

# NUMERICAL SOLUTION OF THE HEAT ACCUMULATOR LAYER BY MEANS OF FEM

P. Fiala, I. Běhunek, E. Kadlecová

Department of Theoretical and Experimental Electrical Engineering,  
University of Technology Brno, Kolejní 2906/4, 612 00 Brno, Czech Republic  
e-mail: fialap@feec.vutbr.cz

**Summary** The article deals with one layer of a heat accumulator which is suitable for solar systems. There is a description of the air turbulence, heat transfer, conduction and also phase change of  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$  which is used to increase the density of stored energy. The numerical solution was done with the help of finite element method (FEM) in ANSYS software.

## 1. INTRODUCTION

The model of heat accumulator is conceptually similar to gravel accumulator. Stones of gravel were replaced by plastic enclosures, which contain PCM (Phase Change Material). Accumulator has 8 layers equipped by thermal insulation. In vertical ducts there is a system of swinging distributing flaps. They are able to direct air flow to layers, close and isolate layers etc. The aim is to reach temperature stratification along the overall height of accumulator, store or pump heat to/from any layer.

## 2. APPLICATION OF PCM

Phase changes of materials are a perspective way of thermal energy storage. The application of PCM offers a lot of advantage. We can reach higher density of stored energy. Table 1 shows the calculation for classical materials and PCM. The initial temperature 20 °C and final temperature 50 °C at the end of heating are supposed. Next advantage is a possibility to store heat at low temperature. We don't need to have such good thermal insulation and solar collectors work with better efficiency so the demand for area of collectors decreases.

Tab. 1. Comparison of classical materials and PCM

materiál	density of storage energy [kWh.m <sup>-3</sup> ]
water	34,5
gravel	23,0
paraffine wax	62,4
$\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$	117,4
$\text{Na}_2\text{CO}_3 \cdot 10\text{H}_2\text{O}$	131,7
$\text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$	134,7

Big latent heat, good thermal conductivity and inflammability are the main advantages of inorganic materials. But they cause corrosion and suffer from loss the of water. Incongruent melting and supercooling are the biggest problem of their exploitation. During melting and freezing there are precipitations of other phases, which do not take part in next process of charging and discharging. Poor

nucleation, slow rate of crystal growth or high rate of heat removal may be the reason for supercooling. Impurities have a strong influence on the cooling curves as well.

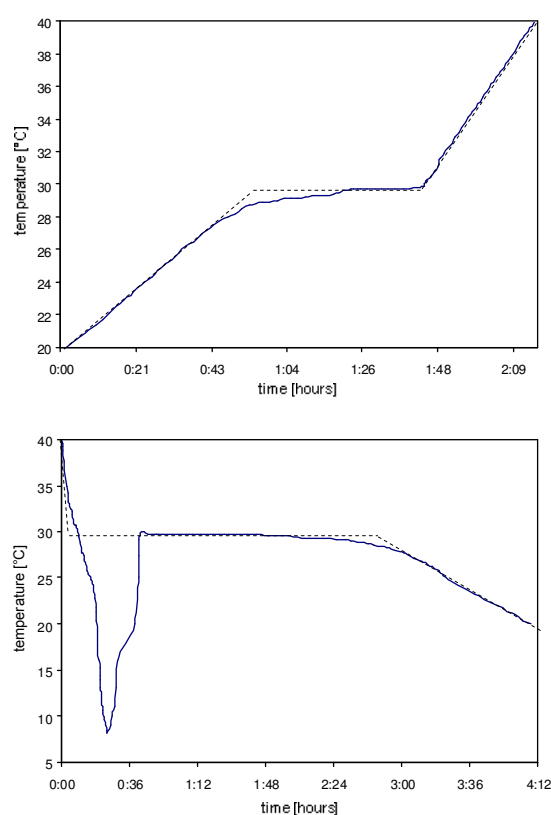


Fig. 1. Phase changes of  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$

In the Fig. 1 there is exhibited the phase change of  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$  during heating and cooling. Dashed lines would show theoretical behaviour if melting and freezing were at constant temperature  $T_m$  – case of pure crystalline substance. Impurity and methodology of measuring (probe always is only in small amount of hexahydrate) are the causes of variances. During solidification the supercooling occurred because of weak nucleation. Crystallization was initiated due to a solid particle of PCM which we put to the measured sample. Otherwise there would not be any crystallization. We can use

plastics, mild steel or copper for enclosures. Aluminium or stainless steel are not suitable.

