CFD Analysis of Nano-Enhanced Phase Change Materials for Energy Storage Applications

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***Abstract*- There has been much emphasis in taking corrective measures to overcome the global warming and integrating the renewables into the energy systems, along with the pathway of the energy storage are the active fields of current research. One of the method is by using thermal energy storage. There are three types of thermal energy storage, namely sensible heat, latent heat and thermal chemical storage system. It is reported that thermal energy storage density for latent heat storage is higher than sensible heat storage. Latent heat storage system using phase change material (PCM) has been widely investigated and explored by various researchers. PCMs offer promising thermal storage characteristic where they can absorb and release large amount of latent heat during phase transition process.**

An CFD investigation of the melting of paraffin wax dispersed with three different metal oxide Alumina (Al2O3), Zirconium Dioxide(ZrO2) & Titanium Dioxide (TiO2) Iterate for different concentration (i.e. 1% & 3% for both) that is heated from one side of rectangular enclosure of dimensions of 25 mm × 75 mm. The melting percentage of PCM having 3% TiO2 concentration is more compared to nanoparticle concentration of 1% (Al2O3, ZrO2 and TiO2) and 3% (Al2O3, ZrO2).It requires 1000 Sec for paraffin wax + TiO2 (3%) to 86% melt while in case of paraffin wax + Al2O3 (3%) to 81% melt and in case of paraffin wax + ZrO2 78% to melt.

Index Terms- Thermal energy storage, Paraffin wax, Nano-enhanced material, CFD, Nanoparticles, Latent Heat.

I. INTRODUCTION

Sustainability engineers are focused on addressing increasing energy demands while reducing greenhouse gas emissions from the use of fossil fuels. Energy storage is a crucial part of any next-generation energy distribution system.

Energy is the key requisite to bring about technological advancement and economic development for the progression of societies all around the world [1]. The unrelenting depletion of non-renewable resources and the escalating scenario of global warming have compelled the trend to be shifted towards the use of sustainable energy resources [2, 3]. Consequently, it is imperative to explore renewable and sustainable resources to meet both electrical and thermal energy conversion and storage requirements. The de-carbonization of the energy sector can be made possible by integrating renewable energy resources with various thermal energy storage systems which possess round-trip efficiency of >96% [4, 5]. Currently, over 18% of the global energy consumption is derived from the renewables [6]. There has been much emphasis in taking corrective measures to overcome the global warming and integrating the renewables into the energy systems, along with the pathway of the energy storage are the active fields of current research.

One of the method is by using thermal energy storage. The main idea of using thermal energy storage system is to store thermal energy for later usage instead of releasing it to the environment. There are three (3) types of thermal energy storage, namely sensible heat, latent heat and thermal chemical storage system [1–2]. Each of the system has their own advantages and disadvantages.

It is reported that thermal energy storage density for latent heat storage is higher than sensible heat storage [2–3]. Latent heat storage system using phase change material (PCM) has been widely investigated and explored by various researchers. PCMs offer promising thermal storage characteristic where they can absorb and release large amount of latent heat during phase transition process. During phase change process, the temperature of these materials remains constant.

Organic PCM offers lower thermal conductivity compared to that of inorganic PCM. Thermal conductivity of paraffin wax is about 0.24 W/ m-K [8]. This characteristic prevents the energy (heat) stored in the PCM to be released to the surrounding for useful purpose.

PCM doped with nanoparticles is known as nano-enhanced PCM. Nanoparticles such as carbon nanotubes, graphite, graphene, metal and metal oxide can be dispersed in PCM [14]. It is worth noting that inclusion of nanoparticles will not only alter thermal conductivity characteristic of PCM but also other characteristics as well, including latent heat capacity, sub-cooling, phase change temperature and its duration, density and viscosity.

II. LITERATURE REVIEW

Choi [1995] is the first researcher who worked on nano particles at the Argonne National Laboratory, USA. He demonstrated that nanofluids exhibit an increased thermal conductivity compared to the host fluid.

