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## **NUMERICAL SIMULATION OF HEAT TRANSFER IN THE SINGLE HEAT STORAGE ELEMENT WITH PHASE CHANGE MATERIAL**

The paper presents a short description of a numerical simulation for the transient heat transfer in a single heat storage element with phase change material PCM (Stefan problem – melting and solidification phenomena). Enthalpy method – a finite difference numerical discretization and explicit temporal discretization scheme – was chosen for the transient 3-D model. The results of numerical calculation of 3-D temperature fields for heating a single PCM vessel are presented in the graphic form.

### **NOMENCLATURE**

- $c_p$  – specific heat
- $L$  – latent heat
- $i$  – enthalpy
- $T$  – temperature
- $\tau$  – time
- $r$  – radial coordinate
- $z$  – axial coordinate
- $\lambda$  – thermal conductivity
- $\rho$  – density
- $Q$  – heat flux
- $\alpha$  – the heat transfer coefficient

### **INTRODUCTION**

Phase change heat transfer problems occur in various technological, industrial and geophysical processes, such as: TES-PCM Thermal Energy Storage in

Phase Change Material, melting of ice, freezing of water, metal casting, welding, coating and purification of metals, crystal growth from melts and solutions, drying of food, nuclear reactor safety etc.

Problems of phase change heat transfer are of great practical importance (e.g. designing of energy storage units, including waste and solar energy, cooling of electronical devices, improving of indoor thermal comfort) as well as importance for basic knowledge, especially when processes for radically changing Prandtl's values are considered.

The main purpose of computer simulation of physical processes which take place in thermal storage systems is to obtain characteristics of such systems very quickly and with low costs. Numerical simulation of charging and discharging processes of thermal storage system is based on solving an energy equation (with proper boundary and initial conditions) for given geometry of the whole system and individual elements containing phase changing material.

Stefan problem is highly nonlinear due to temperature dependence of thermal properties of PCM. This heat transfer problem is being solved using enthalpy technique in an explicit finite difference form.

Some special numerical procedures for solving heat transfer problem mentioned above were developed. They give the possibility to solve this problem in either twodimensional (e.g. cylinder) or much more complicated geometries (3-D) with different boundary conditions. Also a computer program for estimation performance characteristics of thermal storage system was developed. The system under consideration consists of vertical tubes with PCM and the air is considered as heat transfer fluid [1].

It should be stressed that in many papers published so far constant thermo-physical parameters for both the liquid and the solid phase are considered. In case of significant temperature changes this procedure is not appropriate (e.g. thermal conductivity of liquid can be about 50% thermal conductivity of solid). Therefore, in order to obtain a correct numerical simulation of phase change processes it is essential to know changes of enthalpy and specific heat with temperature for both phases [3,4].

## 1. MATHEMATICAL FORMULATION

To determine unsteady state temperature fields in a vertical tube with PCM, it is necessary to solve heat balance equation (for cylindrical 3-D geometry) that describes the heat transfer during phase change without free convection in a melted region:

$$\rho \frac{di(T)}{dt} = \text{div } \lambda(T) \text{ grad } T \quad (1)$$

Initial condition:

$$T(r, z, \varphi, \tau) = T_0 \quad \text{for } \tau = 0$$

Boundary conditions (between the storage tube and air flow):

– for cylindrical surface:

$$-\lambda \left. \frac{\partial T}{\partial r} \right|_{r=R_z} = \alpha_r (T - T_\infty)$$

where:  $\alpha_r$  – the heat transfer coefficient for the cylindrical surface,

$T_\infty$  – air temperature;

– for frontal surface:

$$-\lambda \left. \frac{\partial T}{\partial z} \right|_{z=\frac{H}{2}} = \alpha_h (T - T_\infty)$$

where:  $\alpha_h$  – the heat transfer coefficient for the frontal surface.

## 2. NUMERICAL METHOD

From several ways of solving problem presented above in mathematical formulations, enthalpy method – a finite difference numerical discretization and explicit temporal discretization scheme – was chosen. The processes of phase change (solidification and melting) are nonlinear in the mathematical sense due to a moving of a solid/liquid interface. The solution of this problem is much more difficult when thermal properties of PCM ( $\lambda$ ,  $c_p$ ) are temperature dependent and when the boundary conditions apply to convection.

