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Energy Procedia 141 (2017) 310–314

Energy Procedia

www.elsevier.com/locate/procedia

4th International Conference on Power and Energy Systems Engineering, CPESE 2017, 25-29 September 2017, Berlin, Germany

Long-term Thermal Energy Storage Using Thermochemical Materials

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Abstract

There are different methods to store thermal energy. The thermochemical heat storage is one of the sufficient thermal energy storage. The energy storage density of the thermo-chemical material (TCM) is higher compared with sensible and latent heat storage method. This paper presents a mathematical simulation of thermochemical energy storage process by using COMSOL Multiphysics modeling Software. The TCM studied is magnesium chloride hexahydrate. The model result is validated with the experimental results, and the temperature distribution in the bed and material are investigated. Two reactor designs are considered; cylinder and truncated cone with different radiuses and heights. The comparison of the performance between them is investigated. The validation shows good agreement between the present work and the literature. The results indicate that the increase in entrance area reduces the charging time and increases the pressure drop at constant volume and height of the bed. Cylinder reactor and truncated cone with small and large diameters of 15.5 cm and 18.4 cm are the best to charge this material with thermal energy.

Keywords: Seasonal storage, Thermochemical; heat storage; Salt hydrates; Magnesium chloride hexahydrate.

1. Introduction

The energy demand for buildings accounts for 25% of the total energy consumption in the world and 51% in Egypt [1]. The domestic sector is considered the highest contribution in energy utilization. Also, space heating and

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Peer-review under responsibility of the scientific committee of the 4th International Conference on Power and Energy Systems Engineering.
10.1016/j.egypro.2017.11.111

hot domestic water account for half of this consumption [2]. Thermochemical Heat Storage (THS) is a quite modern technology promises energy storage field with more efficient and desired results. Thus, selecting thermochemical material process depends on different factors [3]; (1) environmental safety and the toxicity, (2) material cost, (3) energy density, (4) charging and discharging temperature range, (5) corrosiveness, (6) operating pressure, (7) sustainability, and (8) cyclability and stability.

Thermochemical materials storage has distinctive advantages, [3] which they are; (1) THS materials have a high energy storage density, (2) the thermal losses during storage period close to zero when the energy stored in the form of chemical potential, (3) the required volume of material is low and applicable inside houses, (4) variable charging temperature range, and (5) low cost materials. However, the weaknesses of thermochemical materials storage [4] are; (1) heat and mass transfer rate are quite low, (2) recyclability is not available in all materials, and (3) formation of layer like gel during hydration may occur. The storage energy density for the thermochemical material is about 100–500 kW h/m^3.

A reversible reaction occurred for TCM in exceptional conditions, is exo/endothermic reaction. TCM can store thermal energy and release it via hydration/dehydration chemical reaction [5]. In hot summer climate, desorption (dehydration) process occurs as the heated air produced by the solar application passes into adsorbent (porous material). In cold winter climate, adsorption (hydration) process occurs, and the hot outlet air is used in heating requirements. The general equation for the thermochemical reaction is [6]: $C + Heat \leftrightarrow A + B$. Rubino and R. de Boer [5] illustrated a model for the thermo-chemical open reactor to analyze the heat discharge process by using magnesium chloride hexahydrate ($MgCl_2$. $6H_2O$). They showed that the model was useful in studying the effects of reactor design and operating conditions on the heat storage efficiency of the reactor. Michel et al. [7] investigated an open thermochemical storage system experimentally and focused on the design of the bed using $SrBr_2/H_2O$. They concluded that the inlet moist air conditions regulate both moist air outlet temperature and thermal power. In another study [8], during hydration of the magnesium chloride ($MgCl_2.6H_2O$), the layer nearest to the evaporator was over hydrated due to some disturbance in inlet condition. They avoided high-pressure drop by using a suitable carrier material. Marias et al. [9] solved the problem of the formation of a hard layer and examined the pressure drop experimentally when using aluminum potassium sulphate12-hydrate ($KAl(SO_4)_2.12H_2O$).

However, the literature shows different works in seasonal energy storage, but there is no study focused on the design of bed reactor. Furthermore, the studies aiming to improve charging and discharging time are not found. The objective of this work is to investigate theoretically the effect of variation entering and outlet area of thermochemical bed reactor on the temperature range, pressure drop, charging time and hydration time.

