Numerical study of heat transfer in macro-encapsulated phase change material for thermal energy storage

D. B. Dzhonova-Atanasova[1*], A. G. Georgiev[2,4], R. K. Popov[3]

[1]*Institute of Chemical Engineering, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., Bl. 103, 1113, Sofia, Bulgaria.*
[2]*Faculty of Mechanical Engineering, Technical University - Sofia, Plovdiv Branch, 25 Tsanko Diustabanov Str., 4000 Plovdiv, Bulgaria*
[3]*Faculty of Physics, Plovdiv University "Paisii Hilendarski", 24 Tzar Assen Str., 4000 Plovdiv, Bulgaria*
[4]*European Polytechnic University, Dept. of "Green Energy", 23 Kiril and Metodiy str., 2300 Pernik, Bulgaria*

The successful development and implementation of systems using renewable energy sources, which are usually of intermittent character, require cheap and effective thermal energy storing for diurnal or seasonal heat accumulation. Thermal accumulators are also used for increasing the efficiency of conventional fuel dependent systems by storing the waste heat in low consumption periods. Much of the efforts are directed towards creation of compact solutions to replace the presently used hot water tanks requiring very large space. This is especially important for small capacity thermal systems in buildings. There are a lot of suggestions in literature using the latent heat of phase change materials (PCM), but only a few close to commercial stage of implementation. A heat accumulator with paraffin as a PCM is a cost effective innovative solution for low grade heat storage. One of the design approaches is encapsulation of the phase change material in containers with a variety of shapes and materials. The aim of the present work is a 3D numerical simulation of the phase change process in a stainless-steel container filled with commercial E53 paraffin. This is a part of a study directed towards design optimization of a hybrid solar installation with thermal storage. The focus is on development and testing of a time effective method for numerical prediction of the thermal behaviour of the container with paraffin and assessment of the factors influencing the heat transfer process prior to the physical experiment.

Keywords*: latent thermal energy storage, phase change material, paraffin, macro-encapsulation, CFD modelling*

INTRODUCTION

Heat accumulation is a key problem for balancing the discrepancy between energy demand and production from renewable and conventional energy sources. The storage technology using the latent heat of paraffin phase change is under intensive investigation and development. Its main shortcomings are relatively low specific heat capacity, low heat transfer coefficient of the paraffin, and high exergy losses.

Advantages of encapsulation

Paraffins are often used as a phase change material in thermal storage systems due to their availability, suitable phase change temperature range, low cost, and non-corrosiveness. Paraffin wax consists of straight-chain n-alkanes, the crystallisation of which releases a large amount of heat, the melting and solidification temperature increasing with the chain length [1]. The disadvantages of the paraffin for heat storage are low thermal conductivity, non-compatibility with plastic containers and moderate flammability. The encapsulation of the paraffin in containers fights the undesirable effects. It increases the heat transfer area, reduces the reactivity towards the outside environment and controls the volume changes during phase transition.

Over 200 potential phase change heat storage materials (including paraffins) suitable for encapsulation, melting from 10 to 90°C, are reported by Lane [2, 3].

Effect of encapsulation size and geometry

The design of the containers should ensure complete melting or solidification of the PCM in a period corresponding to the energy availability for charging mode and the energy consumption for discharging mode in diurnal or seasonal storage.

Based on size, the PCM encapsulation is classified into nano (0–1000nm), micro (0–1000 µm), and macro (above 1mm) encapsulation.

The present work focuses on the design of containers for macro-encapsulation. The cheapest containers used for that purpose are tin cans and plastic bottles. A variety of containers' shapes and materials are discussed in [1]. The container may be spherical [4, 5], tubular, cylindrical or rectangular [6, 7]. As for the container material, the metallic containers are preferred, when high heat transfer rate should be achieved, else plastic containers are widely used. In both cases the PCM should not react with the container material.

* To whom all correspondence should be sent:
  dzhonova@bas.bg

The improvement of the heat transfer rate with various container geometries including sphere, cylinder, plate and tube was studied in [8] by numerical and experimental techniques. The spherical shape was reported to achieve the highest heat transfer rate. For other geometries, it decreased in the order of cylinder, plate and tube [8].

A large improvement in the heat transfer rate was obtained in a packed bed storage unit with small plastic spheres with PCM [4, 5] at the expense of high pressure drop in the packed bed and high initial cost.

