## Comparative Study between Experimental Analysis and CFD Software Analysis of PCM material in Thermal Energy Storage System

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Abstract—In this Research work, phase change materials are used to store heat energy, which can be utilized for Cold start in automobiles. Various PCMs like Paraffin wax, sodium acetate tri-hydrate and phenolphthalein are considered which are used to absorb heat from the coolant water from the engine. The conduction and convection criterion of heat transfer enable the PCM to store this heat as latent heat. The temperature change and thereby heat absorbed by the PCM is first studied experimentally. Then the amount of convection and temperature change brought about due to the heat flux has been simulated and studied in detail using GAMBIT and FLUENT. The experimental results and the simulation results have been compared and found to be similar. This has enabled us to identify the better PCM relative to the other PCMs which were studied.

*Index Terms*—Latent heat storage capacity, phase change materials, paraffin wax, sodium acetate tri-hydrate, phenolphthalein

#### I. INTRODUCTION

The world is looking for an alternative to reduce environmental pollution as it has emerged as the most important problem of this century. During Cold start in internal combustion engines, various problems such as increased fuel consumption resulting from heterogonous combustion, increasing concentration of toxins in emissions, increase in lubricant viscosity and resistance to motion and thereby increase in load on the accumulator and starter resulting in increased vibration and noise. Energy storage plays a critical and vital role in enhancing performance and reliability of Thermal Energy Systems. Developments of new devices that solve this problem are a necessity. Thermal energy storage system (TESS) is one such device. The TESS uses Phase Change Material's (PCM) latent heat storage capacity for pre-heating the internal combustion engine. The thermal energy storage device (TESD) works on the effect of absorption and rejection of heat during the solid-liquid phase change of heat storage material. The overall function of the TESS is dominated by the PCM. The PCM material should be selected considering the application and the working conditions. Depending on the applications, the PCMs should first be selected based on their melting temperature. Materials

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that melt below 288 K are used for storing coolness in air conditioning applications, while materials that melt above 363 K are used for absorption refrigeration. All other materials that melt between these two temperatures can be applied in solar heating and for heat load leveling applications. Hasan [1] has conducted an experimental investigation of palmitic acid as a PCM for energy storage. The parametric study of phase change transition included transition time, temperature range and propagation of the solid-liquid interface, as well as the heat flow rate characteristics of the employed circular tube storage system. Hydrated salts are attractive materials for use in thermal energy storage due to their high volumetric storage density (350 MJ/m3), relatively high thermal conductivity (0.5 W/m C) and moderate costs compared to paraffin waxes, with few exceptions. Hasnain et al [2] confirmed that the paraffin has excellent thermal stability as neither the cycles nor contact with metals degrades their thermal behavior. Lane [3, 4] has identified over 200 potential phase change heat storage materials melting from 283 to 363 K to be used for encapsulation. Xin-shi et al [5] has employed a compound phase change material, which consists of paraffin as a dispersed phase change material and a high density polyethylene (HDPE) as a supporting material. This new generation phase change material is very suitable for application in direct contact heat exchangers. Gu et al [6] developed a heat recovery system using PCM to recover the rejected heat of air conditioning systems and produce low temperature hot water for washing and bathing. They concluded that the heat recovery system decreases not only the consumption of primary energy for heating domestic hot water but also the calefaction to the surroundings due to the rejection of heat from air conditioning systems. Hong et al [7] tried to improve the accuracy of the T-history method for measuring heat of fusion of various materials and many of the PCMs were taken under study. Duffy et al [8] proposed a numerical simulation of porous latent heat thermal energy storage device for thermoelectric cooling under different porosities of the aluminum matrix. They used a porous aluminum matrix as a way of improving the performance of the system, enhancing heat conduction without reducing significantly the stored energy. Ravikumar et al [9] has proposed Cool storage system using phase change materials can be used for peak load shifting. Regin et al [10] proposed a paper in analyzing the behavior of a packed bed latent heat thermal energy storage system. The packed bed is composed of spherical capsules filled with paraffin wax as PCM usable with a solar water heating system and the phase change phenomena of PCM inside the capsules are analyzed by using enthalpy method. The equations are numerically solved, and the results obtained are used for the thermal performance analysis of both charging and discharging processes. Mahmud et al [11] studied a theoretical investigation of thermal and physical properties of a phase change material which consists of paraffin wax with 5% aluminum powder, this composite used as a thermal storage system for solar applications. Demirbas et al [12] studied about thermal energy storage materials and phase change materials and concluded that paraffin waxes are cheap and have moderate TES density but low thermal conductivity and, hence, require a large surface area. Hydrated salts have a larger energy storage density and a higher thermal conductivity. Amin et al [13] proposed and optimized usage of PCMs encapsulated in slabs. Using a validated numerical model of the system, a parametric study was undertaken to investigate the impact of the slab thickness, gap between slabs and the mass flow rate. Sari et al [14] studied determination of proper amount of paraffin absorbed into expanded graphite to obtain form-stable composite as phase change material. Zhang et al [15] found that expanded graphite composite phase change material had a large thermal storage capacity and improved thermal conductivity and did not experience liquid leakage during its solid-liquid phase change. He obtained a thermal conductivity which was higher than that of the paraffin, due to the combination with the expanded graphite that had a high thermal conductivity.

