Numerical Investigations of Phase Change Materials (PCMs) for Thermal Energy Storage Systems: An Overview

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Abstract

In this work, recent numerical studies on energy storage in phase change materials(PCMs) have been reviewed.In recent years, thermal energy storage in phase change materials(PCMs) has been very popular in terms of storing energy and supplying when its needed.High thermal capacity of PCMs, due to large enthalpy of phase change(latent heat), increase the potentiel of these materials for heat accumulation, but also modifies heat transfer in transient states what improves their insulating characteristics. Many simple models have been developed for numerical simulations of energy storage units. Computaional Fluids Dynamics (CFD) tools such as Ansys Fluent have been used for most of the numerical studies. Numerical studies have resulted improving the energy storage potential of PCMs.

Keywords: Thermal energy storage; Phase change material; Heat transfer; Solar energy

1. Introduction

Increasing the use of clean energy and improving energy efficiency have become a worldwide strategy for sustainable development to preserve energy resources [1].Thermal energy storage is a useful tool to achieve these goals. Thermal energy can be stored directly as internal energy of a material through sensible heat, latent heat, and thermochemical heat or any of their combinations [2].The second type is widely preferred because of the high energy density and the small temperature drop during the charge and the discharge processes [3]. For storing and recovering heat, Phase change materials (PCMs) can serve a suitable medium during melting and solidification [4]. They can store and release huge amounts of latent heat while changing their state in a narrow temperature range [5].

Latent thermal energy storage (LTES) system is considered to be the best due to its high energy storage density and storing energy at constant temperature corresponding to the phase transition of PCM. LTES can be achieved by three different phase change processes such as solid–liquid, liquid–gas, and solid–gas [6-8]. Solidliquid phase change is of great interest when compared with other two phase transformations [9]. Because, both liquid-gas and solid-gas processes would require more volume for given energy storage [10].The phasetransformation characteristics of PCM during melting and solidification processes have been reported in many literatures [11-15]. In the melting process, heat is transferred initially by conduction and later by natural convection through the PCM. This is due to the fact that thermal conductivity of PCM in liquid state is less than that of PCM in solid state; thereby the heat transfer by conduction is negligible as the melting process progresses. Unlike melting process, in the solidification process, heat is transferred by convection at the beginning and later by conduction only. This is due to the fact that the solid region is formed at the heat transfer surface and this acts as the resistance to heat transfer. For accelerating the both processes, heat transfer enhancement techniques have been recommended. Thereby, energy storage and release capacity of the PCM can be increased further and as a result of this, energy conservation canalso be achieved considerably. In recent times, more researches have been going on in this regard to make the energy storage systems suitable for large scale practical applications [16].

2. Heat Transfer Enhancement Methods

2.1. Enhancement using fins

There are several methods to enhance the heat transfer in a latent heat thermal store. The use of finned tubes with different configurations has been proposed by various researchers such as Morcos [17], Sadasuke and Naokatsu [18], Costa et al. [19], Padmanabhan and Krisha Murthy[20], Velrajet al. [21,22] and Ismail et al. [23] use finned tubes in thermal storage systems.

Abdiet al. [24], numerically investigates the effect of vertical fins on the power enhancement in the melting process and the energy density of a LTES system. The melting process in a two-dimensional rectangular cavity is simulated using the commercial ANSYS Fluent software. Regarding the length and number of fins, parametric study is carried out. Three 1-, 3- and 5- fins configurations were simulated. At each configuration, fin length is varied from 0.25 to 0.75 of the cavity height.The influence of different fin configurations on contributing natural convection patterns are analyzed. Also, the effects on melting time, enhanced heat transfer rate and accumulated energy are assessed.The details of investigated cases are stated by Table 1.

Table 1. Simulation cases [24].

Simulation case	**Number of fin**	**Dimensionless length=l/H***
Case 1	No fin	No fin
Case 2	1	0.25
Case 3	1	0.5
Case 4	1	0.75
Case 5	3	0.25
Case 6	3	0.5
Case 7	3	0.75
Case 8	5	0.25
Case 9	5	0.5
Case 10	5	0.75

As shown in Figure 1, for the cavity with bottom surface maintained at fixed temperature of70˚C, beside the formed Benard convection cells initiating melting from the bottom of cavity,the natural convection flows along the side walls causes a melting process at the top. Inserting a vertical fin in the middle of the cavity, causes convective flow patterns along the fin length, as illustrated in Figure 2. As the melting progresses, the aforementioned flows split the solid bulk of PCM, shaping two separate solid bulk sections. The longer the fin length, the quicker division of the solid bulk happens. Observing the melt front evolution,the influence of convective flow initiated by the fin is greater than the effect of connective flow along the side walls.