The commercialization of encapsulated PCM based systems is connected with overcoming the following main challenges [9]:

(1) High cost of encapsulation connected with proper selection of the shell material, encapsulation method and size according to the application;

(2) Decreased system performance after a certain number of thermal cycles because of deterioration of the thermo-physical properties, leading to reduction in structural and thermal stability of the PCM;

(3) Precise prediction of thermal behaviour of heat storage, connected with calculating the moving solid liquid boundary during the phase change process.

Results and conclusions on the thermal behaviour of PCM enclosed in rectangular containers were reported in [10, 11]. The numerical simulation in [10] compared the effect of cylindrical and rectangular containers on the performance of air heat energy storage. It showed that at equal PCM volume and heat transfer area, the rectangular container required half of the melting time of the cylindrical container. Therefore in that case it is preferable to use rectangular containers for PCM encapsulation. The melting and solidification of PCM in rectangular containers was simulated in [11] for studying the following effects: effect of the working fluid temperature on the melting behaviour of $CaCl_2.6H_2O$ and paraffin wax C18; effect of the working fluid convection coefficient; effect of the container thickness; effect of the mass of macro-encapsulated PCM. It was found that the time for complete melting was inversely proportional to the temperature and the convective heat transfer coefficient of the heat transfer fluid (HTF); the rectangular encapsulated $CaCl_2.6H_2O$ could store much more energy than C18 paraffin with the same volume, but with longer melting time; the usage of salt hydrates could save space and cost since less volume and consequently less number of blocks were needed to provide the

required storage capacity compared to paraffin wax because of the higher volumetric energy storage density of the inorganic PCMs.

The aim of the present work is to develop a fast numerical method for prediction of the thermal behaviour of PCM enclosed in a container with a specific geometry, designed as an active element in a test thermal accumulator at the Technical University Sofia, Plovdiv Branch, Fig.1 [12]. The HTF is water entering from three tangential inlet pipes at the top of the tank and leaving from three tangential outlet pipes at the bottom. This device is a part of an experimental thermal solar installation with heat storage. The typical HTF inlet temperature is $65^{o}C$ (from the solar collector) in charging mode and $15^{o}C$ (tap water) in discharging mode.

The purpose of the present numerical simulation is to assess prior to the physical experiment the effect on the phase change process of the following factors: external temperature, HTF convection coefficient and natural convection inside the container.
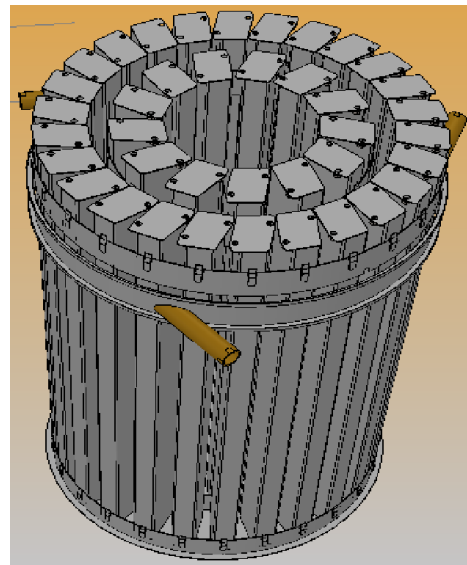

Fig.1. Inner construction of the latent thermal storage of the experimental thermal solar installation [12]

NUMERICAL EXPERIMENT

Numerical Model

The accepted approach for modelling the solidification/melting process is the enthalpy-porosity technique proposed in [13], employed in ANSYS Fluent [14]. This approach avoids tracking explicitly the melt interface. The fraction of the cell volume which is in liquid form, called the liquid fraction, is computed at each iteration based on the

enthalpy balance. The mushy zone, where the liquid fraction lies between 0 and 1, is modelled as a "pseudo" porous medium in which the porosity in each cell is set equal to the liquid fraction and decreases from 1 to 0 as the material solidifies, and hence the velocity drops to zero for solid state.