The first step in the computational process is to subdivide an investigated tube into a definite number of small balance elements. The differential grid consists of  $(NI \cdot NJ \cdot NK)$  nodal points – where  $NI$  is a number of nodal points along a radius of the tube,  $NJ$  is a number of nodal points along  $z$  coordinate and  $NK$  is a number of nodal points along perimeter. The nodal point of a differential grid is located inside the balance element. The balance element has inside diameter  $R_k$ , outside diameter  $R_l$ , height  $\Delta Z$  and angle  $\Delta \varphi$ . The  $I$  and  $J$  and  $K$  indicate positions of balance elements (nodal points) in a differential grid. Fig. 1 shows the shape of the balance element and a part of the differential grid. The temperature in particular nodal points of a grid (average temperature in balance elements) at time  $\tau + 1$  is obtained from a balance of heat fluxes at the boundary:

$$V_i \rho_i \frac{di}{d\tau} = \sum_j (Q_{ji} + Q_{Bj})$$

$$\text{where: } \frac{di}{d\tau} = c_p(T) \frac{T_i^{\tau+1} - T_i^{\tau}}{\Delta\tau},$$

$$Q_{ji} = \frac{1}{R_{ji}} (T_j - T_i) \text{ for internal elements,}$$

$$Q_{Bj} = \alpha_j S_j (T_{\infty}^{\tau} - T_j^{\tau}) \text{ for boundary elements,}$$

$R_{ji}$  – thermal resistance for internal elements,

$\alpha_j$  – the heat transfer coefficient on surface of  $j$  differential boundary element,

$S_j$  – the external surface of  $j$  differential element.

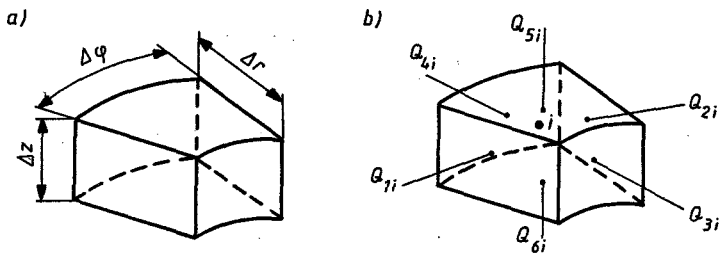


Fig. 1. A shape of the balance element and a part of the differential grid

In the calculations, the melting or solidifying properties of storage materials were taken from measurements, especially characteristics of enthalpy (latent heat) and specific heat vs. temperature. DSC (Differential Scanning Calorimetry) was used to measure the heat effects [3].

### 3. NUMERICAL RESULTS FOR A SINGLE VERTICAL TUBE

A list of considered phase-change materials and some thermodynamic properties are given in Table 1.

Table 1

Material	Density $\rho$ [kg/m <sup>3</sup> ]	Melting point $T_m$ [°C]	Thermal Conductivity $\lambda$ [W/(m·K)]	
			solid	liquid
wax – PPW-20	850	56	0,25	0,15
wax – REW-II	800	70	0,2	0,2

In the numerical charge test a vertical tube of diameter 0,04 m and height 0,4 m, filled with PCM (wax PPW-20 or REW-II) was considered.

Calculations were carried out for following initial and boundary conditions:

- wax PPW-20
  - initial temperature  $T_0 = 30^\circ\text{C}$ , air temperature  $T_\infty = 70^\circ\text{C}$ , heat transfer coefficient on the upper and lower surface  $\alpha_h = 5 \text{ W}/(\text{m}^2\cdot\text{K})$  and side surface  $\alpha_r = 5 \div 25 \text{ W}/(\text{m}^2\cdot\text{K})$ ;
- wax REW-II
  - initial temperature  $T_0 = 30^\circ\text{C}$ , air temperature  $T_\infty = 90^\circ\text{C}$ , heat transfer coefficient on the upper and lower surface  $\alpha_h = 5 \text{ W}/(\text{m}^2\cdot\text{K})$  and side surface  $\alpha_r = 10 \div 20 \text{ W}/(\text{m}^2\cdot\text{K})$ .

