Numerical simulation of thermal energy storage based on phase change materials

A. Seitov[1], B. Akhmetov[1*], A. G. Georgiev[2,5], A. Kaltayev[1], R. K. Popov[3], D. B. Dzhonova-Atanasova[4], M. S. Tungatarova[1]

[1]*Al-Farabi Kazakh National University, Almaty, 050000, Kazakhstan*
[2]*Technical University of Sofia, Plovdiv Branch, Dept. of Mechanics, 25 Tsanko Diustabanov Str, 4000 Plovdiv, Bulgaria*
[3]*Faculty of Physics, Plovdiv University "Paisii Hilendarski", 24 Tzar Assen Str., 4000 Plovdiv, Bulgaria*
[4]*Institute of Chemical Engineering, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., Bl. 103, 1113, Sofia, Bulgaria*
[5]*European Polytechnic University, Dept. of "Green Energy", 23 Kiril and Metodiy str., 2300 Pernik, Bulgaria*

One of the main problems related to the application of thermal energy gained from renewable energy sources is the absence of effective storage system. If we could store, for instance, solar thermal energy which is harnessed during day time, it would be possible to use it at night for space heating, ventilation, air conditioning or hot water systems. Therefore, this paper reports on the numerical analysis of heat transfer and fluid flow processes in a thermal energy storage based on phase change material designed and developed by the authors. Such study is very important in understanding of advantages and disadvantages of the design features and efficiency of the latent heat storage.

Keywords: phase change materials, thermal energy storage, latent heat storage

INTRODUCTION

Various studies indicate that built environment significantly contributes to global energy consumption and production of greenhouse gases. Within built environment, buildings consume about 40% of world's total energy and contribute to release of greenhouse gases up to 35% [1]. There are many energy consumers in buildings. But, heating ventilation and air conditioning (HVAC), and domestic hot water (DHW) systems are generally responsible for significant proportion of total building energy consumption [2].

According to the energy consumption breakdown of buildings [3], typical HVAC and DHW systems accounts for approximately 55% of total energy consumption for residential, and 35 % for non-residential buildings (Table 1). Therefore, developing carbon free heat storage that can provide thermal energy to HVAC and DHW systems of buildings is very important in terms of efficiency and environmental safety.

Renewable energy sources show significant promise in assisting to preserve many of the natural resources that we currently use as sources of energy for built environment, decrease the amount of toxins, by-products of energy use and keep the planet clean for future generation. Unlike many other renewable energy sources, solar power is by far the cleanest and it has a large potential for heating/ cooling of buildings, providing hot water, etc. Unfortunately solar energy value is periodic and unpredictable - for better use it must be accumulated into storage for further utilization [4].

Table 1. Breakdown of building energy use [3]

Residential Energy Use	Commercial Energy Use
1% – Computers	2% – Cooking
5% – Cooking	3% – Computers
5% – Wet clean	4% – Refrigeration
7% – Electronics	6% – Officeequipment
8% – Refrigeration	6% – Ventilation
11% – Lights	26% – Lighting
12% – Cooling	13% – Cooling
12% – Water heat	7% – Water heat
31% – Heating	14% – Heating

Thermal energy storage plays important role in effective application of gained thermal energy from renewable energy sources [5]. It permits to equalize instantaneous differences between demand and supply of thermal energy using off-peak excess energy which may be lost otherwise.

Among the methods for heat accumulation, thermal storage in the form of latent heat is very attractive one [6]. Latent heat storage relies on storage materials which absorbs/ releases heat while undergoes phase transition. Such PCMs has higher energy storage density and narrower temperature range between storing and releasing heat compared to sensible heat storage. Among PCMs which can be used for heating/ cooling and hot water systems of buildings, materials such as

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* To whom all correspondence should be sent:
eng.akhmetov@gmail.com

paraffin or molten salt have been considered as the most appropriate material for heat storage due to their efficient thermal properties. Thus, using latent heat storage filled with PCM gives opportunity to develop effective daily thermal energy supplier for HVAC and DHW systems [7].

The co-author, Prof. A. Georgiev and his team from the Technical University of Sofia, Plovdiv Branch, designed and developed latent heat storage (Fig.1). Aim of the current study is concentrated on numerical analysis of heat transfer and fluid flow processes during charging and discharging regimes of the latent heat storage. Such study is very important in understanding of advantages and disadvantages of the design features of the latent heat storage and its efficiency.