The transient thermal behavior of a single container with paraffin, a constituent part of the accumulator in Fig. 1, is considered. The mesh of the 3D computational domain comprises 26 000 tetrahedral elements. For the phase change process of the PCM in the container, the density difference between the solid and liquid phase is assumed negligible. The natural convection is expected to play an important role especially in a tall vertical tube like the unit under consideration, Fig. 1. The buoyant forces are modelled by the Boussinesq approximation; the reference temperature is equal to the melting temperature. The liquid phase of the PCM is assumed to be Newtonian and incompressible and the flow is laminar. In charging/discharging process, the governing equations for the liquid PCM [14] can be written as:

Continuity equation:
$$\nabla \boldsymbol{v} = 0. \tag{1}$$

Momentum equation:
$$\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \nabla(\rho \boldsymbol{v}\boldsymbol{v}) = -\nabla p + \nabla \boldsymbol{\tau} + \rho \boldsymbol{g} + \boldsymbol{F}, \tag{2}$$

where $\boldsymbol{v}$ is the velocity vector, p is the static pressure, $\boldsymbol{\tau}$ is the stress tensor and $\rho \boldsymbol{g}$ and $\boldsymbol{F}$ are the vectors of gravitational and external body forces.

The momentum sink due to the reduced porosity in the mushy zone takes the following form:

$$\boldsymbol{S} = \frac{(1-\beta)^2}{(\beta^3+\varepsilon)} A_{mush} \boldsymbol{v}, \tag{3}$$

where β is the liquid volume fraction, ε is a small number (0.0001) to prevent division by zero, $A_{mush} = 10^5$ is the mushy zone constant.

Energy equation:
$$\frac{\partial}{\partial t}(\rho H) + \nabla(\rho \boldsymbol{v} H) = \nabla(k\nabla T). \tag{4}$$

The enthalpy H consists of sensible enthalpy h and latent heat ΔH

$$H = h + \Delta H, \tag{5}$$

where $h = h_{ref} + \int_{T_{ref}}^{T} c_p dT$,

$\Delta H = \beta L$.

The latent heat content can vary between zero for solid and L for liquid. The liquid fraction can be defined as:

$\beta = 0$ if $T < T_s$

$\beta = 1$ if $T > T_l$

$\beta = \frac{T - T_s}{T_l - T_s}$ if $T_s < T < T_l$,

where T_s and T_l are solidus and liquidus temperatures respectively.

Table 1 gives the values of the thermo-physical properties of the paraffin used in the calculations. The accepted constants are based on the data from [15] concerning E53 paraffin. The model does not take into account the experimental observations [15] that the paraffin properties depend on the temperature and the physical state. Moreover, according to the literature data [15], E53 paraffin undergoes two-step phase transition, the lower temperature transition is solid–solid (order-disorder) transition, while the higher temperature transition represents the solid-liquid phase change process. The present model assumes that in heating and cooling only solid–liquid transition occurs over the higher temperature range of 52-59°C, yet the accepted value of the latent heat is the cumulative value of the two steps.

The container, made of stainless steel, is placed vertically, Fig.1, and its external dimensions are 40x80x950mm, the wall thickness is 1.5mm. The thermal accumulator in Fig. 1 is a part of an experimental hybrid solar system with heat storage. The equations are solved using the CFD software ANSYS FLUENT 13.0, based on finite volume technique. The following boundary conditions are assumed: no-slip conditions at the container's wall and constant temperature at all external surfaces $T = T_{wall}$. In charging mode the initial conditions are solid PCM with temperature $T_{in} = 51$°C, one degree lower than the solidus temperature, given in Table 1, in discharging mode $T_{in} = 60$ °C, one degree higher than the liquidus temperature, Table 1.

The details of the employed solution methods are as follows: (1) SIMPLE scheme of pressure-velocity coupling; (2) spatial discretization: Green-Gauss cell based for gradient, PRESTO for pressure, first order upwind for momentum and energy; (3) first order implicit transient

formulation. The under relaxation factors assumed for solution controls are: 0.3 for pressure, 1 for density and body forces, 0.2 for momentum, and 0.9 for liquid fraction update. For convergence absolute criteria, the values of the scaled residuals are: 10^{-4} for the continuity and velocity and 10^{-6} for the energy equation.

Table 1. Paraffin thermo-physical properties used in the calculations

Solidus temperature, E53 [15], T_s, °C	52
Liquidus temperature, E53 [15], T_l, °C	59
Density(solid), E53 [15], kg/m³	920
Dynamic viscosity, kg/ms	0.003
Specific heat (solid), E53 [15], J/kgK	1550
Thermal conductivity (solid), E53 [15], W/mK	0.34
Latent heat of fusion, E53 [15], J/kg	194110
Thermal expansion coefficient, 1/K	0.0001

Model verification

Similar set of ANSYS Fluent solution methods and settings was used in [16]. The computational model was experimentally verified by comparing the simulation results with experimental data for melting of paraffin wax n-octadecane (28.2°C melting temperature) encapsulated in a spherical container of glass with inside diameter of 101.66 mm. It was found that the prediction of the overall melting process was satisfactory, though the simulation suggested some faster melting rate than the experiment [16].