Phase change material storages are used to balance temporary temperature alternations and to store energy in several practical application areas. PCM storage is preferable to sensible heat storage in applications with a small temperature swing because of its nearly isothermal storing mechanism and high storage density. Phase change materials are employed in different fields of thermal engineering like energy storage, thermal conditioning of buildings, waste heat recovery, off peak power utilization, heat pump systems, space applications, laptop computer cooling, and telecom shelters. When a temperature peak occurs, PCM absorbs the excessive energy by going through a phase transition and releasing the absorbed energy later when the peak has passed off.

The possibility of varying conditions during the design process urges us to design a reliable PCM model which would enable parametric studies to be conducted at speed and would also enable the comparison of several alternatives. This would also preclude the need to build experimental platforms for measurements.

## II. THEORY

Heat transfer in PCM storage is characterized by a moving solid–liquid interface, generally referred to as the "moving boundary" problem. It is a transient, non-linear phenomenon. Analytical solutions for phase change problems are only known for a couple of physical situations which possess a simple geometry and simple boundary conditions, as nonlinearity poses major difficulties in moving boundary problems. Neumann originated the most well-known precise analytical solution for a one-dimensional moving boundary problem, called the Stefan problem. Some analytical approximations for one-dimensional moving boundary problems with different boundary conditions are the quasi-stationary approximation, perturbation methods, the Megerlin method and the Heat-balance-integral method. It has been assumed here that the melting or solidification temperature is constant. However, for example technical grade paraffin has a wide temperature range at the points where melting and solidification occur.

Phase change problems are usually solved with finite difference or finite element methods in accordance with the numerical approach. The phase change phenomenon has to be modeled separately due the non-linear nature of the problem. A wide range of different kinds of numerical methods for solving PCM problems exist. The most common methods used are the enthalpy method and the effective heat capacity method.

## III. THERMAL ENERGY STORAGE SYSTEMS (TESS)

The demand and supply gap for energy sources is widening day by day. Moreover, the fact that the energy can neither be created and nor destroyed has resulted in focusing of scientific research in the direction of storing the different forms of energy using diverse devices. Thermal energy is one such energy which is of interest to researchers worldwide. Thermal energy could have several geneses but storage of solar thermal energy is one of the principal areas of investigation. In recent years, various conventional and unconventional materials are investigated for their capability to store thermal energy. These thermal energy storage devices (TESD) are selected on the basis of some crucial physical, chemical and economic properties. Melting point, heat of fusion, density, heat capacity, thermal conductivity, compatibility with container and cost of production are the chief parameters for selection of TESD. It is a genuine challenge to find out an ultimate TESD as the overall suitability of materials to be used as TESD is governed by a multifaceted interplay between several properties of those materials.