2. Mathematical Model

An open atmospheric reactor is applied in the lab-scale systems because of its simplicity and potential low costs. The porous material fills the reactor, and the hot gas passes through it during dehydration processes. The holes inside porous allow the hot and relatively dry airflow through it. A new material ($MgCl_2$-$4H_2O$) appears as a product with H_2O. The cooled air stream transports out the vapor [10]. Magnesium chloride hydrate is selected as the range of operating temperature is suitable for domestic use and applicable to simple solar systems. The following reactions apply for this TCM [5].

$$Mgcl_2.6H_2O \Leftrightarrow MgCl_2.4H_2O + 2H_2O \quad \text{and} \quad Mgcl_2.4H_2O \Leftrightarrow MgCl_2.2H_2O + 2H_2O \tag{1}$$

The schematic diagram of the reactor model used in the present study is provided in Fig. 1.with one of the studied design (cylinder) The studied model represents a 2D symmetric axis geometry. There are assumptions considered [5]; (1) the side walls are insulated, (2) the air density is constant, (3) the gas and solid phase conductivity is constant, (4) there is no diffusivity between gas and solid, (5) the radiation is negligible, (6) the velocity is constant in the flow direction, (7) the pressure drop via the porous media is related to Darcy's law, (8) the heat transfer by natural convective is negligible, (9) the friction in the energy balance is equal zero, and (10) the mass transfer resistance is negligible on the air side.

2.1. Mass, Momentum and Energy Balance and Reaction Kinetics

During charging, the completely hydrated sample of a crystalline $MgCl_2$-$6H_2O$ is exposed to the hot and relatively dry air stream. The water vapor mass fraction is varying through the porous bed. The cooled air stream

transports out the vapor [10]. The mass conservation equations for vapor and solid are considered [5].
For the porous material, Darcy law governs the momentum conservation. Darcy's law equation describes the flow of fluid through a porous medium. In laminar flows, the pressure drop is proportional to velocity in porous media as the pressure decrease in the direction of the fluid flow. The pressure drop caused by friction between the fluid and porous media along the distance of flow, when $R_e < 1$ is considered [5];

$$u = \frac{K}{\mu}\frac{P}{x} \text{, and for } Re > 1 \text{ Forchheimer's equation [11] } \nabla P = -\frac{\mu}{K}u - C_F K^{-1/2}\rho_F |u| u \quad (2)$$

Where, K, μ, ∇P and C_f are specific permeability (m^2), dynamic viscosity (Pa. s), pressure drop (Pa) and dimensionless form-drag constant respectively and C_f calculated by [12];

$$C_F = 0.55(1 - 5.5\frac{d_p}{D_e}) \text{ and } D_e = \frac{2wh}{w+h} \quad (3)$$

Where d_p, D_e, w and h are particle diameter (m), an equivalent diameter (m), the width (m) and height (m) of the bed. The energy balance for the solid and fluid are;

$$(1-\varepsilon)\rho_s C_s \frac{\partial T_s}{\partial t} = (1-\varepsilon)k_s \nabla^2 T_s + q_s^{\bullet} \text{ and } \varepsilon\rho_F C_{pF}\frac{\partial T_F}{\partial t} + \rho_F C_{pF} u.\nabla T_F = \varepsilon k_s \nabla^2 T_s \quad (4)$$

As there is a thermal equilibrium between solid and gas phase, T_s=T_f=T. From equations (9) and (10);
The reaction rate was suggested by [13] for dehydration;

$$r_w = -C_a \exp(-\frac{E_a}{RT_s})(\frac{P_F - P_{eq}}{P_{eq}}) \quad (5)$$

Where E_a, P_f, P_{eq} and C_a are activation energy (J/mol), fluid pressure (pa), equivalent pressure (pa) and pre-exponential constant. An empirical approach used as there are not known values of reaction constants.

3. Numerical Solution

The solution of the system of equations is carried out by using COMSOL Multiphysics Modeling Software 5.2. The experimental data in the literature of Marias [9] was selected for validation. They selected aluminum potassium sulfate 12-hydrate ($KAl(SO_4).12H_2O$) as a porous material for their work. The Bed dimension and inlet conditions are simulated like the experimental. Fig. 2 illustrates the computational model validation by making a comparison between the simulation outlet temperature with experimental data [9], during dehydration time. All experimental conditions, like, ambient temperature and pressure, inlet temperature and flow rate are used as input data in the model. Reasonable agreement is observed between the present computational results and the obtained experimental data with a maximum relative error of 8 % at the end of charging time.