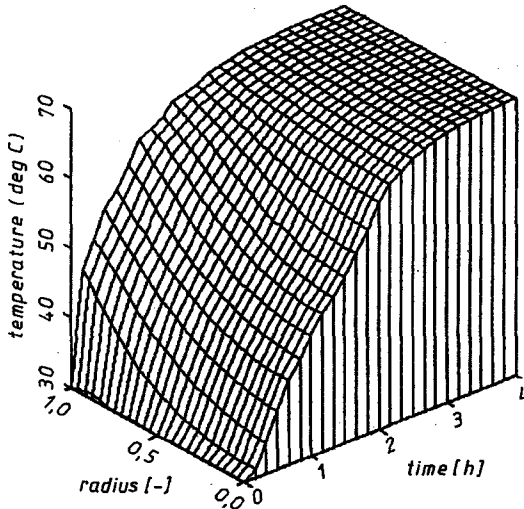


Fig. 2. The 3-D graph presenting temperature field as a function of charge time and radius coordinate for PPW-20 wax (heat transfer coefficient for side surface  $\alpha_r = 20 \text{ W}/(\text{m}^2\cdot\text{K})$ )

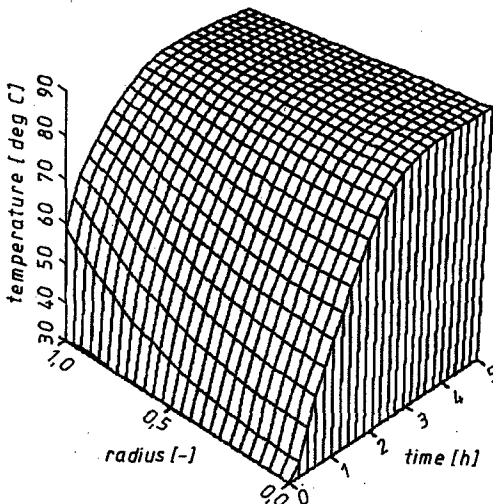


Fig. 3. The 3-D graph presenting temperature field as a function of charge time and radius coordinate for REW-II wax (heat transfer coefficient for side surface  $\alpha_r = 20 \text{ W}/(\text{m}^2\cdot\text{K})$ )

Figures 2 and 3 show 3-D temperature field as a function of charge time and radius coordinate for two waxes: PPW-20 and REW-II.

Results of the numerical simulation of charging single element show (Fig. 4), among others, that there are rather high temperature gradients in the PCM up to the time when material is completely melted. It is a result of rather small thermal conductivity of this materials.