#### IV. PROPERTIES AFFECTING TESS

#### A. Melting Point

Melting point is the temperature at which the first crystal of the material collapses. It is imperative to have the melting point of TESD within the temperature range of application. The melting point as such does not affect the energy storage capacity of a material. However, as a phase change is involved in melting, the inclusion of melting point in temperature range of application can permit the use of phase change as an on-off switch. Melting point lower as well as higher than the temperature range of application prohibits the use of the material in TESD.

#### B. Heat of Fusion $(\Delta H)$

Heat of fusion ( $\Delta$ H) also known as enthalpy of fusion or latent heat of fusion is a very important property useful in selecting a TESD. It refers to the amount of thermal energy that a material must absorb or evolve in order to change its phase from solid to liquid or vice versa. Large values of heat of fusion aid in increasing the efficiency of TESDs.

## C. Heat Capacity

Heat capacity refers to the amount of energy per molecule that a compound can store before the increase in its temperature. This energy is generally stored in translational, vibration and rotational modes. Thus materials with greater number of atoms in its composition are expected to have higher heat capacity.

## D. Thermal Conductivity (K)

Thermal Conductivity (k) measures the ability of a material to conduct heat. Greater values of k imply an efficient heat transfer. Thermal conductivity is a property which needs to be optimized. Since thermal conductivity is phase dependant property, it is important to know values of k in both the solid as well as molten phases. It has been observed that most of molten materials exhibit much higher values of thermal conductivity as compared to that in their solid state. Higher values of thermal conductivity in molten state can facilitate an efficient heat transfer and smooth operation of the thermal circuits in TESD.

## *E.* Density $(\rho)$

Density ( $\rho$ ) of a material refers to its mass per unit volume. Density values can readily be measured using densitometers. Materials with higher density thus occupy less space which in turn increases the energy storage capacity. Materials with high density obviously possess higher energy storage capacity but many of them show a significant decrease in density in their molten state. This is due to the expansion of their volume. Thus, if the TESD is placed in a sealed container in its solid phase, empty space equivalent to its volume expansion must be kept in the container. Considering the above, it can be generalized that materials with high density but very small change in density at the phase change temperature are attractive TESDs.

## F. Required Properties of a PCM

- High latent heat of fusion per unit mass, so that a lesser amount of material stores a given amount of energy.
- High specific heat that provides additional sensible heat storage effect and also avoid sub cooling
- High density, so that a smaller container can hold the material.
- A melting point in the desired operating temperature range.
- The phase change material should be non-poisonous, non-flammable and non-explosive.
- No chemical decomposition, so that the (TESS) system life is assured.
- PCM should exhibit little or no super cooling during freezing.
- No corrosiveness to construction material.

To solve some of the problems inherent in inorganic PCMs, interest has to be tuned towards a new class of material substances such as paraffin, fatty acids and polyethylene glycol. Those materials were more costly than common salt hydrates and they have somewhat lower heat storage capacity per unit volume.

## V. PROPOSED MODEL

A mechanical set up of a coolant box with an inlet and outlet pipe is taken. The PCM material is filled inside the PCM container which is placed in the middle of the coolant heat exchanger as in Fig.1. The coolant water that flows round the engine enters the coolant box with a velocity (V1) temperature (T1) and at a pressure (P1). The coolant water transfers heat within itself to attain an equilibrium temperature as a result of the convection. Conduction of heat takes place at the interface of coolant water and the PCM container which in turn conducts the heat to the PCM material. The PCM material now absorbs heat till its latent heat of fusion is reached. Phase change occurs now. After the phase change occurs, convection of heat takes place within the melted PCM till equilibrium is reached. The heat stored within the PCM can be later on used in purpose of heating up of the engine again while starting up initially.