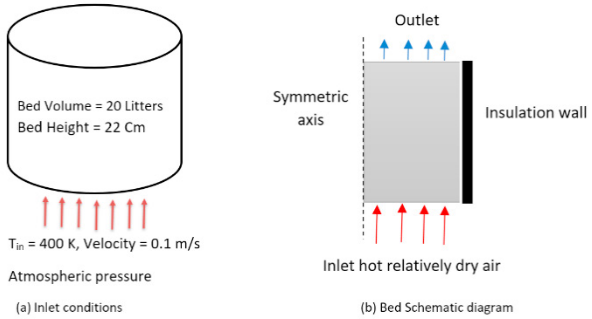


Fig. 1: The reactor schematic diagram.

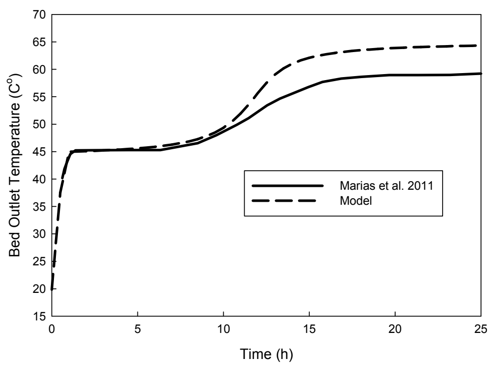


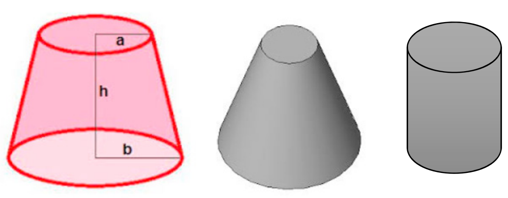
Fig. 2: The validation curve related to Bed outlet temperature in the model and [9].

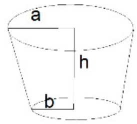
4. Results and Discussions

Between the inlet and outlet gas during dehydration of magnesium chloride hexahydrate is plotted with the operating time for case 1. The other configuration is the truncated cone where the area of bed entrance is increased, and outlet area is reduced. Additionally, 3 cases of the truncated cone are considered (cases 2, 3 and 4) with a different entrance and outlet areas of the bed, and the outlet area is less than the inlet area. Moreover, another three cases (5,6,7) of the truncated cone are considered where the outlet area is greater than the inlet area. The volume and height of the bed for all studied cases are considered equal to 20 liters and 22 Cm respectively. Table. 1 shows the dimensions of all studied cases at constant height and volume of the reactor bed. For case 1, the thermochemical material takes about 50 minutes at the beginning of charging as sensible heating for porous material. The operating time required to charge this volume for case 1, is 25 hours. Fig. 3 shows a comparison between cases 1, 2, 3 and 4 related to the temperature difference between the inlet and outlet air with the operating time. The figure shows that the material of case1 requires about 8 hours to charge the rest (approximately 5%) of magnesium chloride hydrate. The figure illustrates that the operating time for charging magnesium chloride hydrate of case 4 is the lowest (about11.5 hours). For cases 1, 2, 3 and 4, the more entrance area, the less operating time is required.

Table 1: The dimension data for studied cases of the reactor.

h=22 Cm	a (outlet) (Cm)	b (inlet) (Cm)
Case 1	17	17
Case 2	15.5	18.4
Case 3	10.47	20.949
Case 4	9.125	22
Case 5	18.4	15.5
Case 6	20.949	10.47
Case 7	22	9.125





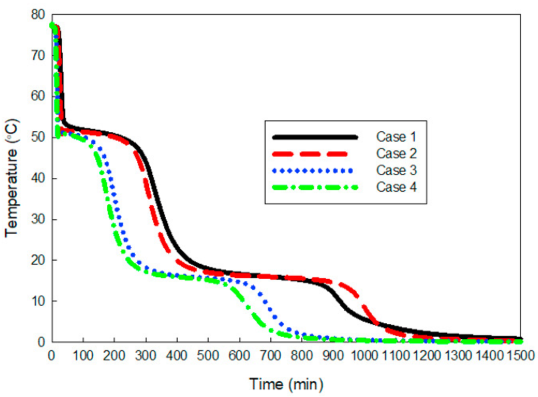


Fig. 3: The temperature difference between inlet and outlet gas stream for cases 1to 4.