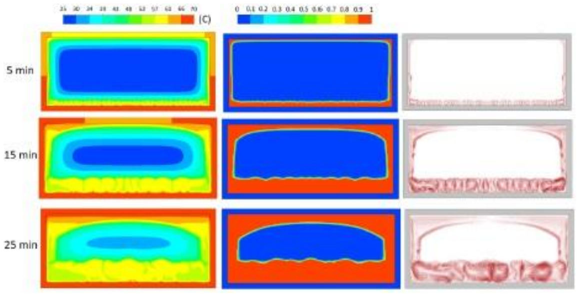

Figure 1. Transient melting for case 1: temperature distribution (left), melt fraction(middle), velocity vectors (right) [24].

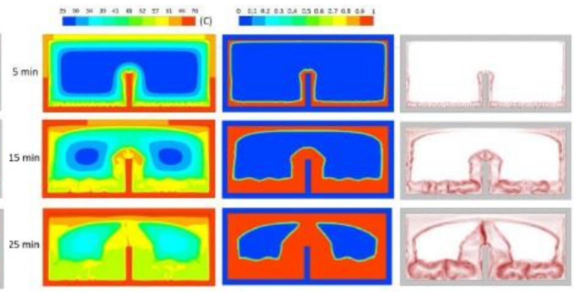

Figure 2. Transient melting for case 3 at Ste=0.55: temperature distribution (left), melt fraction (middle), velocity vectors (right) [24].

Figure 3 shows the decrease in melting time as function of number of fins for dimensionless length of 0.5 and 0.75 under different boundary conditions. As number of fins increases the reduction in melting time is less prominent. As it is shown, for lower wall temperature, Ste=0.36, the decrease in melting time is more significant, whereas for higher wall temperature such as Ste=0.55, the enhancement by increasing the number of fins from three to five is insignificant. Similar trend is observed for longer fins with dimensionless length of 0.75; however, the enhancement effect for all boundary conditions is more pronounced, as compared to dimensionless length of 0.5.

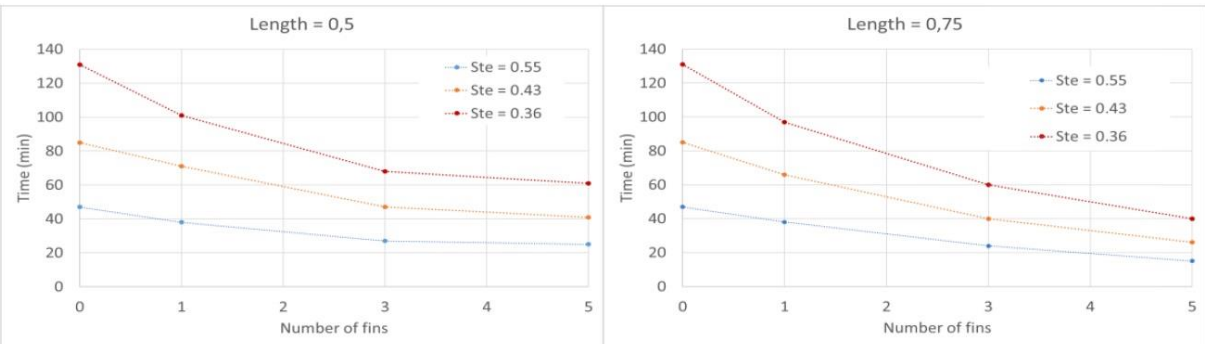

Figure 3. Total melting time as function of number of fins for different Ste number: l=0.5(left), l=0.75(right)[24].

Figure 4(left) shows the accumulative energy for cases 1, 3, 6 and 9. Obviously, it isseen that for all cases the stored energy at every stage of the melting process is above the reference case with no fin. In a similar manner to power curves, in case 9 energy is being stored with a high rate through midway of the melting process and afterward with lower rate, indicating the possibility of partial melting. On the other hand, in cases 3 and 6 heat is being transferred with rather a constant slope. This shows the possibility of these cases to be used in application with constant but low power demand.Figure 4(right) illustrates the stored energy for cases with five fins and increasing length, cases 7, 8 and 9. As the fin length increases, the ability of the storage system to absorb more energy increases. For cases 7 and 8, with dimensionless length of 0.25 and 0.5, respectively, storage of energy is accomplished with quite high rate in areas nearby fins. Further on, heat absorption is continued with lower rate.