Fig.1. Latent heat storage [8]

DESCRIPTION OF THERMAL ENERGY STORAGE AND PHASE CHANGE MATERIALS

Detailed illustration of the latent heat storage and its design features are shown in Fig.2. PCM containers have rectangular cross section with dimensions 950 x 80 x 50 mm. They are placed into the vertical cylinder tank (storage) with 1 m height and 0,3 m radius [8]. The tank and containers are made of stainless steel grade AISI 304L. Number of PCM containers are 39 and they are located coaxially in the storage. There are two concentric circles: external circle contains 26 containers and the inner circle has 13 containers. All the containers are fixed with brackets to the lower and upper parts of the storage tank in order to make them stable during charging and discharging regimes. There are three inlet pipes in the upper side of the storage where the heat carrier fluid flows into the storage. In the base of the storage other three pipes are

connected to the storage to discharge the heat carrier fluid from the storage. The storage is insulated by wrapping with glass wool from the outside.
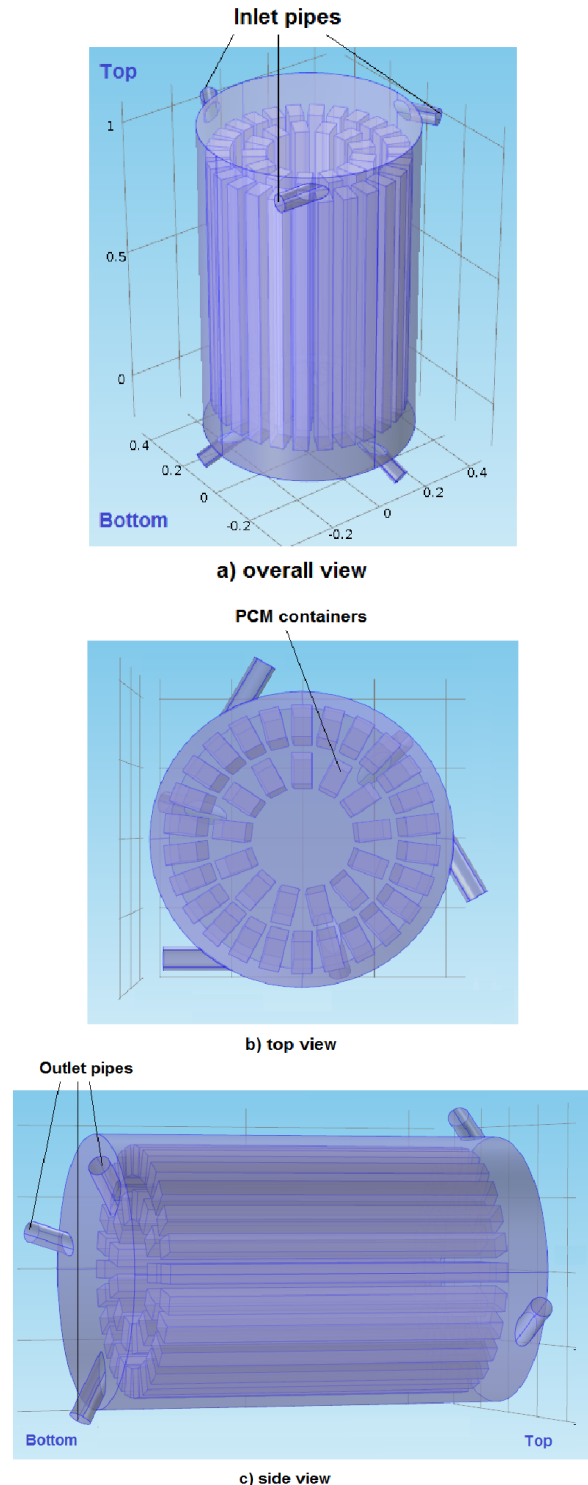

a) overall view

b) top view

c) side view

Fig.2. Design features of the latent heat storage

As a phase change material for the latent heat storage, we used paraffins. Paraffin is considered as effective heat storage material because of its large latent heat of melting (200 kJ/kg or 150 MJ/m³), thermal stability, negligible subcooling, non-toxic,

and low price. There are different types of paraffins. For instance, paraffin waxes, C_nH_{2n+2}, are chain polymers which crystallize in lamellar form. Consequently, properties such as phase change temperature, latent heat, density, and specific heat capacity are particular for each paraffin wax [9].