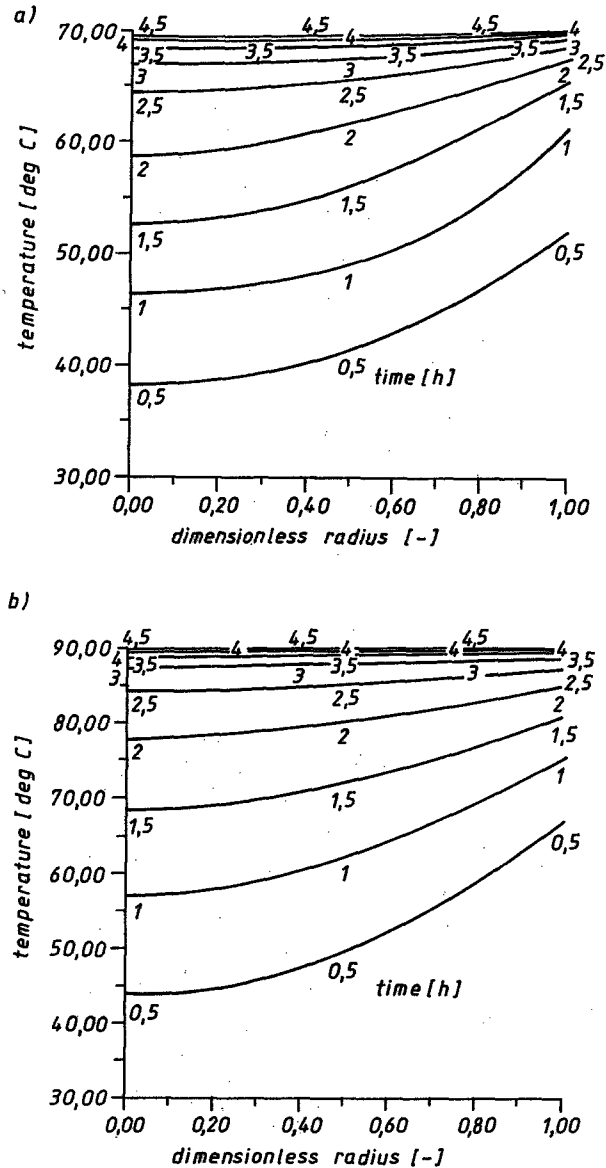


Fig. 4. The temperature distribution inside the cylindrical element with (a) PPW-20 and (b) REW-II along the radius. Heat transfer coefficients for side surface  $\alpha_r = 20 \text{ W}/(\text{m}^2 \cdot \text{K})$