Guo et al. [2013] found that thermal conductivity of expanded graphite (EG) - erythritol is higher than MWCNT-erythritol due to the rapid transfer of phonon in EG network and higher interfacial thermal resistance of MWCNT

Bauer T. et al. [2014] this paper focuses on latent heat storage using a phase change material (PCM). The paper lists of literature and gives the current status of medium working range temperature of 200 to 350oC. In this paper the system with KNO3-NaNO3 is discussed in detail with their thermo-physical properties in the liquid and solid phase. A comparison of literature data and own measurements for the density, heat capacity, thermal diffusivity and thermal conductivity is presented in detail. The melting temperature and enthalpy of the KNO3-NaNO3 is 222oC and 108J/g was identified respectively. Different properties such as thermal conductivity, density are also collected from the different literatures.

Lin and Al-Kayiem [2016] uses Paraffin wax and Cu (0.5, 1.0, 1.5, 2.0 wt. %) as nano enhanced material. Thermal conductivity increases non-linearly with the increase of nanoparticles concentration. 46.3% thermal conductivity augmentation is recorded at 2.0 wt. % of nanoparticles. Latent heat for melting and solidification decreases 14.6% and 13.3% respectively, at 2.0 wt. % of nanoparticles compared to that of pure paraffin wax. Melting (184.2 kJ/kg to 157.3 kJ/kg) Solidification (179.3 kJ/kg to 155.5 kJ/ kg). Melting phase change temperature decreases 4.3% at 2.0 wt. % of nanoparticles concentration compared to that of pure paraffin wax. Melting temperature decreases from 60.42 °C to 57.81 °C. There are slight changes for the solidification phase change temperatures.

M.Auriemma and A. Iazzetta [2016] a numerical study on variations of thermo-physical properties of Phase Change Material (PCM) due to dispersion of nanoparticles is presented in this article. Dispersed metal oxide nanoparticles in paraffin wax might be a solution to improve latent heat thermal storage performance. Thermo-physical properties such as thermal conductivity and latent heat could be changed for different concentration of dispersed nanoparticle. The paper will focus on numerical investigation of the melting of paraffin wax dispersed with three different metal oxide Alumina (Al2O3), Copper Oxide (CuO) and Zinc Oxide (ZnO) that is heated from one side of rectangular enclosure of dimensions of 25 mm × 75 mm. The integrated simulation system ANSYS Workbench 15.0 for the numerical study was used including mesh generation tool ICEM and FLUENT software. In FLUENT, the melting model with Volume of Fluid (VOF) that includes the physical model to disperse nanoparticles in the PCM and their interactions is applied. During melting process, the enhancement of heat transfer is considered. For each nanoparticle analyzed, three different volume fractions are considered and compared. Dispersed nanoparticles in smaller volumetric fractions show a rise the heat transfer rate. The thermal performances are slightly greater using Al2O3 respect both ZnO that CuO nanoparticles.

Mohamed et al.[2017] uses Paraffin wax, microcrystalline wax. α-alumina (0.5, 1, 2 wt.%). Thermal conductivity increases with addition of nanoparticles and temperature for both types of base materials. Latent heat storage increases with addition of nanoparticles for both types of base materials. Paraffin wax (from 159.46 to 210.99 J/g) Microcrystalline wax (from 22.9 to 45.81 J/g). There are very minor changes on phase change temperature (solid-liquid) when both base mater.

III. METHODOLOGY

Dispersed metal oxide nanoparticles in paraffin wax might be a solution to improve latent heat thermal storage performance. Thermo-physical properties such as thermal conductivity and latent heat could be changed for different concentration of dispersed nanoparticle.

The geometry used taken form one of the research scholar’s M.Auriemma and A. Iazzetta (2016) is a rectangular box of size 25 mm × 75mm. It contains paraffin wax or paraffin wax dispersed with 1% and 3% by volume of three different nanoparticles Al2O3, ZrO2 and TiO2. The initial temperature of the nano PCM is 300 K, the hot wall side is at a constant temperature of 330 K (Tmax) and the cold wall, opposite the hot wall, is at 300 K (Tmin) in order, the other two walls are adiabatic.