Bulgarian team and their colleagues studied thermophysical properties of three phase change paraffinic materials by means of differential scanning calorimetry (DSC). Aim of the experimental study was to thermophysically characterize two commercial paraffin waxes (E53 and E46), and a commercial paraffin-ceresine composite (ECP).

Table 2. Phase change temperatures and latent heat of E53, E46, and ECP paraffin samples [9]

| PCM	Cycle	T_{on},°C	T_{max},°C	T_{off},°C	ΔH, J/g
E53	Heating	33.07	39.83	45.33	194.32
		51.79	56.4	59.22	
	Cooling	59.41	57.01	51.93	-194.11
		44.36	39.76	33.02	
E46	Heating	46.67	56.57	61.78	176.77
	Cooling	59.54	56.99	47	-165.69
ECP	Heating	43.85	54.21	64.00	143.891
	Cooling	63.39	55.51	34.03	-142.9

Thermal properties obtained with DSC during heating/ cooling cycle of the three PCMs are presented in Fig.3 and Table 2. It can be seen from Fig.3 that E46 and ECP samples have single peaks while E53 sample has two peaks during heating/cooling process. Indeed, paraffins undergo multiple phase transitions. At lower temperatures phase transition occurs in the form of solid-solid while at higher temperatures solid-liquid melting process takes place. Therefore, latent heat values in Table 2 includes both solid–solid and solid–liquid phase transitions. Thus, obtained thermophysical properties of these paraffinic PCMs will be used for numerical studies.

## MATHEMATICAL FORMULATION OF PHYSICAL PROCESSES IN LATENT HEAT STORAGE

Equations

Simulation is conducted in three dimensional space in a time dependent manner by means of finite element method based on Comsol multiphysics. The geometry used to perform the simulation of charging and discharging of LHS is presented in Fig.2. The containers which enclose

PCM (e.g. paraffins) are thermally insulated at the top and bottom. Moreover, it is assumed that the volume of the PCM does not change during phase transition. Such assumption, allows to introduce simpler mathematical models [10], although, according to the experimental investigations, paraffins change their volume during melting or solidification [9]. Moreover, to avoid intensive numerical calculations, the containers are considered as highly conductive layers [11]. Meshing of PCM containers are shown in Fig.4.
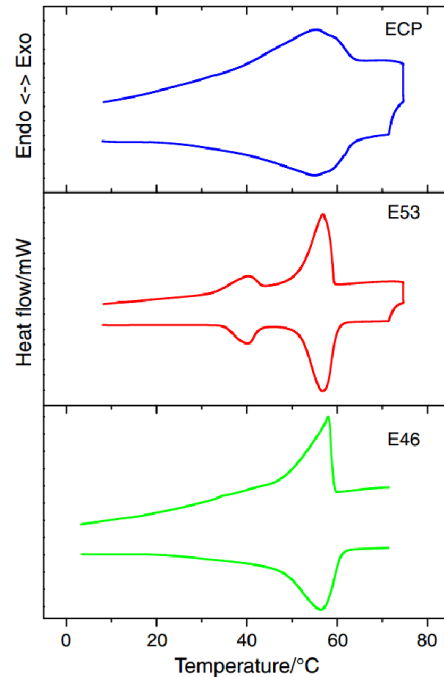
Fig.3. Temperature change of E53, E46, and ECP paraffin samples during heating and cooling cycles at a rate 10°C /min [9]
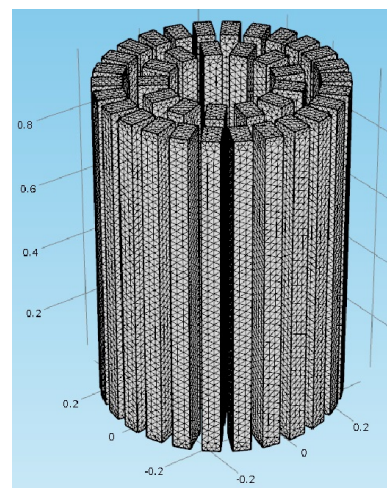
Fig.4. Meshing of the containers with PCM

In order to simulate the dynamic behaviour of the heat carrier fluid flowing inside the LHS, the continuity and Navier-Stokes equations must be

solved simultaneously. Continuity equation takes the form [12]:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \qquad (1)$$

where ρ - density, kg/m³ and u - velocity, m/s. The Navier-Stokes equation which accounts for the conservation of the momentum is given by [12]:

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u = -\frac{1}{\rho}\nabla p + \nu \nabla^2 u + F \qquad (2)$$

where p - pressure in the fluid, Pa, ν - kinematic viscosity, m²/s.