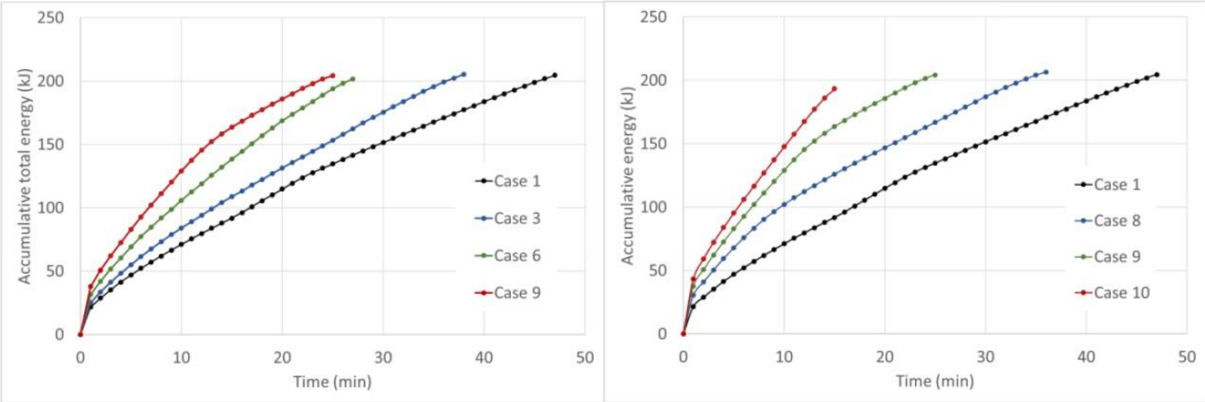

Figure 4. Accumulative energy as function of time at Ste=0.55: cases 1, 3, 6 and 9 (left), cases 1 and 8-10(right) [24].

The results show that installation of fins contributes to the melting process by increasing the heat transfer surface area, and by enhancing the natural convection mechanism. Also, not only fins could enhance the heat transfer performance, but could maintain the same level of total stored energy including latent and sensible energy during melting, or even in some configurations increase the total stored energy slightly.

Tan et al.[25] experimentally and numerically studied the impact of the configuration of spiral aluminium fillers on the PCM's melting performance in a fin type latent heat storage system. A two-dimensional simulation domain was designed using Fluent 6.3 software for both fin type and fine-spiral fillers slab (Figure 5). The numerical results were validated with experimental data, and a good agreement was observed. It was also found that the aluminium spiral fillers have a strong influence on the PCM's melting behaviour. The heat conduction increased due to the rise in the induction area as a result of adding the spiral fillers, whilst the natural convection was reduced.

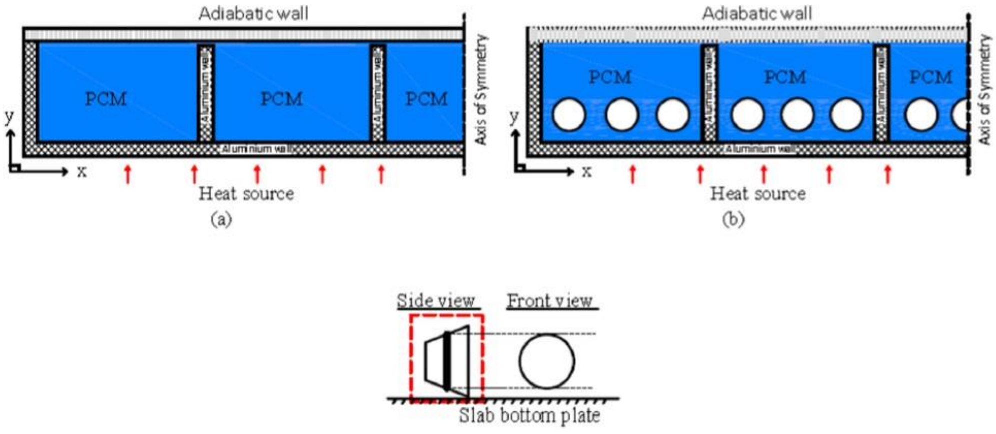

Figure 5. Two-dimensional simulation domain [25].

Ismail et al.[23] presented a numerical model of the solidification process around a vertical axially finned tube immersed in a PCM and the model results were compared with experimental data The study was designed to determine the effect of the fin length, thickness and number, the aspect ratio of the annular space and the difference between the phase change temperature and the wall temperature of the tube. The numerical results were supported by the findings of the experimental work, and these indicated that as the fin length increases, the complete solidification and the solidified mass fraction are reduced significantly. An increase in the fin thickness as well as the number of fins resulted in an increase in the solidified mass fraction and a reduction in the solidification time. The results also demonstrated that an increase in the aspect ratio of the annular space resulted in an increase in both the solidification time and the solidified mass fraction, whilst an increase in the temperature difference resulted in a reduction in the solidification time and the solidified mass fraction.