Sometimes we can see temperature fluctuation above  $T_m$  during solidification (Fig. 2). We found an explanation in the binary diagram (Fig. 3).

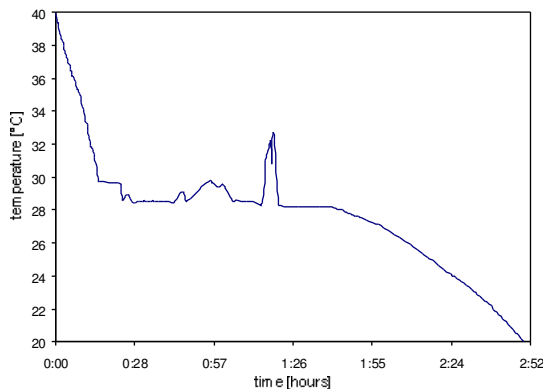


Fig. 2. Phase change of  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$  ( $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$  crystallization)

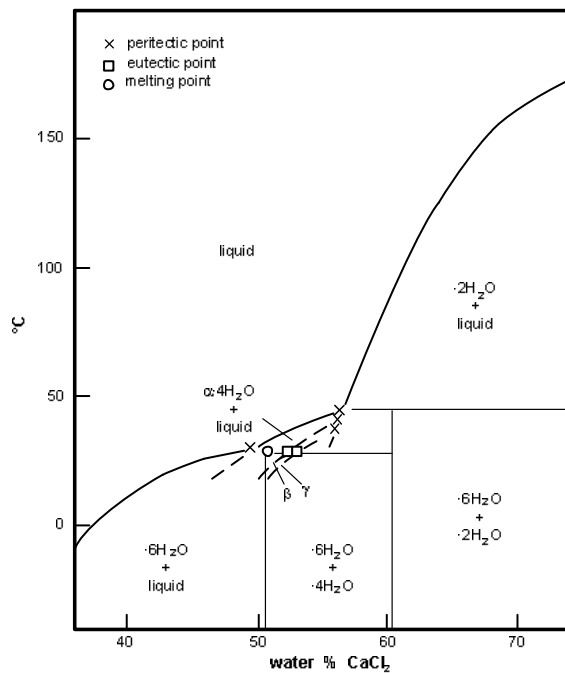


Fig. 3. Binary diagram of  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$  [2]

Figure 3 shows the binary phase diagram of calcium chloride and water. The hexahydrate contains 50,66 wt%  $\text{CaCl}_2$ , and the tetrahydrate 60,63 wt%. The melting point of the hexahydrate is 29,6 °C, and of the tetrahydrate 45,3 °C. The hexahydrate- $\alpha$  tetrahydrate peritectic point is at 49,62 wt%  $\text{CaCl}_2$ -50,38 wt%  $\text{H}_2\text{O}$ , and 29,45 °C. In addition to the stable  $\alpha$  form, there are two monotropic polymorphs of the tetrahydrate salt,  $\beta$  and  $\gamma$ . The latter two are rarely encountered when dealing with the hexahydrate composition; however, the  $\alpha$  tetrahydrate is stable from its liquidus temperature, 32,78 °C down to the peritectic point, 29,45 °C, a span of 3,33 °C. When liquid  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$  is cooled

