An Analytical Model Characterising a Latent Heat Thermal Energy Storage Tank

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Synopsis

This paper details a research study that was undertaken by Babcock ME&S behalf of the UK Defence Science and Technology Laboratory (DSTL) to improve the understanding of cooling performance of Phase Change Materials (PCMs).

The Chilled Water Plants (CWP) on naval platforms are often not optimised to cope with high peak thermal demands whilst operating in challenging climates. The cooling demands on future platforms are set to increase with the introduction of high energy systems such as Laser Directed Energy Weapons (LDEWs), driving the exploration of alternative cooling technologies that have the potential to improve system efficiency and size.

Latent Heat Thermal Energy Storage (LHTES) systems utilise PCMs and have the ability to supplement the Chilled Water (CW) system and smooth cooling loads at peak demand. Phase Change Materials are substances which absorb and release large amounts of latent heat when undergoing a change in physical state.

A LHTES tank representative of scaled down naval system was modelled using 3D computational fluid dynamics (CFD) in ANSYS Fluent. Hydrated salts were chosen as the PCM due to the favourable thermal properties. The thermal characteristics of the tank and the viability as a cooling system were assessed by simulating a variety of thermal load profiles. The computational model acts as a digital twin of an experimental setup, which will later be used for validation. This paper is primarily focussed on the approach to modelling the tank, model parameters and findings.

Keywords: Computational Fluid Dynamics, Thermal Energy Storage, Phase Change Materials, Latent Heat

1. Introduction

The thermal demands on Naval platforms are becoming increasingly challenging due to operational environments and the introduction of laser directed energy weapons and high-powered radars. It is critical the thermal management of such systems are sufficiently capable to maintain operational integrity and provide a continuous platform functionality.

The thermal demands on-board a Naval vessel are traditionally met with chilled water or sea water cooling. These systems are often limited by spatial constraints and environmental conditions.

The thermal characteristics for a laser directed energy weapon are stochastic by nature with peak demands that exceeds traditional cooling capacity. The implementation of a Latent Heat Thermal Energy Storage (LHTES) system utilising Phase Change Materials (PCMs) is a potential solution with the ability to supplement a chilled water system and smooth out peak cooling demands; charging up overnight whilst demand is low and deployed during the day.

The capabilities of the thermal storage system are discussed in two papers preceding the project this paper is based upon, "The Potential of Thermal Storage Tanks to Assist in managing Peak Heat Loads on Naval Ships [Dawe T, 2020] and "Advanced Cooling Methods for Naval Laser Directed Energy Weapons" [Dubey L, Hook A 2020].

This paper details the approach to modelling a thermal energy storage tank which contributes towards the continued development and research into a thermal energy storage system for Naval systems. To assess the viability of a thermal energy storage system, a LHTES tank representative of scaled down naval system was modelled using Computational Fluid Dynamics (CFD) along with a physical experiment. The model acts as a digital twin of the experimental setup, which will later be used for validation.

Author's Biography

Lewis Godiff is a Mechanical Design Engineer working for Babcock International Group – Marine Engineering & Systems, based on HMNB Devonport, Plymouth, where he began his engineering career in 2017 as a graduate engineer. He is currently part of the mechanical engineering group and primarily involved in undertaking thermal and HVAC design and analysis for vessels in the Royal Navy's fleet.

2. Modelling and Experimental Methodology

A LHTES tank and control system were designed to replicate a scaled-down version of a ship's on-board tank in a laboratory setting. The experimental conditions were controlled, and data capture instrumentation was installed to analyse and monitor the tank and PCM performance and determine its effectiveness at providing cooling to variable load inputs.

The experiments are to be carried out at the Power Demonstration Networks Centre (PNDC) at the University of Strathclyde. A detailed schematic diagram of the experimental setup is shown in Figure 1.

The system can be configured depending on the test cycle, heating, cooling or pulse load. There are three 12 kW in-line heaters which replicate a constant thermal load profile. These can be independently operated to test the tank against different load profiles, 12 kW, 24 kW and 36 kW. Chilled water is supplied by a 30 kW chiller. The pulse load cycle is achieved by alternating between a pre-charged hot and cold Intermediate Bulk Container (IBC). There is a flow meter on the inlet and outlet measuring flow rate and temperature, the system flow rate is controlled by three diaphragm valves.