RESULTS AND DISCUSSION

Macro-encapsulated E53 paraffin in a stainless steel container was considered as an active unit for thermal energy storage. The simulation studied the thermal behaviour of the unit at various temperatures of the external surfaces of the container, T_{wall}=15°C for discharging mode, T_{wall}= 65°C and 80°C for charging mode. All the surfaces were at constant temperature. Fig.2 shows the contour plots of the liquid fraction at 10, 15 and 20 min of the charging process in the middle-width plane parallel to the 80 mm face of the container. After 20 min charging the liquid fraction is 88%, and due to the buoyant forces the paraffin is stratified, liquid at the top, solid at the bottom. The stratification is illustrated by the contour plots of the temperature in Fig.3a. It can be seen in Fig.3b from the contour plots of the velocity y-component that, due to natural convection, there is an upward

flow along the side walls of the container, and a downward flow in the central volume. Therefore, the convective heat transfer, often neglected in the simulations, affects substantially the picture of the melting process. However, as expected, it has negligible effect on the solidification in the container. This is illustrated by the identical patterns in the upper and bottom halves of the container in Fig.4, which presents solidification at 15°C of the external surfaces after 10min, 15min and 20min. This picture confirms that the natural convection in the container should be taken into consideration when organizing the fluid flows in the accumulator. Tan et al. [16] computationally and experimentally demonstrated that while conductive heat transfer was dominant in the initial stage of the phase change process, natural convection became dominant with the progress of the melting process. Ettouney et al. [17] found that natural convection was dominant during melting for upward flow of HTF and negligible for downward flow. It was observed there that the solidification process was dominated by conduction and independent of flow direction of HTF.
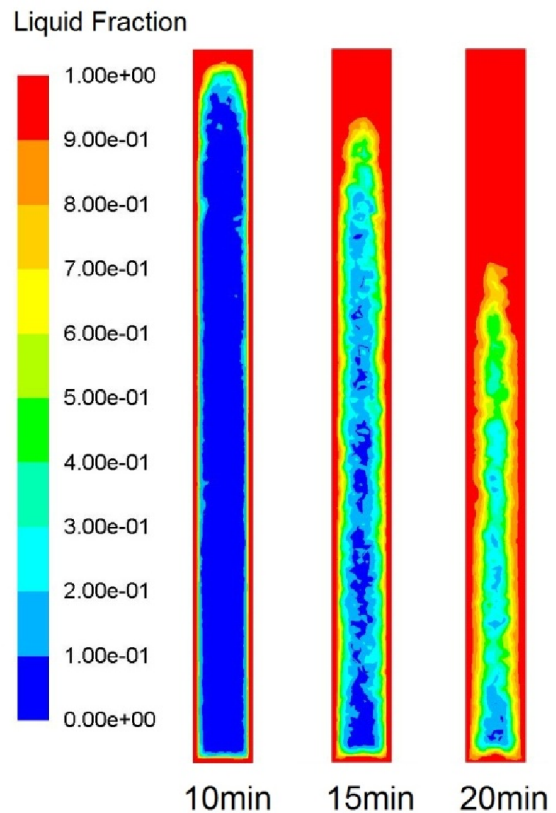