at equilibrium, a  $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$  can begin to crystallize at 32,78 °C. When the peritectic is reached at 29,45 °C the tetrahydrate hydrates further to form hexahydrate, and the material freezes. The maximum amount of tetrahydrate which can be formed is 9,45 wt%, calculated by the lever rule. This process is reversed when solid  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$  is heated at equilibrium. At 29,45 °C the peritectic reaction occurs, forming 9,45% a  $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$  and liquid of the peritectic composition. As the temperature increases further, the tetrahydrate melts, disappearing completely at 32,78 °C. Under actual freezing and melting conditions, the equilibrium processes described above may occur only partially, or not at all. Supercooling of the tetrahydrate may lead to initial crystallization of the hexahydrate at 29,6 °C, or lower if this phase also supercools.

Modification is possible to do by additives. From number of potential candidates  $\text{Ba}(\text{OH})_2$ ,  $\text{BaCO}_3$ , and  $\text{Sr}(\text{OH})_2$  were chosen. They seemed to be feasible. When we used  $\text{Ba}(\text{OH})_2$  and  $\text{Sr}(\text{OH})_2$  at 1% part by weight there was no supercooling. We could increase stability of the equilibrium condition with addition of KCl (2 wt%) and NaCl. NaCl is weak soluble in  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$ , therefore part by weight is only about 0,5%. Disadvantage is that melting point decreases about 3 °C at 26-27 °C. The melting point of pure  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$  is 29,6 °C. Due to availability on the market and price we chose for modification  $\text{BaCO}_3$ . We obtained the best results for 1,2 wt%. In Fig. 1 we can see that supercooling is 3-4 °C but then crystallization started spontaneously and temperature increased at 28-29 °C. It is obvious that nucleation is slower in comparison with pure crystalline matter. Supercooling is not considered as a disadvantage. If we use  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$  in the heat accumulator we will be able to store energy at lower temperature (about 26 °C) and suppress heat losses. Next disadvantage of  $\text{BaCO}_3$  is that it carbonates because of atmospheric CO and  $\text{CO}_2$ . This means the loss of properties. In our case  $\text{BaCO}_3$  will be isolated from surrounding environment.

### 3. NUMERICAL MODEL OF HEAT ACCUMULATOR LAYER

There is geometric model of one layer of accumulator in the figure 4. It consists from 26 PVC pipes in the square configuration. Inside of pipes there are 9,36 liters of modified  $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$ . The air flows through the layer and transfers heat into pipes. Progress of numerical solution had two parts. First we solved turbulence model and got heat transfer film coefficients. These results were the input of solution for second part when thermal model was calculated. Time dependence of temperature distribution in the layer is final result.

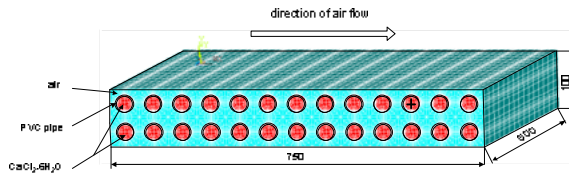


Fig. 4. Geometric model of layer with mesh of elements

Initial and boundary conditions

- inlet temperature of the air is 50 °C
- inlet velocity of the air is 0,4 m.s<sup>-1</sup>
- outlet pressure is 101,3 kPa + 10 Pa
- initial temperature of the air, PVC and CaCl<sub>2</sub>.6H<sub>2</sub>O is 20 °C

There are distributions of velocity in Fig. 5 and next results for distribution of the turbulent kinetic energy, dissipation, temperature, and pressure.