Zhang and Faghri [26,27]developed theoretical methods to study the heat transfer enhancement in a latent heat thermal energy storage unit using tubes with internal longitudinal fins (Figure 6a) and external radial finned tubes (Figure 6b). The most interesting finding was that the use of internal fins provided stronger effect of enhancing the melting heat transfer for transfer fluids at low Reynolds numbers. Another important finding for the externally finned case was that the tube wall temperature and Nusselt number were increased significantly when the thickness of the wall increased, but the latter had no significant effect on the molten liquid volume. On the other hand, the fin height had a significant impact on the molten volume fraction (MVF).

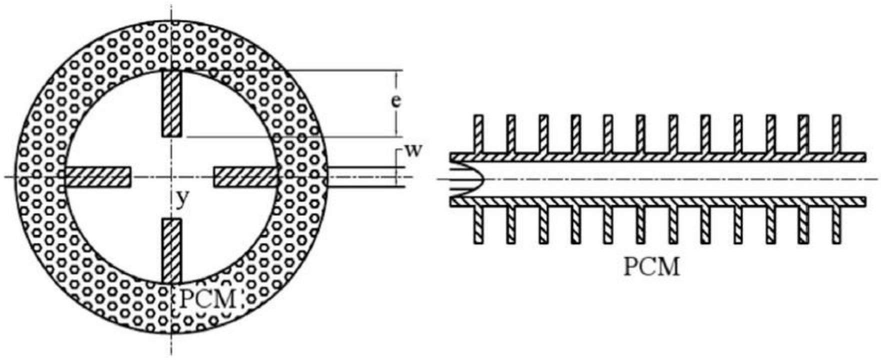

Figure 6. Schematic of internally and externally finned tubes deployed in [26] and [27].

Works by Costa et al. [19] study numerically a two-dimensional rectangular area, using energy equations in solid and liquid phases, continuity, momentum and Stefan's equation in the boundary. Three PCM are analysed: paraffin (n-octadecanol) and metals (gallium and tin). They put forward a numerical resolution method called SIMPLEC (semi-implicit method for pressurelinked equations consistent) and compare the results with those obtained in the literature. In the case of octadecanol, there is poor agreement with the experimental results in the upper zone where the liquid which melts at the sides fills the upper empty cavity and accelerates melting in this area. Costa indicates that the reasons of the discrepancies between the experimental andtheoretical results are due to thermal inertia, instability in the systems, thermal losses, lack of reliable information about the physical properties of the materials, three-dimensional behaviour, consideration of constant thermophysical properties, variations in density, long calculation periods and significant variations in viscosity with the temperature.

2.2. Enhancement using multiple PCM

Using multiple PCMs to form cascaded or multi-stage LHS system is an efficient method to improve the uniformity of heat transfer process [28–29]. The schematic for cascaded LHS system is shown in Figure 7.In this method, PCMs are arranged in the decreasing order of their melting points and then nearly a constant temperature difference can be maintained during melting process, even though the HTF temperature decreases in the flow direction [30].

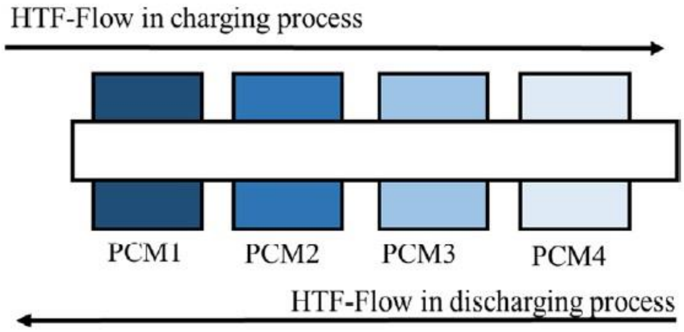

Figure 7. Schematic of multi-stage LHS system [28].

Wu et al. [29] numerically investigated the transient performance of cascaded molten salt packed-bed TES system. The results show that the noncascaded system suffers from a low charging ratio and a long charging time while the cascaded systems especially with 5 cascaded PCMs are found to have both a fast discharging rate and a fast charging rate.Li et al. [31] numerically investigated the performance of a three-stage LHS unit. The instantaneous solid-liquid interface positions and liquid fractions of PCMs were analyzed and the optimum lengths for different stages are recommended.

Shaikh and Lafdi[32] studied the numerical analysis on a combined convection–diffusion phase change heat transfer in varied configurations of composite slabs using multiple PCMs. It wasobserved that the total energy charged rate could be considerably increased by using composite PCMs as compared to the single PCM.Fang and Chen [33] numerically investigated the performance of a shell-and-tube LHS unit using multiple PCMs and found that PCMs' fractions and melting temperatures play importantroles in the performance of the LHS unit. Appropriate choosing of multiple PCMs is very significant for the performance improvement of the LHS unit.