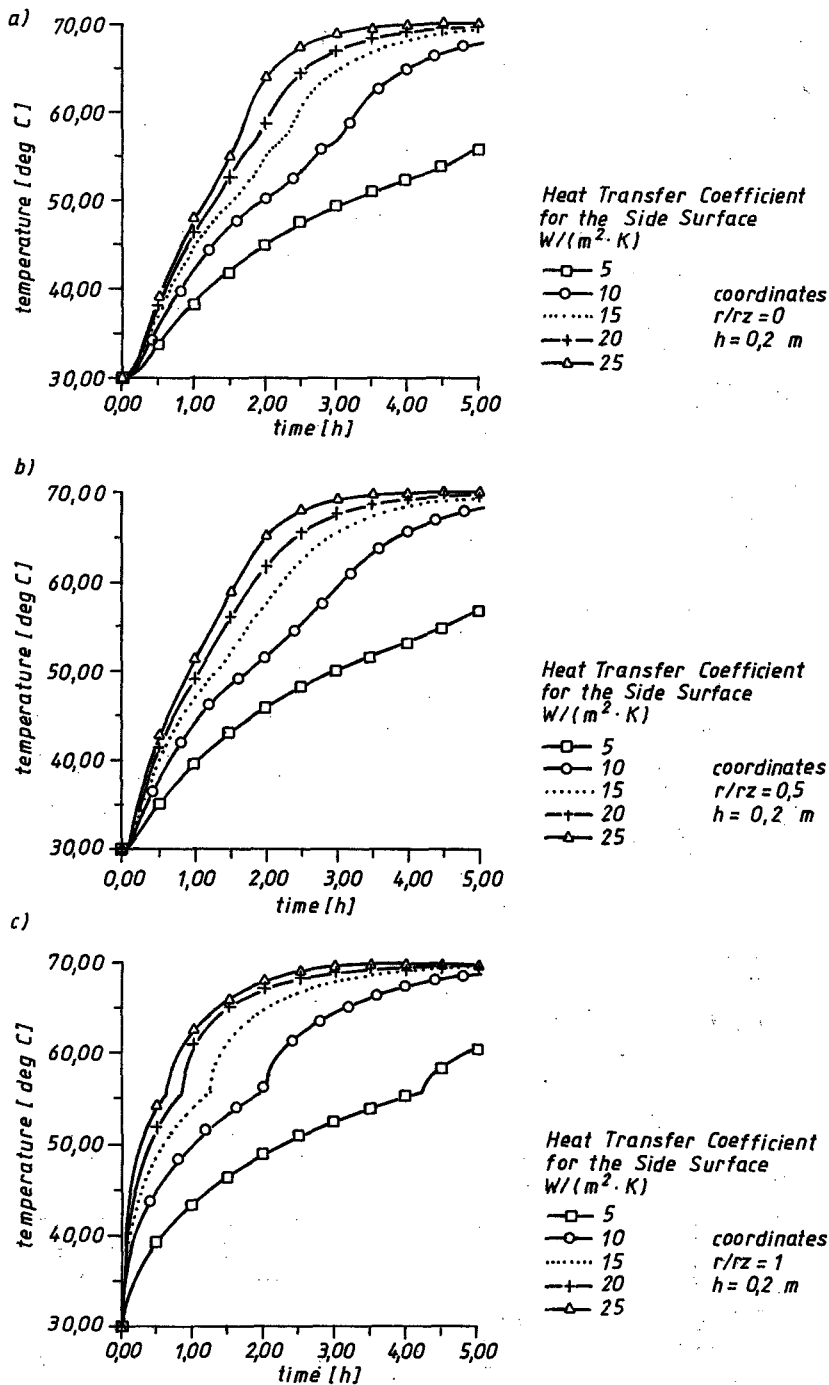


Fig. 5. The temperature distribution inside the cylindrical element (in the middle  $h = 0,2$ ) with PPW-20 for different heat transfer coefficients for side surface  $\alpha_s$ , and 3 points (a) symmetry axis  $r = 0$ , (b) in the middle of radius  $r/r_2 = 0,5$ , (c) surface of the boundary element  $r/r_2 = 1$

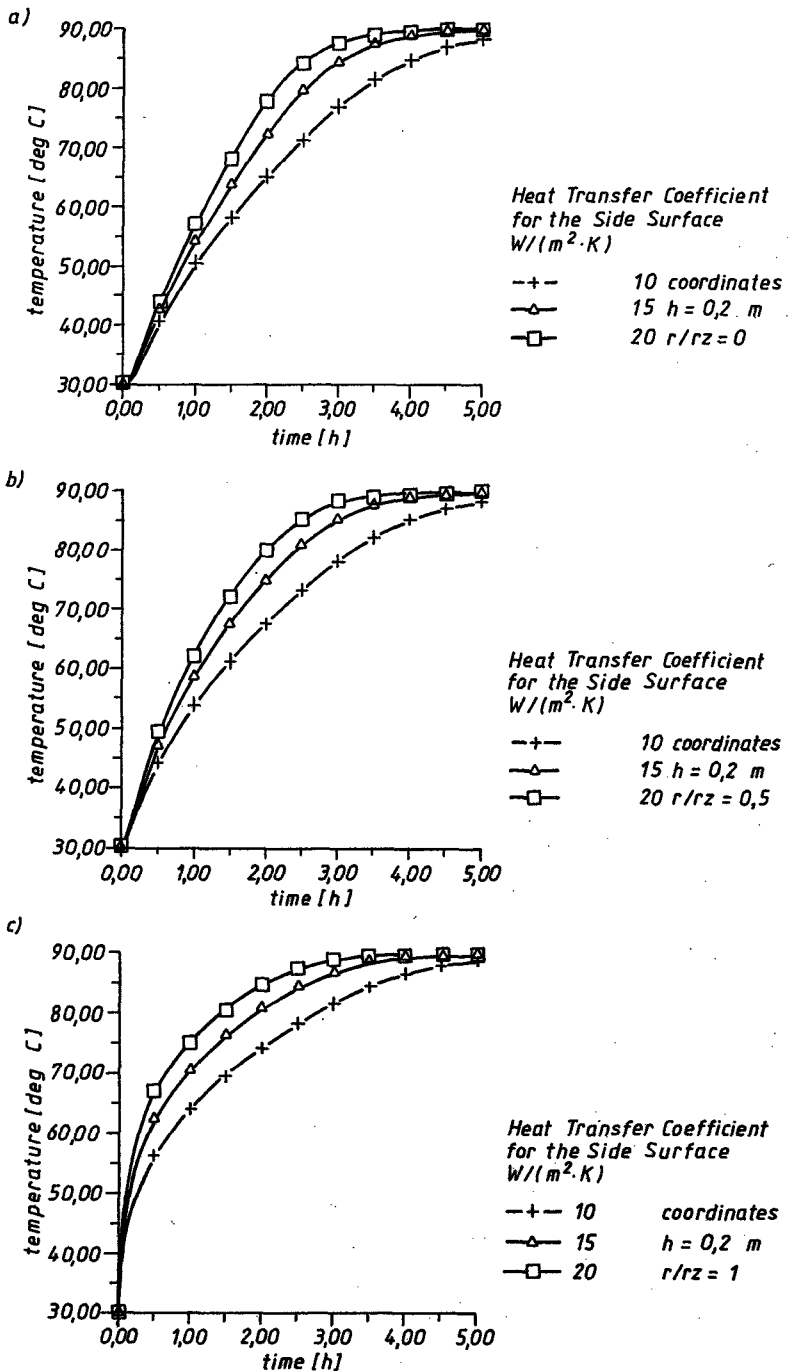


Fig. 6. The temperature distribution inside the cylindrical element (in the middle  $h = 0,2$ ) with REW-II for different heat transfer coefficients for lateral surface  $\alpha$ , and 3 points (a) symmetry axis  $r = 0$ , (b) in the middle of radius  $r/r_z = 0,5$ , (c) boundary element  $r/r_z = 1$