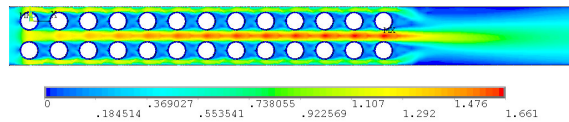


Fig.5. Velocity distribution of the air

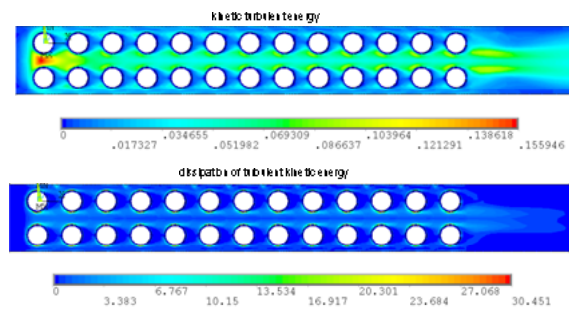


Fig.6. Distribution of kinetic energy, dissipation

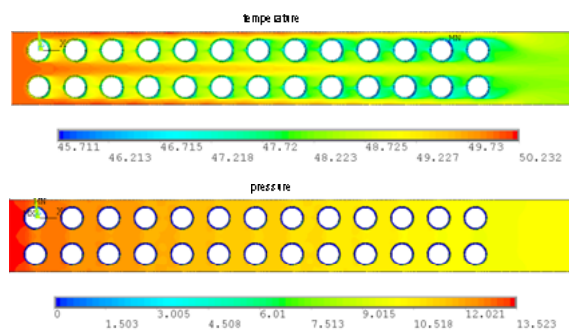


Fig.7. Distribution of temperature and pressure

Calculation of thermal model was done with the same conditions as previous turbulence model. In Fig. 8 there is time dependence of CaCl<sub>2</sub>.6H<sub>2</sub>O temperature in the pipe which is marked with black cross (see Fig. 4). We can compare results obtained by numerical simulation with the measuring. Differences between simulation and measuring are caused due to inaccuracy of model with respect to

reality. We used tabular values of pure CaCl<sub>2</sub>.6H<sub>2</sub>O but in pipes there is modified hexahydrate with 1,2% of BaCO<sub>3</sub>. We would need to know temperature dependence of thermal conductivity, specific heat, and density during phase change exactly.

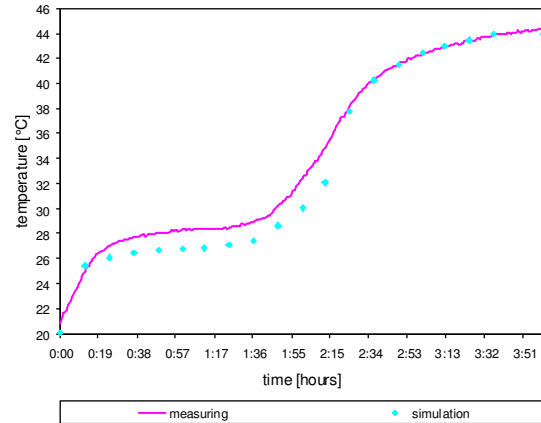


Fig.8. Comparison between measuring and simulation

4. CONCLUSION

There was presented one layer of heat accumulator in the paper which is derived from gravel accumulator. We used pure CaCl<sub>2</sub>.6H<sub>2</sub>O with addition 1,2% of BaCO<sub>3</sub> to increase heat capacity and avoid a supercooling. Numerical model was solved with help of FEM in ANSYS software. If we compare results between simulation and experimental measuring we will see quite good congruence. Exact knowledge of material properties has crucial effect on accuracy of numerical model.

Acknowledgement

The paper was prepared within framework of the research plan No. MSM 0021630516 of the Ministry of Education, Youth and Sports of the Czech Republic.

REFERENCES

- [1] BEHUNEK, I. *Properties of inorganic PCM* In Honeywell EMI conference and competition 2005. Brno: Ing. Zdeněk Novotný CSc., Ondráčkova 105, Brno, 2005. ISBN 80-214-2942-9.
- [2] LANE, G.A. *Solar Heat Storage: Latent Heat Materials, Volume II: Technology*. Boca Raton (Florida, USA): CRC Press, Inc., 1986. ISBN 0-8493-6586-4.
- [3] WILCOX, D.C. *Turbulence modeling for CFD*. La Canada (California, USA): DCW Industries, Inc., 1994. ISBN 0-9636051-0-0.