



Numerical investigations of a continuous thermochemical heat storage reactor



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ABSTRACT

Thermochemical systems are a good alternative to current technologies for long-term heat storage, since the energy is stored as a chemical potential and there is no heat loss during the storage phase. A large number of studies have now been conducted on the development of integrated thermochemical reactors, but fewer studies have investigated separate reactor technologies. The latter present the advantage of dissociating the thermal power and storage capacity of the system, which also increases the energy storage density of the process.

This paper investigates the functioning of an open continuous thermochemical reactor with falling solid flow and humid air cross-flow. A 2D model was developed and set up with the finite element simulation software COMSOL Multiphysics to represent heat and mass transfer phenomena in the reactor.

This study focuses on the influence of the inlet pressure and vapour fraction of the air on the reaction behaviour and the reactor performance (power, temperature). This study also investigates the influence of the reaction front on the pressure drop in the reactor. It highlights the presence of a sharp reaction front between one part of the reactor (bottom) where the solid is completely hydrated and the other part (top) where the solid has not reacted yet. This sharp front is strongly dependent on the inlet air conditions. Also, there is an inertia phenomenon at the entrance of the unreacted solid, which is influenced by inlet air pressure, creating a particular air velocity field.

1. Introduction and context

The energy demand for building applications accounts for about 25% of energy consumption worldwide (40% in Europe) and most of this energy (53% worldwide and 80% in Europe) is used for space heating [1]. Solar thermal systems are a good option to decrease the fossil energy consumption in this sector, but this energy source's production fluctuates. Developing efficient and convenient energy storage systems is an important step toward better management of this renewable energy, because it could join the timing of the resource and demand.

Heat storage technologies available nowadays, using sensible or latent heat, are efficient on the daily and weekly scales, but they present substantial heat loss for longer time scales. Thermochemical technologies are therefore a good alternative for long-term heat storage because the energy is stored as a chemical potential and there is no heat loss during the storage phase [2].

Solid/gas thermochemical energy storage (TES) is based on the use of reversible chemical reactions of the form:



The decomposition of the solid (S1) into (S0) and (G) requires a heat input, Δh_r^0 (endothermic reaction). Therefore, for seasonal storage, the reactive solid is heated by solar energy during summer. This is the “charge” phase of the system. Inversely, during winter, the solid (S0) reacts with the reactant gas (G) to form (S1). This synthesis is exothermic and corresponds to the “discharge” phase of the system (heat recovery period).

The solid reactants must be low-cost, non-toxic, non-corrosive and have sufficient energy storage density to satisfy the needs of large-scale technological development. Several types of reactive pairs exist and different reactive gases can be used for thermochemical systems (NH₃, H₂O, etc.). This paper focuses on a reactive pair using water as the reactive gas.

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Nomenclature		X	Conversion
C _p	Specific heat (J/(kg.K))	$\dot{X}a$	Reaction kinetics (1/s)
D _{ec}	Energy density (kWh/m ³)	y _v	Vapour fraction (mol _v /mol _n)
H	Reactor height (m)	<i>Greek symbols</i>	
h	Convective heat transfer coefficient (W/(m ² .K))	ε	Porosity
Δh _r ⁰	Enthalpy of reaction (J/mol _v)	ν	Stoichiometric coefficient (mol _v /mol _s)
Δs	Entropie of reaction (J/(mol _v .K))	ρ	Bulk density (kg/m ³)
k	Permeability (m ²)	λ _{eff}	Effective thermal conductivity (W/(m.K))
k _{cin}	Reaction kinetic coefficient (1/s)	λ _s	Solid thermal conductivity (W/(m.K))
M	Molar mass (kg/mol)	Φ _v	Vapour sink term (mol _v /(m ³ .s))
n	Molar density (mol/m ³)	<i>Subscripts and superscripts</i>	
p	Pressure (Pa)	a	Dry air
p _{eqSG}	Solid/gas equilibrium pressure (Pa)	h	Humid air
P _q	Power needed for ventilation (W)	v	Vapour
P _{th}	Thermal power of the reactor (W)	s	Solid
p _v	Vapour pressure (Pa)	s0	Dehydrated solid
Δp	Pressure drop (Pa)	s1	Hydrated solid
Q	Volumetric air flow rate (m ³ /h)	in	Inlet
q ₀	Inlet heat flux (W/m ²)	out	Outlet
T	Temperature (K)		
t	Time (s)		
u	Velocity (m/s)		