Heat transfer from the water to the wall of the PCM containers takes place in the form of convection. Therefore, complete energy equation has to be solved by using the velocity field obtained from the solutions of Eqns. (1) and (2). Thus, the energy equation describing the heat transfer process is given by [13]:

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p u \cdot \nabla T = \nabla \cdot (k \nabla T) \qquad (3)$$

c_p - specific heat capacity, J/kgK; k - thermal conductivity of the material, W/mK, T- temperature of the heat carrier fluid, °C. Meshing of the domain between storage vessel and PCM containers, where Eqns. (1)-(3) are solved are illustrated in Fig.5.
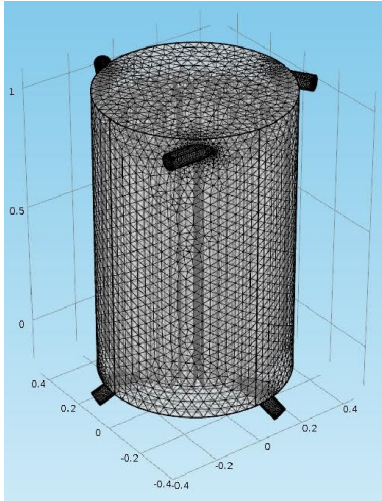

Fig.5. Meshing of the latent heat storage

The energy equation for the phase change material including latent heat transfer during phase change is [14]:

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p u \cdot \nabla T = \nabla \cdot (k \nabla T) \qquad (4)$$

$$k = \theta_1 k_{phase1} + \theta_2 k_{phase2} \qquad (5)$$

$$c_p = \theta_1 c_{p,phase1} + \theta_2 c_{p,phase2} + L\frac{d\alpha}{dT} \qquad (6)$$

$$\rho = \frac{\theta_1 \rho_{phase1} c_{p,phase1} + \theta_2 \rho_{phase2} c_{p,phase2}}{\theta_1 c_{p,phase1} + \theta_2 c_{p,phase2}} \qquad (7)$$

where $\theta_1 = 1 - \alpha$ and $\theta_2 = \alpha$ corresponds to phase 1 and phase 2 respectively. Moreover, L is the latent heat of phase change and α is the liquid volume fraction in the phase change material and it is a function of temperature:

$$\begin{aligned} \alpha &= 0 & T &< T_{solid} \\ \alpha &= \frac{T - T_{solid}}{T_{liquid} - T_{solid}} & T_{solid} &\leq T \leq T_{liquid} \\ \alpha &= 1 & T &> T_{liquid} \end{aligned} \qquad (8)$$

In the PCM containers buoyancy flow of melted part of PCM due to temperature differences was not considered in the model, but only conduction heat transfer happens in both melted and solid part of PCM. Therefore, difference between melted and solid phases is based on their thermal conductivity coefficients k, specific heat capacities c_p and densities ρ. Moreover Eqns. (4) - (7) do not consider modelling of subcooling effects during phase change processes. And, other properties of the phase change paraffinic materials for the modelling purposes were taken from experimental results [9].

Initial and boundary conditions

For the fluid flow, the boundary conditions (BC) at solid surfaces such as inner wall of the storage tank and on the surface of PCM containers are considered as no slip BC. Moreover, it is assumed that the storage tank was perfectly insulated which is given by:

$$-n \cdot (-k\nabla T) = 0 \qquad (9)$$

where n - normal vector to the heat transferring surface. Therefore, heat transfer occurs only by means of inlet and outlet pipes. The containers are considered as highly conductive layers, where heat exchange takes place between heat carrier fluid and phase change material which can be described as:

$$\begin{aligned} -n \cdot (-k\nabla T) = \\ d_s(Q_s - \rho_s c_s \frac{\partial T}{\partial t}) - \nabla_t \cdot (-d_s k_s \nabla_t T) \end{aligned} \qquad (10)$$

where d_s - layer thickness which is taken as 0,01m in our case, Q_s - layer internal heat source and it is

zero in our modeling, J, ρ_s- layer density, kg/m³, c_s - layer specific heat capacity, J/kgK, k_s - layer thermal conductivity, W/mK - they are taken from material properties and it was mentioned above that the PCM containers are made from stainless steel.