Geometry Setup

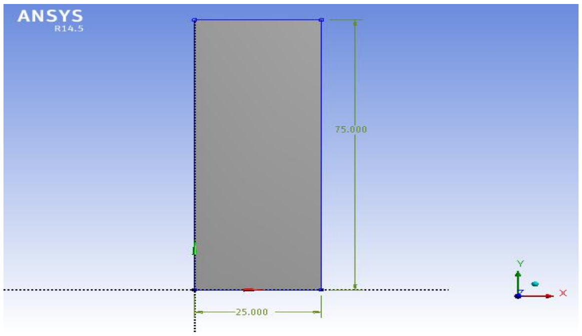

Figure 1 2D wall of the paraffin wax of rectangular enclosure 25mm*75mm.

Meshing and Name Selection

By, default, a coarse mesh is generated by ANSYS software. Mesh contains mixed cells per unit area (ICEM Tetrahedral cells) and quadrilateral at the boundaries.

Number of nodes-2025

Number of elements-1910

Curvature- On

Smooth – Medium

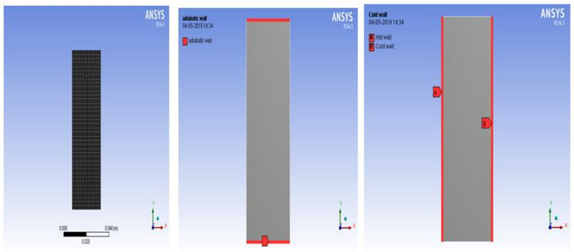

Figure 2 Meshing and name selection of 2D wall of the paraffin wax.

Fluent Setup and Model Selection

The mesh is properly checked and fine mesh is obtained. The analysis type is changed to heat transfer analysis type. The problem type is 2D and type of solver pressure-based solver. The PRESSURE BASED method with the FIRST ORDER UPWIND differencing scheme are used for solving the momentum and energy equations, whereas the PRESTO scheme is adopted for the pressure correction. In model selection only three parameters are selected. Remaining parameter is remained as default. The three parameters are: Energy – on and Viscous – Standard k-e standard wall Fn, mixture, Solidification and melting.

Material Selection

Table 1 Properties of PCM + Metal oxides at different volume fractions.

	Density (Kg/m^3)	Specific Heat (J/Kg-K)	Thermal Conductivity (W/m-K)	Dynamic Viscosity (N-s/m^2)
Paraffin at 300K	764.6429	2890	0.21	0.004123
Paraffin + 1% Al_2O_3	792.9964	2793.53	0.21622	0.00461
Paraffin + 3% Al_2O_3	849.7036	2619.90	0.22913	0.005978
Paraffin + 1% ZrO_2	812.9964	2719.726	0.21622	0.00461
Paraffin + 3% ZrO_2	909.7036	2433.482	0.229039	0.005978
Paraffin + 1% TiO_2	798.5664	2776.518	0.21631	0.00461
Paraffin + 3% TiO_2	866.413	2576.2165	0.22933	0.005978

Boundary Conditions

The boundary and test conditions are prescribed as follows:

- Hot wall T = Tmax

- Cold wall T = Tmin
- Adiabatic walls (Knpcm ΔT) = 0
- Initial condition Ti = Tmin

The simulation process ends after 1000 seconds.

IV RESULTS AND DISCUSSIONS

The thermo-physical properties of nano PCM. Essentially, thermal conductivity of paraffin wax dispersed with 1% and 3%, by volume of nanoparticles Al2O3, ZrO2 and TiO2 are plotted as a function of temperature and volumetric concentration.