The data reported in the literature show that a wide temperature range can be reached using different reactive pairs (from ambient temperature to several hundred degrees) [2] [3]. A large number of studies have been conducted over the last few years in the field of low-temperature TES, especially regarding thermochemical material development and optimization of their chemical and thermal properties (energy storage density, thermal conductivity, cycle stability, etc.) [4–8]. In comparison, few investigations were conducted to develop thermochemical reactor technologies [9–12], even though it is a key issue in enhancing heat and mass transfer during the reaction and thus achieving a maximum conversion of the reactants and increasing the power of the reactor.

The TES technologies using water vapour can work under atmospheric pressure with humid air (open mode) or pure vapour (closed mode), usually at low pressure. The use of pure vapour provides better control of the working conditions and favours the reaction kinetics, but it increases the technical constraints on the process (airtightness, non-standard components, etc.). The open mode, at atmospheric pressure, eliminates these constraints, possibly leading to a simpler and cheaper reactor design [13].

In addition to the operating mode (open or closed system), two different technologies can be distinguished for thermochemical reaction applications:

- integrated reactors
- separate reactors

In an integrated reactor, the material is stored in the same tank where it reacts. On the other hand, with a separate reactor, the chamber where the reaction takes place is separate from the thermochemical material storage tank. Each technology presents advantages and drawbacks. The main advantage of the separate reactor is the dissociation between the thermal power and the installation's storage capacity, which increases the storage density of the process because there is no need for vapour diffusers and heat exchangers integrated into the reactor. Contrary to the integrated reactor systems, the separate reactor technologies can also work in steady-state, which can provide constant thermal power output. In this configuration, the technological constraints are focused on the reactor and the storage functions are simplified. But this technology implies transportation of the solid material

and as a consequence the addition of mechanical components. Transportation can also damage the material and have an impact on its cycling stability.

Until now, the separate reactor technology has not been fully investigated. Indeed, most of the studies in the TES field examine integrated reactor technologies, mainly in closed systems [14,15] and recently in open systems [9,16]. Many studies on integrated reactor technology have investigated packed bed technologies, but the fluidized bed reactor [10,17] and a rotary kiln reactor [11] have also been adapted to thermochemical storage.

In this study, the choice of the reactor adapted to solid/gas thermochemical reactions was made according to the following criteria:

- technological simplicity of the process components,
- good contact between the solid and the gaseous phases to improve heat and mass transfers,
- low energy consumption, which implies in particular a low pressure drop for air flow,
- no stirring device, which can cause the attrition of the solid,
- reduction of the air volume according to the solid phase volume in the reactor, in order to reach the highest storage density and the highest outlet air temperature during the discharge phase.

Regarding all these aspects, the choice was made to develop an open mode moving bed reactor with humid air as the reactive and heat-carrying fluid, which is described in the next section. This technology has already been investigated by the Institute for Thermodynamics and Technical Engineering (ITW) [12] for space heating applications using zeolite as the storage material. This study confirmed that the moving bed reactor is adapted for solid/gas adsorption heat storage.

However, the use of zeolite in adsorption storage systems is not adapted to a wide panel of applications because of the narrow range of discharge temperatures that can be reached (40–80 °C). Thermochemical salts should allow reaching higher temperatures. Moreover, adsorption materials present a lower energy density compared to thermochemical hydrated salts, as the enthalpies of chemical sorption phenomena are higher than in the case of physical adsorption [18]. In addition, a chemical reaction is monovariant, whereas the physical adsorption process is divariant. Finally, the bed behaviour is different for the two materials: in the case of adsorption, the physical

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