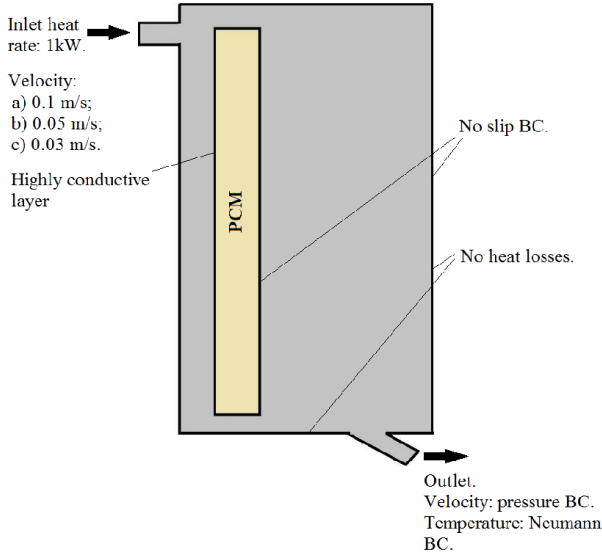**Fig.6.** Schematic description of boundary conditions

Table 3. Study cases for the simulation

Case	Number of inlet pipes used	Number of outlet pipes used	Inlet velocity
a)	1	1	0,100 m/s
b)	2	2	0,050 m/s
c)	3	3	0,033 m/s

In case of the simulation of charging process, initially it is assumed that the temperatures of the PCM and working fluid filling the storage tank are 20 ^{0}C. Inlet velocities were taken as depending on the number of inlet pipes (Table 3). The storage was charged with the net heat rate of 1kW through the inlet pipes (Fig.6). For instance, in case of one inlet pipe, heat rate from the inlet is 1 kW and in case of two inlet pipes, heat rate from each pipe is 0,5 kW. Purpose of such heat rate establishment was to estimate the effectiveness of the storage depending on different number of inlet and outlet pipe working conditions, and visualize by the simulation tools, intensive heat transferring zones in the storage and PCM containers. Conversely, during discharging case, initial temperate of the storage and PCM was 80 ^{0}C and 1 kW of thermal energy started to be discharged from outlet pipes. Moreover, inlet flow was maintained at 20 ^{0}C during simulation of the discharging process.

Outlet BCs for the velocity was set up in terms of the pressure with suppress backflow which adjusts the outlet pressure in order to prevent fluid from entering the domain through the boundary. And, temperature BC is Neumann type:

$$-n \cdot (-k\nabla T) = 0 \qquad (11)$$

RESULTS AND DISCUSSION

Three dimensional transient heat transfer simulations with PCM phase change were performed for the cases shown in Table 3. Durations of both charging and discharging simulations were three hours long since it was enough to conduct heat transfer analysis in the storage. Note that not all the simulation results are shown in the paper but only selected simulation results are presented and discussed.
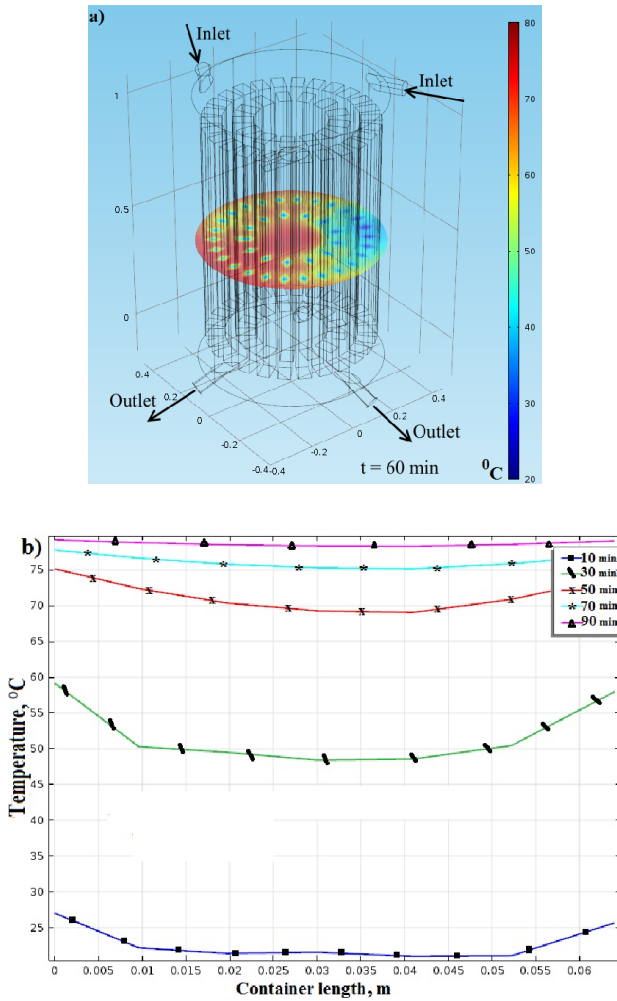
In Fig.7 simulation results are illustrated for the case-a where only one inlet and one outlet pipe was used for charging process. Moreover, paraffin E46 was considered as PCM in the simulation since it has more thermal stability than other two. Velocity of the heat carrier fluid at the inlet pipe was 0,1 m/s and thought the inlet pipe the fluid transferred into the storage 1kJ thermal energy at every second. It can be seen from Fig.7a that thermal energy came from the inlet pipe starts to charge the PCM containers which are opposite to the inlet pipe. This is true since heat carrier fluid flows to that area first but after circulation over the PCM containers most part of the fluid flows downward through the centre of the storage thus charging coaxially located PCM containers of the inner circle. Main streamlines where actively heat transfer process occurred are shown in Fig.7b. After 180 min still temperature distribution inside the storage was uneven and the PCM containers were not fully charged yet - Fig.7c.