Fig. 1. Schematic view of the TESD



Fig. 2. Position of TESD in engine system

## A. Location of TESD

The basic scheme of the TESD connection to the cooling system of the engine is in Fig.2. The TESD can be connected to the engine water jacket. During charge period, liquid moves through the TESD, the water jacket of the engine and radiator with the help of the water pump of engine. During discharging, because the thermostat is closed cooling liquid moves through only the TESD and the water jacket of the engine with the help of the electrical pump. The TESS for preheating of the engine consists of the TESD.

# *B. Grid Generation and Numerical Solutions by Fluent* 6.2

CFD techniques consist of numerical solutions of mass, Momentum and energy conservation with other equations like species transport. Solution to CFD problems is obtained in two main stages. The PCM volume is divided into small control volumes called mesh in the first stage. The structure of the TESD is created with the PCM storage tank inside it. Using Boolean operations of subtraction in Gambit, we subtracted the PCM volume from the TESD volume. This volume was meshed as shown in Fig.3.



Fig. 3. GAMBIT model of the TESD

The PCM volume was recreated and meshed separately. This allowed us to obtain the exact volumes of the TESD and PCM container for meshing purposes. Next part is the numerical solutions of mass, Momentum and energy conservation equations. In this case, unsteady energy balance equation has been solved in solid phase and unsteady momentum and energy balance equation have been solved simultaneously in liquid phase for each control volume. After making intricate meshing in gambit, it is exported to Fluent and in 3D, simulations were made using the material properties in Table 1.

FABLE I: PROPERTIES OF PCM MATERIA	١LS
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Physical	Phase Change Material			
Parameters	Paraffin Wax	Sodium Acetate Tri-hydrate	Naphthalene	
Wall Temperature in Kelvin (K)	343	343	343	
Viscosity (kg/m.s)	1.90	-	-	
Density (kg/m <sup>3)</sup>	900	1450	1140	
Heat conduction (W/m.K)	0.24	0.5	0.1221	
Specific heat capacity (C <sub>P</sub> ) (J/kg.K)	2900	1088	1720	

<u>NOTE\*</u>: These values of viscosity are not required as sodium acetate tri-hydrate doesn't melt and naphthalene sublimes.

- VI. EXPERIMENTALLY OBTAINED RESULTS AND DISCUSSION
- A. Results Obtained for Paraffin Wax:

TABLE 2. TEMPERATURE VARIATION OF THE TESD IN CHARGE PERIOD:			
S.no.	Time (S)	Temperature of paraffin wax (°C)	Temperature of coolant water (°C)
1.	0	27	70
2.	100	28.8	68.6
3.	200	30.5	67.2
4.	300	31.9	65.8
5.	400	33.8	64.5
6.	500	35.7	63.2
7.	600	36.9	62.3
8.	700	38.8	61.6
9.	800	40.6	60.9
10.	900	41.9	60.4
11.	1000	43.7	59.8
12.	1100	45.2	59.4
13.	1200	46.7	59.1
14.	1300	48.1	59.0

TABLE 3. TEMPERATURE VARIATION OF THE TESD IN DISCHARGE PERIOD

S.no.	Time (S)	Temperature of paraffin wax (°C)	Temperature of coolant water (°C)
1.	0	46.0	57.0
2.	100	44.5	58.4
3.	200	41.6	59.6
4.	300	40.0	60.3
5.	400	37.8	61.6
6.	500	36.1	62.8
7.	600	35.2	63.6
8.	700	34.0	64.9
9.	800	32.7	65.7
10.	900	31.4	66.3
11.	1000	30.2	67.2
12.	1100	29.1	68.0
13.	1200	28.6	68.4
14.	1300	27.5	68.5



Fig. 4. Temperature variation of the TESD in charge period

It is clear from table 2 that in the charge period, paraffin wax's temperature increases from 27 °C (300 K) to 48.1 °C (321.1 K) and temperature of coolant water decreases from 70 °C (343 K) to 59 °C (332 K). The graph in fig. 4 clearly shows the variation in temperature of paraffin wax and coolant water over a period of 1300 seconds.