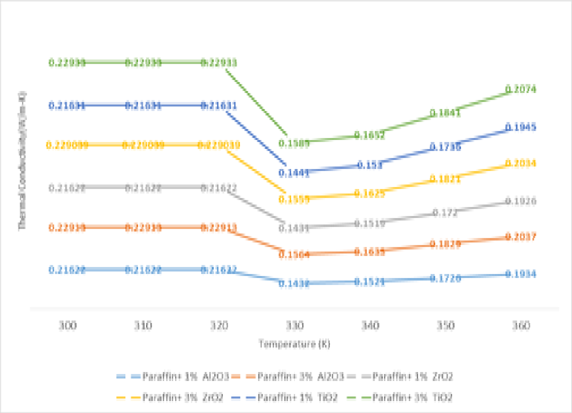

Figure 3 Thermal Conductivity for volumetric concentration of nanoparticle 1% and 3%.

It can observe that the thermal conductivity enhancement of the nanoparticles dispersed in paraffin can be seen markedly augmented with increasing temperature, (range 330K–360 K). This event, typically observed for the nanofluids, is due to the increased Brownian motion of nanoparticles in the base fluid having considerably reduced viscosity following a rise in temperature.

Table 2 Melting processes of paraffin wax and Al2O3 at nanoparticle concentration of 1% and 3%

Time (in seconds)	Liquid Fraction	
	Paraffin+ 1% Al_2O_3	Paraffin+ 3% Al_2O_3
200	0.09	0.11
400	0.16	0.19
600	0.28	0.31
800	0.54	0.58
1000	0.77	0.81

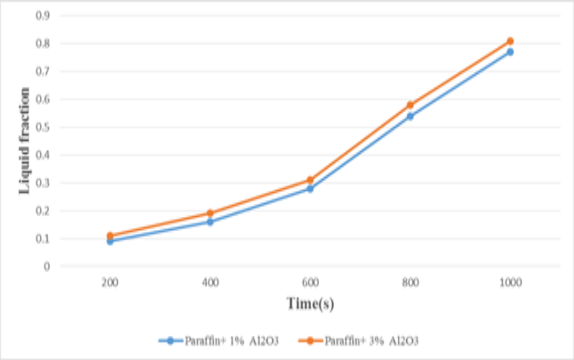

Figure 4 Melting processes of paraffin wax and Al2O3 at nanoparticle concentration of 1% and 3%

Table 3 Melting processes of paraffin wax and ZrO2 at nanoparticle concentration of 1% and 3%

Time (in seconds)	Liquid Fraction	
	Paraffin+ 1% ZrO_2	Paraffin+ 3% ZrO_2
200	0.085	0.105
400	0.145	0.17
600	0.26	0.3
800	0.51	0.57
1000	0.74	0.78

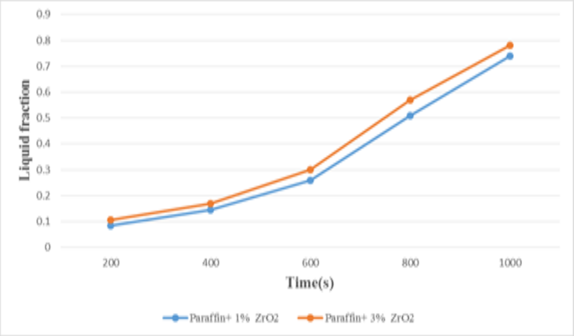

Figure 5 Melting processes of paraffin wax and ZrO2 at nanoparticle concentration of 1% and 3%

Table 4 Melting processes of paraffin wax and TiO2 at nanoparticle concentration of 1% and 3%

Time (in seconds)	Liquid Fraction	
	Paraffin+ 1% TiO_2	Paraffin+ 3% TiO_2
200	0.09	0.11
400	0.16	0.19
600	0.28	0.31
800	0.54	0.58
1000	0.77	0.81