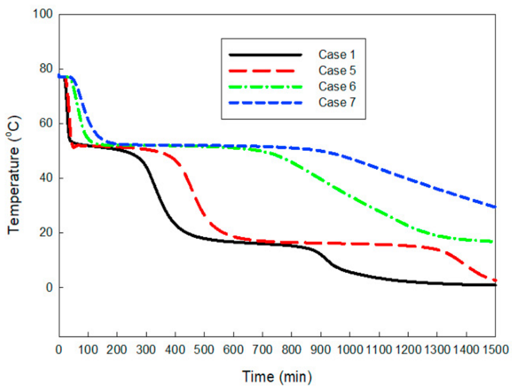


Fig. 4: The temperature difference between inlet and outlet gas stream for cases 1, 5, 6 and 7.

A comparison between the temperature difference of cases 1, 5, 6 and 7 with operating time is illustrated in fig.4. This figure shows that the operating time for charging magnesium chloride hydrate for case1 has the lowest operating time, compared with cases 5, 6 and 7. The pressure drop is a significant issue in thermochemical heat storage during hydration and dehydration. Figure 5 and 6 show the pressure drop during dehydration for cases 1 to 4 and 1, 5-7 respectively with time. The figure indicates that the pressure drop increases with operating time during dehydration, due to the decreasing in vapour content inside the magnesium chloride which decreases the porosity of it. Despite, the design change of the truncated cone from case1 to case 4 improve the charging time, but it increases the pressure drop via material bed. Moreover, the cylindrical shape (case1) has the least pressure drop, compared with case2, 3 and 4 because of the effect of throttling at the outlet. The reaction rate in case 4 is higher than other cases. Increase pressure drop increases cost, because the system required a more powerful fan. Designs 3 and 4 are preferred at a condition which the time is the main important factor in the storage system. In fig. 6, cases 6 and 7 require more operating time for charging. For cases 1 and 5, the operating time for charging the material is close approximately to 25 hours. The rise in pressure drop in case 1 is three times more than it in cases 6 and 7. In consequence, case 5 has an improvement in pressure drop without effect on operating time during charging. This result is due to the low difference in pressure drop, compared to case 1, and this difference is not enough to decrease the reaction operating time. Thus, the reaction operating time for cases 1 and 5 are equal.

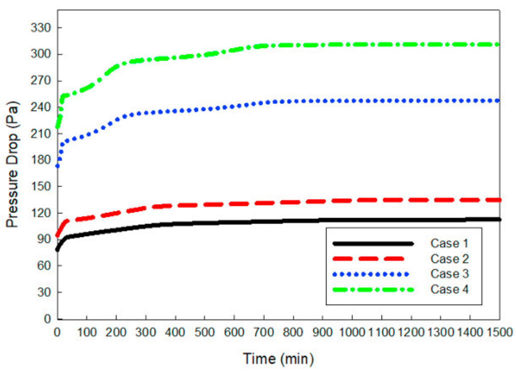


Fig. **5**: The pressure drop for case1, 2, 3 and 4 for the reactor design.

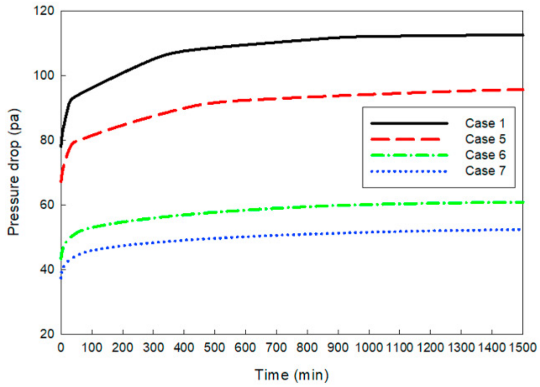


Fig.**6**: The pressure drop for case1, 5, 6 and 7 for the reactor design.

5. Conclusions

The effect of different reactor configurations (cylinder and truncated cone) on the charging time and pressure drop is investigated at constant reactor volume and height. The effect of variation in entrance and outlet area of the truncated cone reactor on the pressure drop and charging time during dehydration process is also considered. A comparison between the studied cases shows that the increase in entrance area reduces the charging time and increases the pressure drop. However, cases 2, 3 and 4 used in which the time is the main factor in the system, cases 6 and 7 are important when the heat source is operating at a temperature lower than 100 °C. The results show that Cases 1 and 5 are the best design of the seven studied designs.

Acknowledgements

The authors are beholden to the Ministry of Higher Education (MoHE) – Egypt and Egypt - Japan University of Science and Technology (E-JUST) for supporting this work and providing tools.

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