It is clear from table 3 that in the discharge period, paraffin wax's temperature decreases from 46 °C (319 K) to 27.5 °C (300.5 K) and temperature of coolant water increases from 57 °C (330 K) to 68.5 °C (341.5 K). The graph in fig. 5 clearly shows the variation in temperature of paraffin wax and coolant water over a period of 1300 seconds.



Fig. 5. Temperature variation of the TESD in discharge period

B. Results obtained for Sodium acetate Tri-hydrate:

S.no.	Time (S)	Temperature of Sodium Acetate Trihydrate (°C)	Temperature of coolant water (°C)
1.	0	27.0	70.0
2.	100	31.2	68.1
3.	200	35.8	65.8
4.	300	40.5	63.2
5.	400	44.8	61.1
6.	500	47.9	58.7
7.	600	51.6	56.2
8.	700	55.2	54.5
9.	800	57.8	53.4
10.	900	59.9	52.6
11.	1000	63.2	52.1
12.	1100	65.1	51.7
13.	1200	66.7	51.5
14.	1300	66.8	51.3



Fig. 6. Temperature variation of the TESD in charge period



Fig. 7. Temperature variation of the TESD in discharge period

It is clear from table 4 that in the charge period, sodium acetate tri-hydrate's temperature increases from 27  $^{\circ}$ C (300 K) to 66.8  $^{\circ}$ C (339.8 K) and temperature of coolant water decreases from 70  $^{\circ}$ C (343 K) to 51.3  $^{\circ}$ C (324.3 K). The graph in fig. 6 clearly shows the variation in temperature of sodium acetate tri-hydrate and coolant water over a period of 1300 seconds.

S.no.	Time (S)	Temperature of Sodium Acetate Trihydrate (°C)	Temperature of coolant water (°C)
1.	0	64.0	49.0
2.	100	60.1	52.5
3.	200	56.3	54.2
4.	300	52.2	56.1
5.	400	49.3	57.8
6.	500	45.6	59.5
7.	600	41.2	61.3
8.	700	37.4	62.6
9.	800	34.6	64.5
10.	900	31.8	65.7
11.	1000	29.4	66.1
12.	1100	28.1	66.6
13.	1200	27.6	67.0
14.	1300	27.6	67.1

TABLE 5. TEMPERATURE VARIATION OF THE TESD IN DISCHARGE PERIOD

TABLE 6. TEMPERATURE VARIATION OF THE TESD IN CHARGE PERIOD

S.no.	Time (S)	Temperature of Naphthalene (°C)	Temperature of coolant water (°C)
1.	0	27.0	70.0
2.	100	30.2	68.2
3.	200	33.4	64.4
4.	300	36.1	63.2
5.	400	39.4	61.7
6.	500	42.2	60.3
7.	600	45.5	59.1
8.	700	47.2	58.2
9.	800	49.3	57.1
10.	900	52.4	56.4
11.	1000	53.2	55.9
12.	1100	54.6	55.2
13.	1200	55.4	54.7
14.	1300	55.4	54.6

It is clear from table 5 that in the discharge period, sodium acetate tri-hydrate's temperature decreases from 64 °C (337 K) to 27.6 °C (300.6 K) and temperature of coolant water increases from 49 °C (322 K) to 67.1 °C (340.1 K). The graph in fig. 7 clearly shows the variation in temperature of sodium acetate tri-hydrate and coolant water over a period of 1300 seconds.

#### A. Results Obtained for Naphthalene:

It is clear from table 6 that in the charge period, naphthalene's temperature increases from 27 °C (300 K) to

55.4 °C (328.4 K) and temperature of coolant water decreases from 70 °C (343 K) to 54.6 °C (327.6 K). The graph in fig. 8 clearly shows the variation in temperature of naphthalene and coolant water over a period of 1300 seconds.