Seeniraj and Narasimhan [34] numerically studied the performance of a LHS unit with both finned-tube and multiple PCMs. The results show that the unit can obtain appreciable energy storage in the form of latent heat and a nearly uniform HTF exit temperature as compared to a single PCM unit.Mosaffa et al. [35,36] numerically investigated the performance enhancement of a free cooling system using a LHS unit employing multiple PCMs, where the energy and exergy analyses were also performed.

2.3. Enhancement using nano-fluid, nano-particles and microencapsulation

Nanofluids are new suspensions that are produced by dispersing the solid nanoparticles in conventional liquids [37,38]. In general, the main purpose of preparing nanofluids is to improve thermal conductivity of industrial liquids such as water and engine oil because these fluids possess a low thermal conductivity. In fact, use of the nanoparticles that have a superior thermal conductivity enhances thermal characteristics of ordinary liquids.Many researchers have employed nanofluids in different applied situations such as heat exchangers, power plants, nuclear reactors, electronics cooling, transportation, and so forth. Moreover, several review papers have been presented by the relevant scholars, and it was concluded that applying nanofluids can improve the performance of various thermal devices [39].

Numerical simulations using FLUENT software were carried out by Arasu et al.[40] to investigate the effect of AL2O3 nano-particles on paraffin wax in a concentric double pipe heat exchanger. The computed thermo-physical properties of paraffin saturated with AL2O3 nano-particles were compared with Ho and Gao's measurements in [41] and a good agreement was observed between these two data sets. The results demonstrated that the AL2O3 nano-particles in paraffin wax had a significant effect on the charging-discharging rates of the thermal energy compared to the case with pure paraffin. A similar enhancement in the thermal conductivity of the composite materials and in the heat transfer rate was also found. Furthermore, the viscosity of the composite materials increased as the volumetric fraction of AL2O3 nano-particles rose, thus improving the natural convection heat transfer effectiveness.Seeniraj et al. [42] proposed a theoretical expression for the energy storage and heat flux for cases with and without dispersed particles in the PCM and identified the optimum fraction of dispersed particles to maximise the energy storage and heat flux. The schematic arrangement used in this study is shown in Figure 8. It was reported that the cumulative energy storage capacity was decreased as the particle fraction was increased, due to the particles reducing the volume occupied within the PCM. However, the addition of particles increased the instantaneous surface heat flux and hence accelerated the energy storage process. The results also revealed that the optimum fraction of dispersed particles to maximise the stored energy depends on the thermal conductivity of the dispersed fraction.

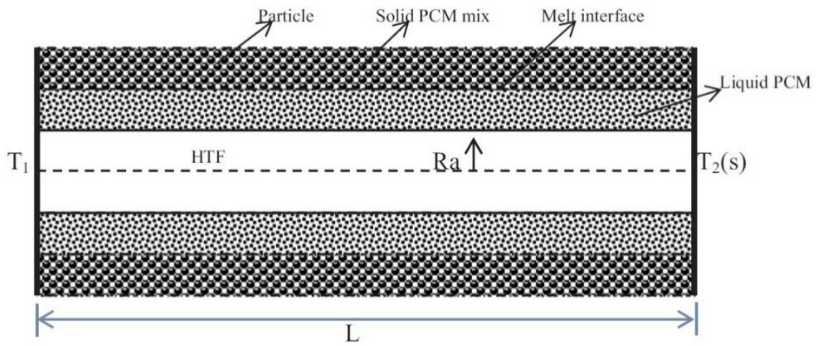

Figure 8. Schematic of the storage unit containing dispersed particles [42].

Shaikh et al. [43] carried out an experimental and a numerical study of the latent energy storage with a PCM containing dispersed single wall carbon nanotubes (SWCNTs), multiwall CNTs (MWCNTs) and carbon nano-fibres (CNFs). The results of the numerical model were compared to experimental results and a good agreement was found. Figure 9 illustrates the physical model and the 2-D arrangement of carbon nanotubes (CNTs) used in the theoretical model. From the experimental results, the maximum value of the latent heat enhancement was found to be in the wax/SWCNTs composite followed by the wax/ MWCNTs composite, whilst the minimum enhancement was found inthe wax/CNFs composite. The theoretical model also examined the effect of nanoparticle mass fraction, size and type on the intermolecular attraction within the mixture. It was concluded that the molecular density of the SWCNTs was higher compared to that of MWCNTs and CNFs, resulting in the enhanced latent energy.