Fig.2. Contours of liquid fraction in the middle-width plane parallel to the 80 mm face, in charging at T_{wall} = 80 °C
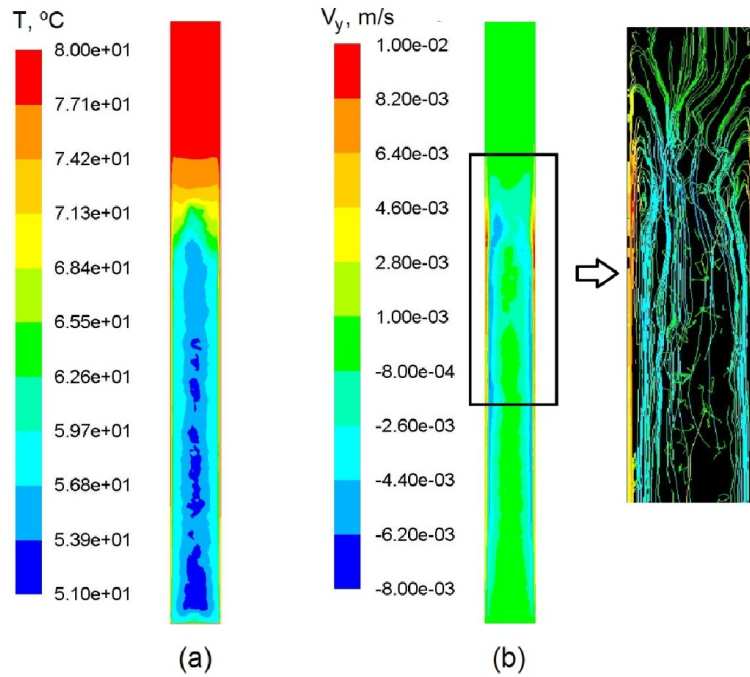
Fig.3. Contours of temperature T (a) and y-component of velocity v_y (b) in the middle-width plane parallel to the 80 mm face, in charging after 20 min at T_{wall}=80°C
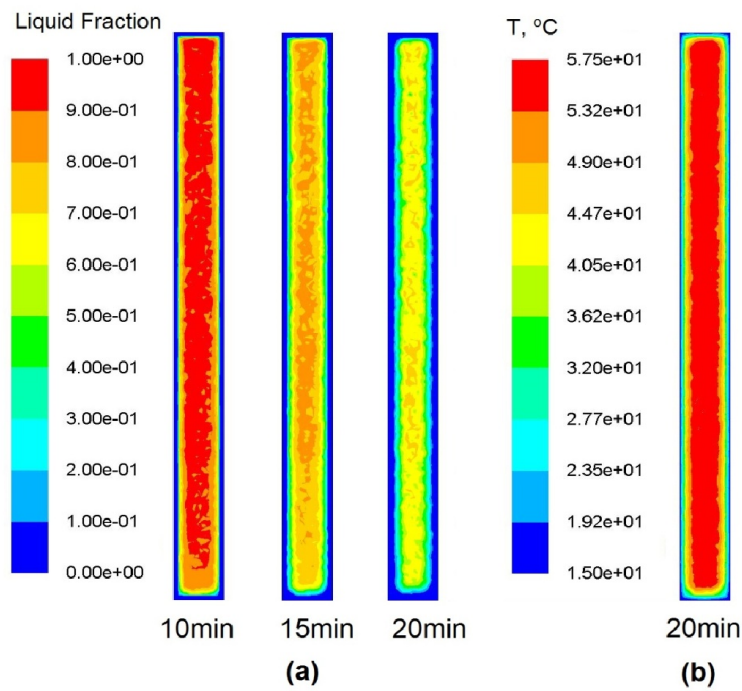

Fig.4. Contours of liquid fraction (a) and temperature T (b) in the middle-width plane parallel to the 80 mm face, in discharging at T_{wall}=15°C

Fig.5 illustrates the effect of the external temperatures on the duration of the phase change process. During the phase transition, the liquid fraction in the total volume of the container lies between 0 when the total volume is in solid state and 1 when the total volume is in liquid state. A simulation was performed at a constant heat flux through the wall with a convective heat transfer coefficient α=3000 W/m²K, calculated by the relation [18] for laminar boundary layer of water flow on a flat surface at a bulk fluid temperature T_{fl}=65°C. The results in Fig.5 in that case coincide with those calculated at a constant wall temperature T_{wall}=65°C. The explanation is that the thermal

resistance at the fluid-solid interface is low and the temperature difference between the fluid bulk and the solid surface of the container is negligibly small. The same was the reason for the observations in [11], where it was demonstrated that the storage material melting time was inversely proportional to the air convective heat transfer coefficient. However, it had major effect at lower values (10 and 15 W/m^2K, [11]) and less effect at higher convection coefficients (30 and 35 W/m^2K, [11]).
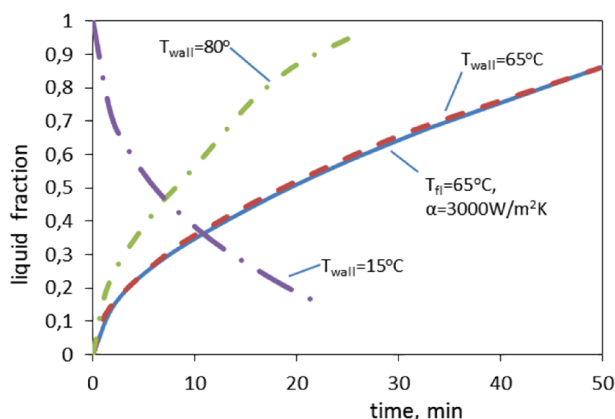