Fig. 8. Temperature variation of the TESD In charge period

TABLE 7. TEMPERATURE VARIATION	OF THE TESD IN DISCHARGE PERIOD
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S.no.	Time (S)	Temperature of Naphthalene (°C)	Temperature of coolant water (°C)
1.	0	52.0	53.0
2.	100	49.3	54.8
3.	200	47.2	56.6
4.	300	45.1	58.5
5.	400	43.4	59.7
6.	500	41.3	61.2
7.	600	39.3	62.3
8.	700	37.5	63.1
9.	800	35.3	64.2
10.	900	33.1	65.1
11.	1000	31.2	66.0
12.	1100	30.5	66.5
13.	1200	28.8	66.9
14.	1300	28.8	67.0



Fig. 9. Temperature variation of the TESD In discharge period

It is clear from table 7 that in the discharge period, naphthalene's temperature decreases from 52 oC (325 K) to 28.8 oC (301.8 K) and temperature of coolant water increases from 53 oC (326 K) to 67 oC (340 K). The graph in fig. 9 clearly shows the variation in temperature of naphthalene and coolant water over a period of 1300 seconds.

## VII. RESULTS AND DISCUSSION FROM SOFTWARE ANALYSIS OF PCM MATERIAL IN TESS

The transient temperature profiles have been obtained by solving unsteady energy balance equation using Fluent 6.2 version. The temperatures profiles have been estimated. As the natural convection was considered in liquid phase therefore, unsteady momentum and energy balance equation have been solved simultaneously in liquid phase.

A. Results Obtained for Paraffin Wax





Fig. 11. Temperature contours of TESD containing paraffin wax

The temperature contours in Fig. 10 and Fig. 11 clearly show the decrease in temperature of the coolant water from 343 K to 332 K. The PCM exhibits a temperature change of almost 16 K as observed from the above graphical images obtained through fluent analysis.

B. Results Obtained for Sodium Acetate Tri-Hydrate



Fig. 12. Temperature contours of sodium acetate tri-hydrate



Fig. 13. Temperature contours of TESD containing SOdium acetate tri-hydrate

We observe that the temperature contours in Fig. 12 and Fig. 13 clearly show the decrease in temperature of the coolant water from 343 K to 324 K. The PCM exhibits a temperature change of almost 25 K. as observed from the above graphical images obtained through fluent analysis.

C. Results Obtained for Naphthalene:



Fig 14. Temperature contours of naphthalene



Fig. 15. Temperature contours of TESD containing naphthalene

The temperature contours in Fig. 14 and Fig. 15 clearly show the decrease in temperature of the coolant water from 343 K to 327 K. The PCM exhibits a temperature change of almost 20 K. as observed from the above graphical images obtained through fluent analysis.

#### VIII. CONCLUSION

Successful analysis of the transient heat transfer characteristics of phase change material has been carried out. From the temperature profiles we observe that sodium acetate tri-hydrate gives us the most promising results when compared to paraffin wax and naphthalene. Coolant water loses maximum heat to sodium acetate tri-hydrate which is obtained as drop in temperature from 343 K to 324K (in the coolant water) from the graphs obtained. This fact is verified from the experimentally obtained values where coolant water loses maximum heat to sodium acetate tri-hydrate which is obtained as drop in temperature of coolant water from70 °C (343 K) to 51.3 °C (324.3 K) and rise in temperature of sodium acetate tri-hydrate from 27 °C (300 K) to 66.8 °C (339.8 K) which is found to be more than the values obtained by using paraffin wax and naphthalene. In the software analysis, it is observed that the heat absorption in the PCM material decreases gradually as we travel from the inlet of coolant water towards the outlet of coolant water. The phase

change near wall is noted by the formation of a flat plateau regime on temperature vs. time plot. Different contours were generated by using Fluent. The temperatures profiles have been estimated.

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