Figures 5 and 6 show the temperature-time history inside the cylindrical element with PPW-20 and REW-II for different heat transfer coefficients and 3 different points. It is shown that for high heat transfer coefficients temperature gradients inside the storage element are not so big. It also can be noticed that for very small heat transfer coefficients loading time is too long from practical point of view. Additionally, when the heat transfer coefficient is high enough, the loading time is almost constant. In that case it is not necessary to increase this value.

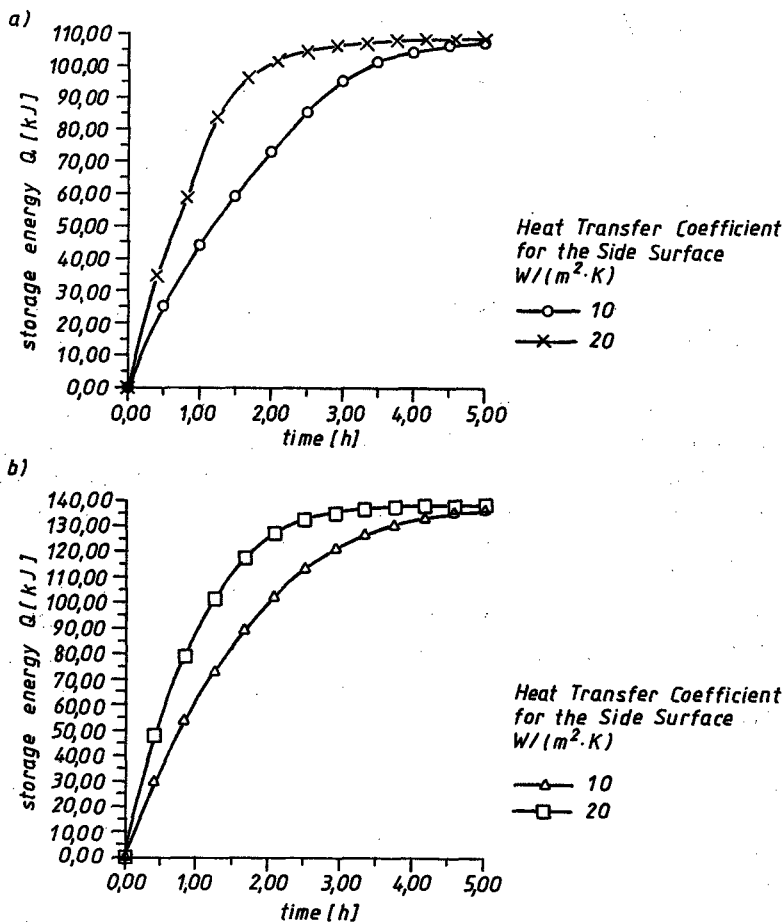


Fig. 7. Storage energy vs. charging time for cylindrical element with (a) PPW-20, (b) REW-II for two different heat transfer coefficients for side surface  $\alpha_s$ .

Figure 7 shows stored energy during charging time for the cylindrical element with two waxes. As it is shown amount of stored energy approaches the maximum energy  $Q_{\max}$  which is expressed:

$$Q_{\max} = \rho V \Delta i_{\max}$$

where:  $\rho$  – wax's density,  
 $V$  – volume of the storage element,  
 $\Delta i_{\max}$  – the maximum change of enthalpy.

