by calcium sulfoaluminate cement hydration [4].

Concrete solutions for thermal energy storage are usually based on sensible heat transfer and thermal inertia [5,6], and sometimes they are enhanced with PCMs solutions [7,8]. An ettringite based material, capable of storing thermal energy by a reversible dehydration/hydration cycle, was produced by hydration of a mixture of sulfoaluminate clinker, anhydrite and aluminium powder [9]. Thermal energy storage by ettringite material is a physicochemical process usable in both the short (daily, weekly) and long (seasonal) term. In the charge phase, heat is stored by endothermic processes (desorption and dehydration) and is not restored as long as the material remains dry. In the discharge phase, the heat stored in the material is released by exothermic adsorption (adsorption and hydration). The chemical part of the energy storage process

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http://dx.doi.org/10.1016/j.applthermaleng.2016.08.157
1359-4311/

Nomenclature

a_g	thermal diffusivity of steam (m^2/s)
a_f	thermal diffusivity of fluid (m^2/s)
c_w	specific heat of liquid water (J/(kg K))
c_g	specific heat of water vapour (J/(kg K))
c_s	specific heat of material (J/(kg K))
c_h	volumetric heat of three phases (J/(kg K))
d	diameter (m)
dz	length of longitudinal mesh (m)
dr_f	length of radial mesh in the tube (m)
dr_s	length of radial mesh in material (m)
D_v	diffusion coefficient of stream (m^2/s)
RH	relative humidity (%)
K	gas permeability of material (m^2)
K_{LDF}	mass transfer coefficient (1/s)
L	length of the reactor (m)
M	molar mass of adsorbed phase (kg/mol)
n_f	number of radial meshes in material
n_s	number of radial meshes in material
n_z	number of longitudinal meshes
NUT	number of transfer units
p	water vapour pressure (Pa)
p_{vs}	saturation vapour pressure (Pa)
q	water uptake (kg/m^3)
q_{equ}	water uptake at equilibrium (kg/m^3)
r	radial coordinate (m)
R	gas constant (J/(mol K))
R_1	inner radius of the metal tube (m)
R_2	outer radius of the metal tube (m)
R_3	outer radius of the material (m)
t	time (s)
T	temperature (K)
u	gas phase velocity in the material (m/s)
v	fluid velocity in the metal tube (m/s)
z	axial coordinate (m)

Greek letters

ε	porosity
ρ	density (kg/m^3)
λ	thermal conductivity (W/(m K))
ΔH	heat of sorption (J/kg)
μ	dynamic viscosity (Pa s)

Subscripts

equ	equilibrium
f	heat transfer fluid
g	gaseous phase (water vapour)
h	three phases homogenized
in	inlet
LDF	linear driving force
m	maximum
s	solid material
w	liquid phase (water)
0	initial

is related to the reversible conversion of ettringite ($3CaO{\cdot}Al_2O_3{\cdot}3CaSO_4{\cdot}30H_2O$) to metaettringite ($3CaO{\cdot}Al_2O_3{\cdot}3CaSO_4{\cdot}12H_2O$).

The first objective of this study is to predict the behaviour of the ettringite-based material in a thermochemical reactor (cylindrical adsorber) during the heat storage process, by simulating the spatiotemporal variation of the temperature and the water vapour pressure inside the storage material. Then the second aim is to carry out an experimental validation by testing a prototype. To reach this goal, the physical, thermal and hygrometric properties of the material were measured, using standardized tests, and used in an energy storage model [10,11].

Several 1D or 2D energy storage models based on adsorbent materials such as zeolites can be found in the literature [12–16]. To predict the spatiotemporal behaviour of the storage system during heat charging and discharging, a two-dimensional model taking the specificities of cementitious material into account was developed. The heat and mass balance in the thermochemical reactor (cylindrical adsorber) generated a system of non-linear and strongly coupled differential equations. They were solved numerically, first by spatial discretization using the finite difference method [17], and then by temporal integration of state variables (temperature and water vapour pressure) using the Gear method [18–20] in MatLab.

The simulation of this model using measured properties of the ettringite material (physical, thermal and hygrometric properties) provided the evolution of temperature and water vapour partial pressure in the thermochemical reactor during charge and discharge of heat. The evolution of the variables observed during charge and discharge of heat corresponded to the desorption and adsorption phases, respectively. This numerical study gave a complete prediction that allowed us not only to understand the material behaviour better, but also to determine the optimal operating conditions of heat storage. This helped to build the thermochemical reaction prototype for heat storage tests in both the charging and discharging phases.

To store solar heat (daily or seasonal storage), for example, it was necessary to connect the thermochemical reactor with a heat source (e.g. solar collector) to charge it in the storage phase. During the discharging phase, a humidification source was required to release the heat. To perform the storage tests in the laboratory, the reactor was connected to an electric water heater and a humidifier (bubbler) simulating the charge and discharge of heat, respectively. The test bed installed in the laboratory reproduced the storage system functioning during both phases. The comparison between numerical and experimental results validated the numerical model and served as proof of concept.

2. Thermochemical reactor description and principle

The two-dimensional modelling of heat storage was based exclusively on the thermochemical reactor, which was the key element of the heat storage system. The thermochemical reactor (Fig. 1) consisted of a thin metal tube (R_2 - R_1) where the heat transfer fluid (hot water) heated the ettringite-based material placed around the tube (ettringite material between R_2 and R_3) during the charging period. The ettringite material was then insulated from the surrounding environment to avoid heat loss.

A cylindrical adsorber, filled with zeolite, is often used to store heat using a longitudinal humidification system [12,16]. Longitudinal humidification means that the water vapour is introduced at both ends of the storage material. That is to say, the humidified gas (water in vapour phase) circulates through the material porosity in the longitudinal direction (z). The moist input gas ($z = 0$) dries progressively as a result of the adsorption of water vapour by the material and the outlet gas ($z = L$) is thus dry. Furthermore, a radial humidification system, i.e., around the storage material, has the advantage of quickly creating a uniform water vapour pressure in the adsorber [13,21]. Therefore, a thermochemical reactor filled with ettringite-based material with a radial humidification