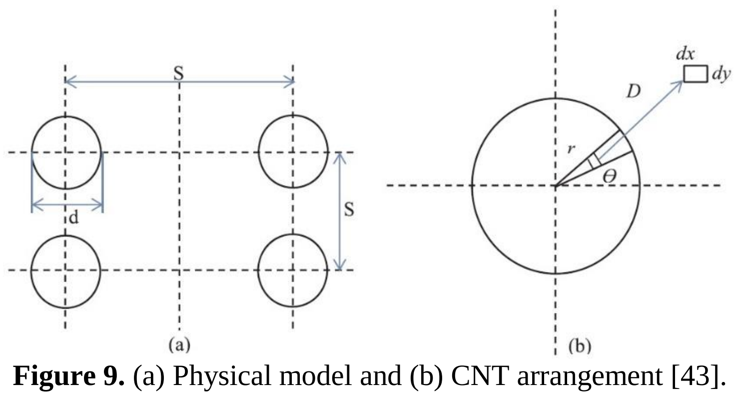

Figure 9. (a) Physical model and (b) CNT arrangement [43].

Minea [44], summarised the recent numerical studies onthe preparation, thermophysical properties, correlations and heat transfer characteristics of hybrid nanofluids and compared between hybrid nanofluids with that of pure water. It can be noticed from the numerical results that hybrid nanofluid significantly improves the conventional heat transfer capacity. This is because the suspension ofhybrid nanoparticles highly improved the thermal conductivity of the nanofluid. On the other hand, this study outlined the advantages and disadvantages of using hybrid nanofluids compared to water in term of heat transfer enhancement.

Ho et al. [45] numerically examined different models of the effect of thedynamic viscosity and thermal conductivity of nano-fluids on natural convection heat transfer. Numerical 2D modelling was carried out for a vertical square enclosure (Figure 10), with a water-alumina (AL_2O_3) mixture chosen as the working nano-fluid. Results indicated that the heat transfer across the enclosure was improved with respect to the base fluid.

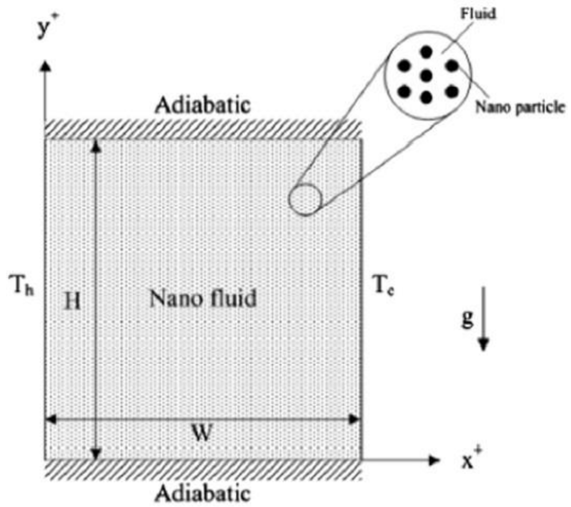

Figure 10. Schematic of a vertical enclosure system [45].

Hu and Zhang [46] carried out a numerical investigation of the enhancement of convective heat transfer in a microencapsulated PCM. The model analysed the effect of various factors on the heat transfer enhancement in a laminar flow in a circular tube with a constant wall temperature.The numerical simulation results show that the Stefan number, mass flow rate of HTF and volumetric concentration of microcapsules can improve the heat transfer rate.

3. Solar Thermal Energy Storage Systems with PCM

Many research studies have shown that applying PCMs can provide much higher energy density while reducing the costs considerably. Due to this fact, many investigations have employed PCMs to improve the performance of solar collectors [39].

3.1.Solar water-heating systems

Solar water heater is getting popularity since they are relatively inexpensive and simple to fabricate and maintain [47,48]. Hamed et al. [49] conducted a numerical work on an integrated solar water heater using PCMs. The objectives were drawn to reach the maximum outlet temperature by providing the complete melting and solidification processes and evaluating thepossibility of using solar collector system after the sun shining such as during night. They utilized MATLAB software to simulate the problem using explicit finite difference method. The performance of the system showed that the PCM could reduce the charging temperature and increase the discharging temperature.

Huang et al. [50] performed a numerical work on a solar water heater using PCMs. $NaSO_4$. $10H_2O$, $CaCl_2$. $6H_2O$ with capric acid were used as the new type of PCM (Figure 11). A 2D mathematical model was developed to analyze heat transfer rate by ANSYS software based on the enthalpy and finite element methods (Figure 12). They finally reported that around 38000 kJ heat releases within 16 h for a room which has an area of 11 m^2, without using any pump. According to their results, 47.7% energy supplied was reached through the process improvement.