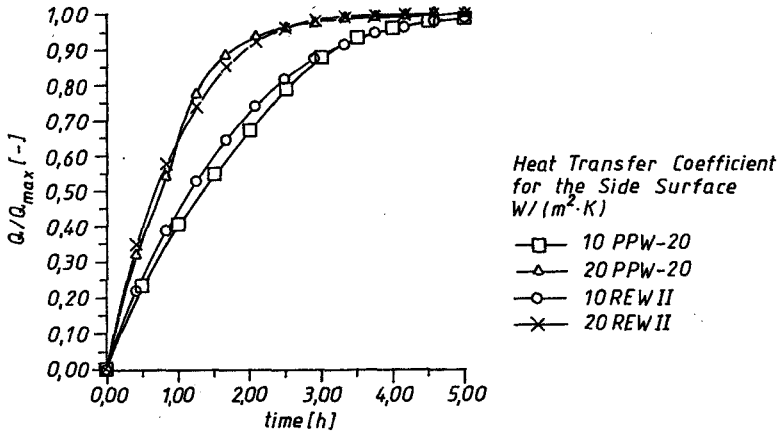


Fig. 8. Dimensionless storage energy ( $Q/Q_{\max}$ ) vs. charging time for cylindrical element with PPW-20 and REW-II for two different heat transfer coefficients for the side surface  $\alpha_s$ ,

Figure 8 shows dimensionless stored energy ( $Q/Q_{\max}$ ) vs. charging time for cylindrical element with PPW-20 and REW-II for two different heat transfer coefficients of lateral surface  $\alpha_s$ . It can be said that the storage element can be loaded very fast (in 2 hours) or very slowly (in 4 hours). It depends on boundary conditions – heat transfer coefficients. For both waxes charging time is very similar. Waxes can be used in many applications, especially in solar heat storage systems, because they work in the temperature range 25–150°C, are very stable and have a good performance. One of their disadvantages, low thermal conductivity, can be improved by embedding a metal matrix structure in the PCM [5].

## CONCLUSION

In this paper some aspects of thermal energy storage in a vertical, cylindrical element are discussed. The theoretical model of the diffusion phase change (without free convection in a melted region) has been analyzed numerically.

In order to determine the main parameters of TES system (such as its dimensions, mass of PCM, flow rate of heat transfer fluid and so on), it is necessary to use a computer program for determining the temperature fields of PCM in unsteady state of charging and discharging thermal energy storage in the cylindrical element. It was shown that waxes have very good thermal properties

for TES. In very short time the element with a wax can be completely charged. It is necessary to mention that these results have been checked by comparison with experimental results [4]. A good agreement has been achieved. Numerical simulation of 2-D and 3-D temperature field is a very powerful and useful tool for prediction of behavior of a single PCM storage unit and subsequently can be used as a tool for designing the storage system. It is useful to investigate waxes with different melting points (difference between the highest and the lowest melting point can be about 20°C) in order to use them in thermal storage units with wide range of the operating temperature. The energetic efficiency of such systems can be improved.

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## SYMULACJA NUMERYCZNA PROCESÓW PRZEWODZENIA CIEPŁA W POJEDYNCZYM ELEMENTCIE MAGAZYNUJĄCYM CIEPŁO W MATERIAŁACH ULEGAJĄCYCH PRZEMIANOM FAZOWYM

### Streszczenie

W artykule zaprezentowano krótki opis symulacji numerycznej modelu nieustalonego przewodzenia ciepła w materiale ulegającym przemianie fazowej (PCM), umieszczonym w pojedynczym elemencie magazynującym ciepło (problem Stefana – zjawisko topnienia i solidifikacji). Wybrano metodę entalpową – numeryczna dyskretyzacja różnicami skończonymi i schemat jawny kroczenia w czasie – do rozwiązania 3-D przewodzenia z przemianą fazową. Wyniki obliczeń numerycznych trójwymiarowego pola temperatury przedstawiono dla grzanego materiału (PCM) w pojedynczym cylindrze.

## **ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ПРОЦЕССОВ ТЕПЛОПРОВОДНОСТИ В ОТДЕЛЬНОМ ЭЛЕМЕНТЕ СОБИРАЮЩЕМ ТЕПЛО В МАТЕРИАЛАХ ПОДВЕРГАЮЩИХСЯ ФАЗОВЫМ ПРЕВРАЩЕНИЯМ**

### **Краткое содержание**

В работе представлена численная модель нестационарной теплопроводности с фазовым превращением материала (условие Стефана – явление плавления и затвердевания).

Объектом анализа является вальцовый элемент системы аккумулирующей тепло, использующей тепло фазового перехода.

Эта трехмерная задача теплопроводности была решена с помощью метода конечных разностей и баланса энергии. Представлены результаты численных расчетов нестационарного поля температуры в исследованном элементе.