Fig.5. Computed liquid fraction in the total PCM volume (0 when the total volume is in solid state and 1 when the total volume is in liquid state) versus time in the phase change process

CONCLUSIONS

The present simulation has obtained the flow pattern and temperature distribution in macro-encapsulated paraffin inside a rectangular container with specific dimensions designed as an active unit in a test heat accumulator of a thermal solar system. It demonstrates the effects on the melting/solidification process of the external temperature, the HTF conduction coefficient and the natural convection inside the PCM. A time efficient method using the ANSYS Fluent techniques for prediction of phase change processes has been tested. The calculated results correspond to the observations in the literature about the factors affecting PCM encapsulation. The simulations add information for better understanding and more precise prediction of the phase change process, which is necessary for the design of thermal energy storage systems.

REFERENCES:

1 A. Sharma, V.V. Tyagi, C.R. Chen D. Buddhi, Review on thermal energy storage with phase change materials and applications, *Renewable and Sustainable Energy Reviews* 13, 318–345 (2009)

2 G.A. Lane, Encapsulation of heat of fusion storage materials. In: Proceedings of 2nd Southeastern *Conference on Application of Solar Energy*, 442–50 (1976).

3 G.A. Lane, Low temperature heat storage with phase change materials. *Int J Ambient Energy* 1, 155–68 (1980).

4 R.J. Wood, S.D. Gladwell, P.W.O. Callahar, S.D. Probert, Low temperature thermal energy storage using packed beds of encapsulated phase-change materials. In: *Proceedings of the International Conference on Energy Storage*, Brighton, UK, 145–58 (1981)

5 T. Saitoh, K. Hirose, High-performance of phase change thermal energy storage using spherical capsules. *Chem. Eng. Commun.* 41, 39–58 (1986)

6 /www.pcmproducts.net/

7 /www.rubitherm.com.

8 J. Wei, Y Kawaguchi, S Hirano, H. Takeuchi, Study on a PCM heat storage system for rapid heat supply, *Applied Thermal Engineering* 25, 2903–20 (2005).

9 P. B. Salunkhe, P. S. Shembekar, A review on effect of phase change material encapsulation on the thermal performance of a system, *Renewable and Sustainable Energy Reviews* 16 5603–16 (2012)

10 B. Zivkovic, I. Fuji, An analysis of isothermal phase change material within rectangular and cylindrical containers, *Solar Energy* 70, No. 1, 51–61 (2001)

11 M. Jradi, M. Gillott, S. Riffat, Simulation of the transient behaviour of encapsulated organic and inorganic phase change materials for low-temperature energy storage, *Applied Thermal Engineering* 59, 211-222 (2013)

12 A. Stoyanov, A. Georgiev, R. Popov, Experimental installation for investigation of latent heat accumulator as a part of hybrid system for air-conditioning, *Toplotehnika,* Tech. Univ. Varna 4, 2, 28 (2013)

13 V. R. Voller, C. Prakash, A fixed-grid numerical modelling methodology for convection-diffusion mushy region phase-change problems. *Int. J. Heat Mass Transfer* 30, 1709–20 (1987).

14 Theory Guide ANSYS Fluent v. 13.0.

15 E. M. Anghel, A. Georgiev, S. Petrescu, R. Popov, M. Constantinescu, Thermo-physical characterization of some paraffins used as phase change materials for thermal energy storage, *J Therm. Anal. Calorim.*, 117, 557–566 (2014)

16 F.L. Tan, S.F. Hosseinizadeh, J.M. Khodadadi, L. Fan, Experimental and computational study of constrained melting of phase change materials (PCM) inside a spherical capsule, *International Journal of Heat and Mass Transfer* 52, 3464–72 (2009)

17 H. Ettouney, H El-Dessouky, E. Al-Kandari, Heat transfer characteristics during melting and solidification of phase change energy storage process, *Industrial and Engineering Chemistry Research* 43, 5350–7 (2004)

18 J. H. Leinhard IV, J .H. Leinhard V, A heat transfer textbook, 3rd ed. Cambridge MA, Phlogiston press (2008)