When two inlet (inlet fluid velocity is 0,05 m/s at each inlet pipe) and two outlet pipes were used to charge the storage thermal energy still unevenly distributed in the storage (Fig.8a) but heat carrier fluid could charge more PCM containers both in outer and inner circles. Moreover, it can be noticed from heat carrier fluid flow streamlines in Fig.8b that active fluid flow process took place between inner and outer circles of PCM containers. In other words, transfer of the heat carrier fluid into the storage by two inlet pipes and two outlet pipes increased flow active areas in the storage, as a consequence, more PCM containers started to be charged during the process. When charging process reached 180 min, almost all PCM containers were fully charged (Fig.8c).
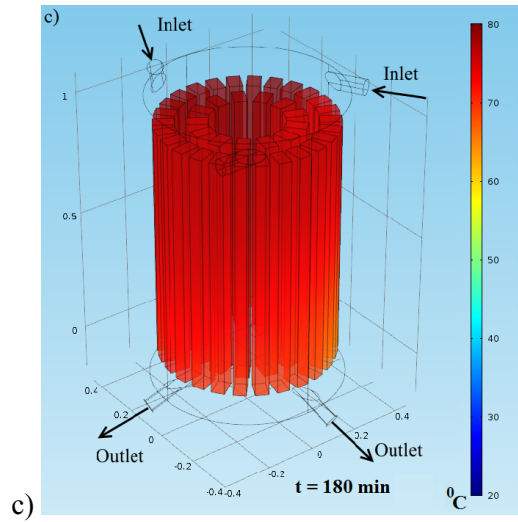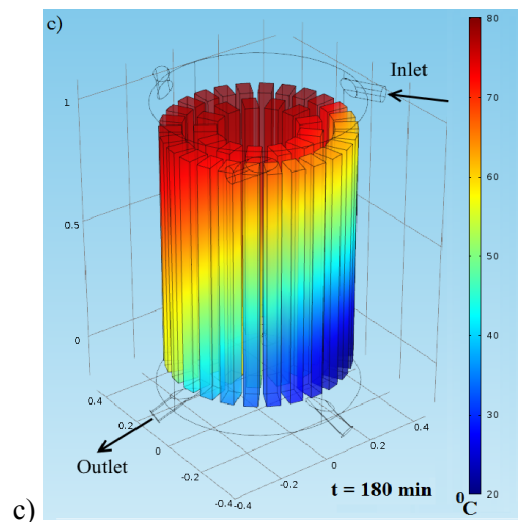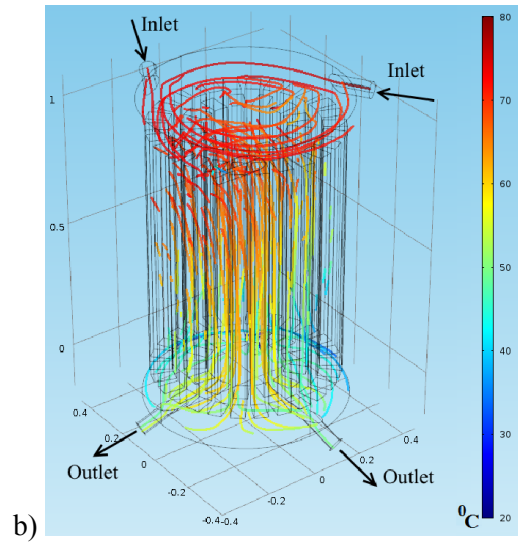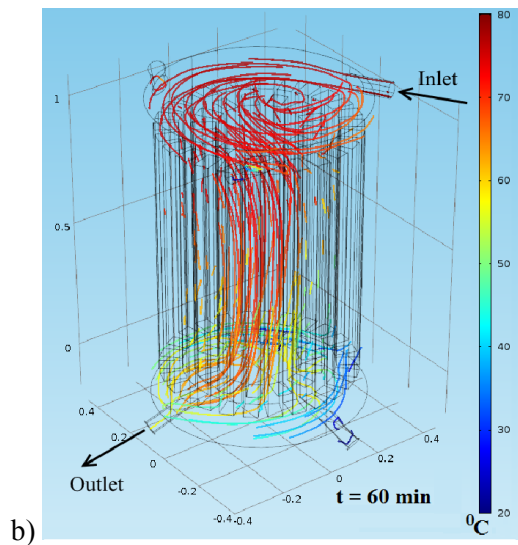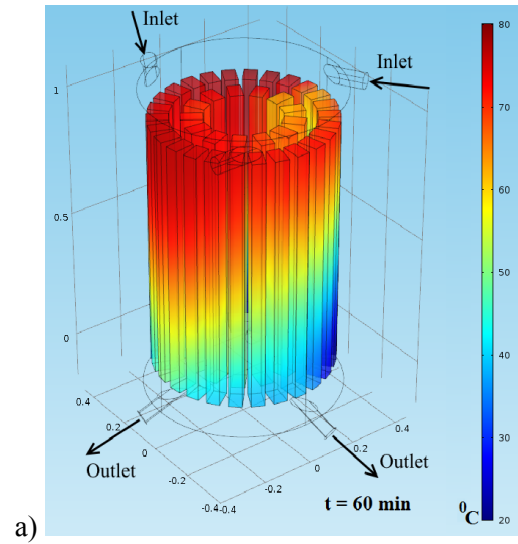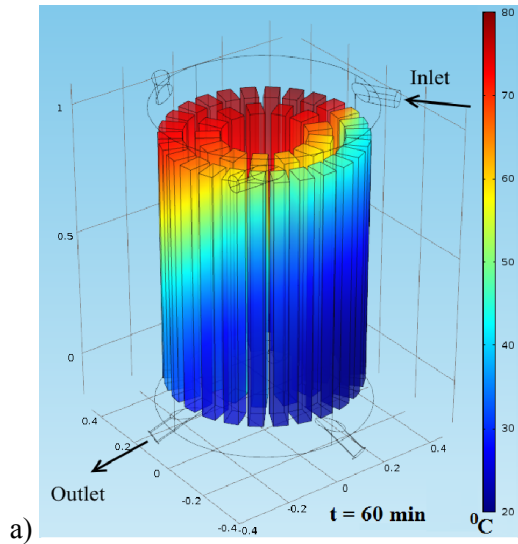
Fig.7. Charging process with single inlet and outlet pipes: a) Thermal energy distribution in the PCM containers after 60 min; b) Heat carrier fluid flow streamlines with thermal effect at 60 min; c) Thermal energy distribution in the PCM containers at 180 min

Fig.8. Charging process with two inlet and outlet pipes: a) Thermal energy distribution in the PCM containers at 60 min; b) Heat carrier fluid flow streamlines at 60 min; and c) Thermal energy distribution in the PCM containers at 180 min