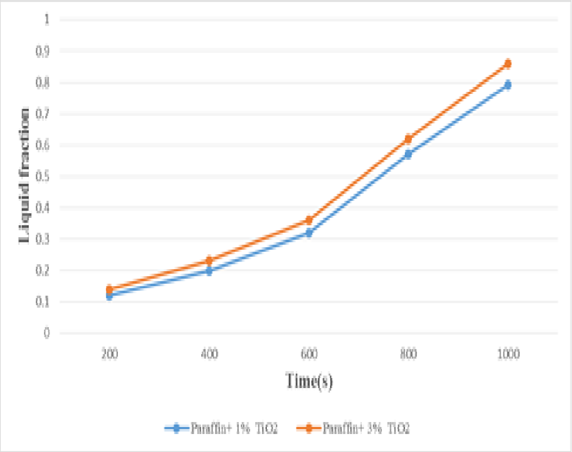

Figure 6 Melting processes of paraffin wax and TiO2 at nanoparticle concentration of 1% and 3%.

Table 5 Melting processes of paraffin wax and Al2O3, ZrO2 and TiO2 at nanoparticle concentration of 1% and 3%

Time (in seconds)	Liquid Fraction					
	Paraffin+ 1% TiO2	Paraffin+ 3% TiO2	Paraffin+ 1% ZrO2	Paraffin+ 3% ZrO2	Paraffin+ 1% Al2O3	Paraffin+ 3% Al_2O_3
200	0.12	0.14	0.085	0.105	0.09	0.11
400	0.2	0.23	0.145	0.17	0.16	0.19
600	0.32	0.36	0.26	0.3	0.28	0.31
800	0.57	0.62	0.51	0.57	0.54	0.58
1000	0.792	0.86	0.74	0.78	0.77	0.81

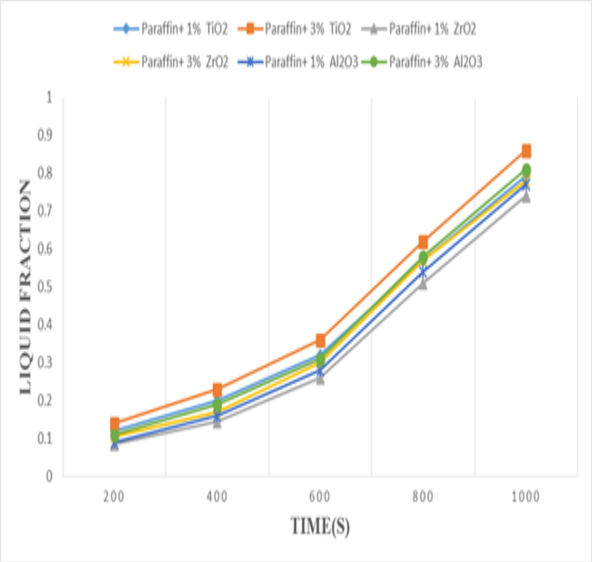

Figure 7 Melting processes of paraffin wax and Al2O3, ZrO2 and TiO2 at nanoparticle concentration of 1% and 3%

V. CONCLUSIONS

From the results mentioned in the previous chapter following conclusion can be drawn:

- Thermal conductivity of nano-enhanced PCM increases with the increase of nanoparticles concentration. However, it is observed that the effect of temperature on thermal conductivity of nano-enhanced PCM is similar to the characteristic of pristine PCM towards temperature changes.
- Thermal conductivity of nano-enhanced PCM depends on size or shape of nanoparticles.
- Density of PCM increases with the increase of nanoparticles concentration based on mixture model. Addition of nanoparticles in liquid PCM increases its viscosity behavior.
- Addition of nanoparticles reduces effect of sub-cooling and phase change duration.
- In the early stages of the melting process the heat transfer take place mainly by conduction process and after further heating it changes to natural convection.
- The melting percentage of PCM having 3% TiO2 concentration is more compared to nanoparticle concentration of 1% (Al2O3, ZrO2 and TiO2) and 3% (Al2O3, ZrO2).
- It requires 1000 Sec for paraffin wax + TiO2 (3%) to 86% melt while in case of paraffin wax + Al2O3 (3%) to 81% melt and in case of paraffin wax + ZrO2 78% to melt.

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