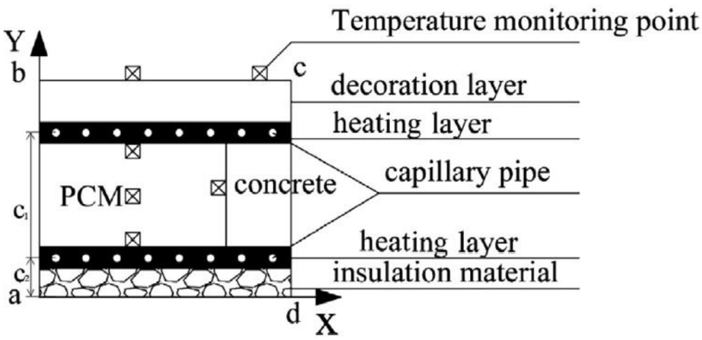

Figure 11. Configuration of the novel PCM floor [50].

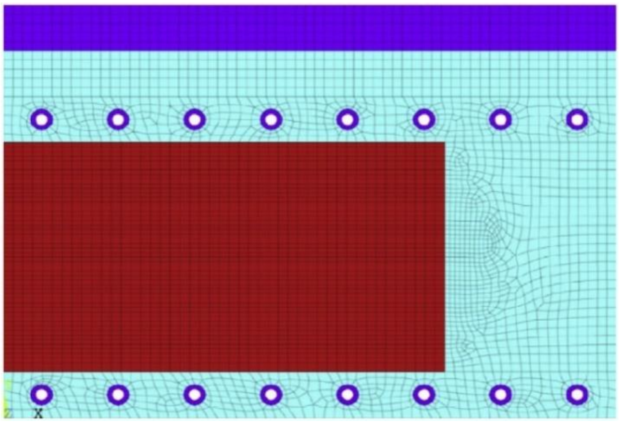
Figure 12. Finite element model [50]

A cylindrical storage unit in the closed loop with a flat plate collector has been theoretically studied by Bansal and Buddhi [51] for its charging and discharging mode. The calculations for the interface moving boundary and fluid temperature were made by using paraffin wax (p-116) and stearic acid as phase change materials. A comparative study of solar energy storage systems based on the latent heat and sensible heat technique has been carried out to preserve the solar heated hot water for night duration by Chaurasia et al. [52]. For this purpose, two identical storage units were used. One storage unit contained 17.5 kg paraffin wax (m.p. about 54˚C) as the storage material packed in a heat exchanger made of the aluminum tubes and another unit simply contained the water as a storage material in a GI tank. Both units were separately charged during the day with the help of the flat plate solar collectors having same absorbing area. This study has revealed that the latent heat storage system comparatively yields more hot water on the next day morning as compared tosensible storage system.

Ibanez et al. [53] numerically studied the incorporation of two cylindrical PCM capsules into the solar storage tank of a domestic hot water (DHW) system. They produced a new TRNSYS component based on previously developed components to simulate and validate the water temperature in the tank. The predicted results agreed with those of the experiment. Padovan and Manzan [54] generated an optimization tool for PCM thermal energy storage in a DHW system to enhance energy saving and to reduce the volume/space required by the system. They analyzed different designing para- meters, such as tank dimensions, PCM melting temperature point, and insulation thickness. The findings indicated that the effects of tank geometry and insulation thickness on energy saving in thermal storage are limited.

Kousksou et al. [55] numericallyanalyzed the benefits of PCM in a DHW system and made recommendations to improve the thermal performance of the PCM storage system. As per the results, the utilization of PCM in DHW system may not be considerably beneficial. Thus, an optimization tool must be established during the early stages of design because PCM integration into DHW may be enhanced by selecting proper design parameters, such as PCM melting temperature point.

Nkwetta et al. [56] numerically studied the performance of a DHW tank integrated with different PCM types in various this models was validated experimentally and used to determine the effect of PCM location on the thermal performance of the tank given three actual profiles of hot water consumption. The results indicated that the discharge times wereconsistent at the different draw-off intervals between predictions. The stored energy increased with the increase in PCM. Hence, the integration of PCM in hot water tanks improves storage capacity. Furthermore, it may provide energy, shift, and/or smooth peak power demand. Moreover, the PCM composed of sodium acetate trihydrate + 10% graphite displayed the highest storage potential at a shorter charging time compared with industrial-grade granulated paraffin wax and RT58-Rubitherm.