Fig.10. Charging process with three inlet and outlet pipes (case-c): Temperature field of PCM containers at 80 min
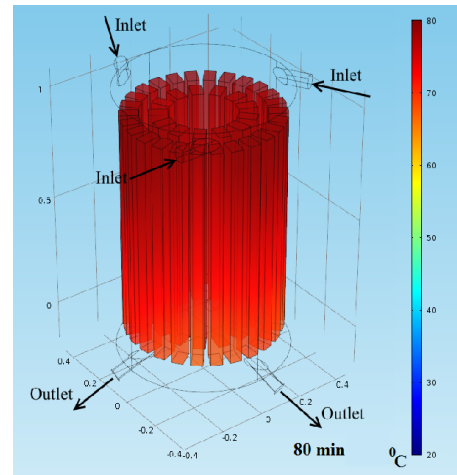
Fig.9. a) Temperature field at 60 min in the form of a cut plane to demonstrate the phase change process in the containers; b) Temperature change along the length of one of the containers during charging
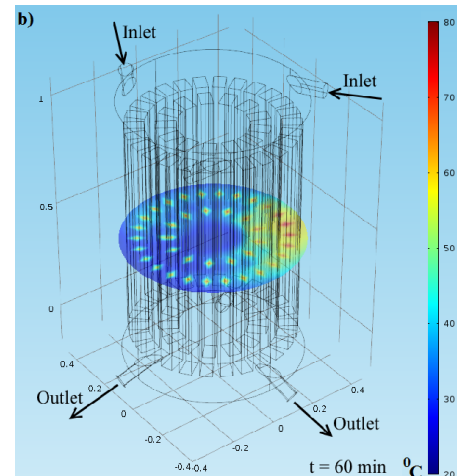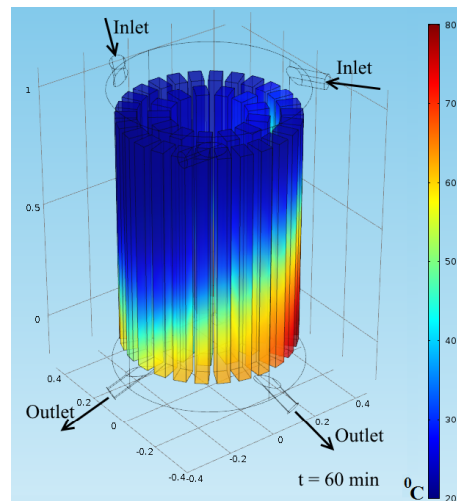
In Fig.9a temperature field demonstrated using cut plane to see phase change processes in the PCM containers and in Fig.9b we can see temperature change over time along the length of one of the PCM containers in the inner circle at 0,5 m height.

In case of three inlet and three outlet pipes, full charging time was reduced approximately by half, that is, 80 min compared to results of case b). Simulation result in case of three outlet and three inlet pipes, shown in Fig.10 where only final temperature field is presented.

Discharging process also studied using numerical simulation in same manner as charging process. In other words, cases presented in Table 3 also were studied for discharging process. From the results of the simulation, it was noticed that in case b) where two inlet and outlet pipes were used for discharging process was more effective than other two cases. Therefore, in the Fig.11 we presented results of simulation results related to case b).

Fig.11. a) Thermal energy distribution during discharging case at 60 min; b) cut plane to show phase change process in the PCM containers. Note that inflow temperature is 200 °C and velocity corresponds to Table 3, case b) - two inlet and two outlet pipes

CONCLUSIONS

In this paper, we presented charging and discharging processes of the latent heat storage in terms of simulation tools, Comsol, taking into account fluid flow and heat transfer physics in the storage tank and phase change processes in the PCM containers.

Three cases were studied in terms of numerical simulation. The results are illustrated in terms of temperature field to investigate how PCM containers were charged and velocity streamlines to understand how fluid flow process took place in the storage domain. From the results, it can be concluded that two inlet and two outlet pipes are enough to charge or discharge such LHS in enough short time, that is, three hours. Moreover, the PCM containers which are in the inner circle charged first in a short time and outer circle containers were charged after that. It can be concluded that outer circle PCM containers are very close to the storage tank walls, therefore, those areas does not allow fluid flow and heat transfer processes to be intensive.

Towards end of 2016, it is planed to build latent heat storage at Al-Farabi Kazakh National University, Almaty, Kazakhstan. Therefore, studies in this paper based on numerical simulation tools are very important in developing design features of the planned storage.

ACKNOWLEDGMENTS

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