The specific apparent heat capacity Cp^{app} techniquehas been successfully validated with the work of Talmatsky et al. [57] who have performed a physical model to describe the heat storage tank with and without PCM. They carried out annual simulations to compare the performance of a storage tank with PCM to a standard tank without PCM. Talmatsky et al. [57] suggested a system that consists of a storage tank with PCM, collector, pump, controller and auxiliary heater. They have reported that the beneficial impact of PCM is not guaranteed since the gains observed over the day period brought by the presence of PCMs to store the solar energy were compensated by the losses undergone by the storage tank during the night.

3.2. Solar air-heating systems

Morrison, Abdel Khalik and Jurinak [58,59] in their different studiesevaluated the performance of air-based solar heating systems utilizing phase change energy storage unit. The main objectives of their work were: (i) to determine the effect of the PCM latent heat and melting temperature on the thermal performance of air-based solar heating systems and (ii) todevelop empirical model of significant phase change energystorage (PCES) units. The main conclusion was that the PCM should be selected on the basis of melting point rather than its latent heat and also found that air-based system utilizing sodium sulfate decahydrate as a storage medium requires roughly one-fourth the storage volume of a pebble bed and onehalf the storage volume of a water tank. Ghoneim and Klein [60] compared theoretically the performance of phase change and sensible heat storage for air and water based solar heatingsystems.

Zhou et al. [61] investigated numerically the performance of a hybrid heating-system combined with thermal storage by shape-stabilized phase-change material (SSPCM) plates. A direct gain passive-solar house in Beijing is considered: it includes SSPCM plates as inner linings of walls and the ceiling. Unsteady simulation is performed using a verified enthalpy model, with a time period covering the winter heating-season. Additional heat supply is employed during load hours at late night and early morning or during the whole day necessary to keep the minimum indoor air temperature above 18 8C. The results indicate the thermal-storage effect of SSPCM plates, which improves the indoor thermal comfort level and saves about 47% of normal-and-peak-hour energy use and 12% of total energy consumption in winter. This hybrid heating system can level the electrical load for power plants and would providesignificant economic benefits in areas where night and day electricity tariff policy is used.

3.3.Solar absorption refrigeration systems

Although there are numerous absorption refrigeration cycles (like half, single or multi-effect absorption systems; absorption heat transformer, absorption refrigeration cycle with GAX or absorber-heatrecovery, sorption-resorption cycle; diffusion, self-circulation, osmotic membrane, combined ejector and combined vapor absorption systems), only a few are studied extensively due to their promising outcomes [62]. Ullah et al. [63] compiled various solar thermal refrigeration systems with emphasis on absorption and adsorption refrigeration systems. The current study focuses on aqua-ammonia and LiBr-water absorption systems (operating temperatures) due to plentiful investigations and diversified techniques used.

4.5 kW LiBr-H_2O absorption chiller was designed by Agyenim et al. [64] at anaverage COP of 0.58 with a cold storage of 1000 ltr for chilled water at almost 7 °C. They made a critical analysis on each component of the system with daily measurements of thermodynamic properties and suggested to use 60–90 ltr of cold storage per square meter of vacuum tube collectors, or 80–150 ltr of for every kW chiller capacity to produce chilled water. Recently, He [65] modified the system with additional thermal storage unit with PCM (Erythritol) to enhance the COP of the system. He reported that the only disadvantage of using erythritol is low thermal conductivity. He also suggested that longitudinal and multitubes are most suitable for charging and discharging of erythritol.

Pintaldi et al. [66] numerically evaluated thermal energy storage options for a triple effect solar absorption system. They compared sensible and latent heat storage using transient simulation and finally reported a high storage efficiency for latent heat materials. Brancato et al. [67] recently investigated few PCMs with melting temperatures between 80 and 100 °C for application of solar cooling. They found that those PCM (with high latent heat) characterized by them still have some issues like subcooling, incongruent melting, allotropic phase transition; and that the commercially available (PlusIce A82, S83 & S89) eutectic mixtures are much stable with lower heat of fusion.Serale et al. [68] numerically studied a slurry PCM based flat plate collector with an efficiency improvement of +0.08 compared to conventional water based technology. A 20% −40% improvement in heat conversion was seen on average, throughout the year. Their concern with the 50% or more concentration of PCM was not possible due to increased demand in pumping energy (design constrain).

4. Conclusions

- Many simple models have been developed for numerical simulations of energy storage units. Computaional Fluids Dynamics (CFD) tools such as Ansys Fluent have been used for most of the numerical studies.

- Many research studies have shown that PCMs improve the performance of solar collectors.

- This review work would be helpful to choose appropriate heat transfer enhancement method to achieve better thermal performance for PCM based latent heat storage system.

- Also, this paper would kindle the researchers to develop larger energy storage density PCMs with improved heat transfer capabilities dedicated for possible latent thermal energy storage applications in the near future.

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