Note, at the time of writing this paper, the experiment is currently being setup and commissioned, therefore no results are available to compare with the digital model.

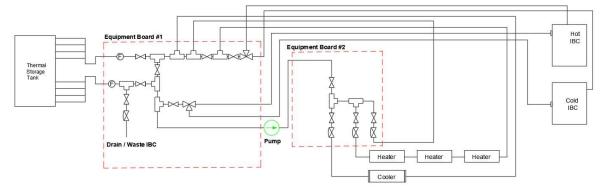


Figure 1: Schematic view of the experimental set-up

A computational model of the LHTES was created using ANSYS Fluent v2020 R2. The model acts as a digital twin of the tank, it does not account for the ancillary pipework or control system as shown above. The experimental outputs are used to validate the computational model. Post validation, the intention is to use the model for additional load cycles and operating scenarios.

2.1. Design Parameters

The TES tank acts as a thermal battery once charged to an initial starting temperature. For heating cycle (solid to liquid) an initial starting temperature of 12 deg.C was chosen as this is achievable from the operating conditions of an on-board CWP.

The operating parameters for the TES tank were designed for a specific heat exchanger. The system flow rate was set at 70 litres per minute. Unlike a traditional heat exchanger, the outlet temperature of a TES tank continually increases. As the PCM undergoes a phase transition and increases in temperature, the rate of heat transfer between the PCM and water decreases reducing the overall cooling capacity of the tank. The tank is classified as fully utilised when the outlet temperature reaches 20 deg.C due to the heat exchanger requirements.

3. Phase Change Material and Selection

Phase Change Materials (PCMs) are substances which absorb or release large amounts of latent heat when undergoing a change in physical state. The principle of latent heat thermal energy storage is to utilise the PCM as a storage medium of thermal energy by exploiting the latent heat during the phase transition as shown in Figure 2.

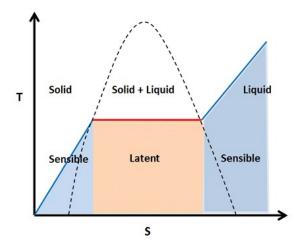


Figure 2: Sensible and latent heat during phase change of material

A latent heat energy storage tank possesses at least the following components:

- 1. A PCM with a melting point in the desired temperature range,
- 2. A surface in which the PCM material is contained,
- 3. A fluid medium with which to exchange heat with the PCM and external systems,
- 4. A vessel in which the PCM and heat exchange fluid are housed.

A conventional thermal energy storage tank uses water to store energy. Phase change material storage tanks can increase the stored energy density per unit volume. One experimental study shows the energy storage capacity for a rectangular tank filled with PCM increased by 35.5% compared to the same tank filled with water [Moreno et al, 2014]. The increase in capacity is proportional to the type and relative volume of PCM material.

The PCM can be selected so that the phase change temperature is suited around a specified system temperature profile. The LHTES tank in this paper has a thermal energy capacity of approximately 390% that of an equivalent water tank (water tank approximate capacity of 65,000 kJ, TES PCM tank approximately 320,000 kJ).

A hydrated salt solution was chosen as the PCM material. Hydrated salts are inorganic salts that contact with water molecules and undergo a change in their crystalline structure. They have advantageous characteristics for a TES tank such as a high latent heat to energy density ratio, non-flammable, well defined phase change temperature, relatively high thermal conductivity, and low cost.

PCM Products Ltd were chosen as the material supplier being able to supply an off the shelf product which comprises of salt hydrate PCM hermetically sealed in HDPE containers known as FlatICE (Figure 3). These modules are designed to be stacked in a tank environment (see nodules in Figure 3).



Figure 3: FlatICE module (Left - underside) (Right - topside)

The FlatICE modules are filled with PlusICE S17 (Hydrated Salt) PCM solution, utilising the melting phase change between solid and liquid. Salt Hydrates expand when solidified and therefore the internal cavity is approximately 90% filled with PlusICE S17, with an air gap to avoid over pressurisation and bursting of the module when it undergoes freezing.

The thermo-physical properties for PlusICE S17 PCM are shown in Table 1. The PCM is enclosed in a High Density Polyethylene (HDPE) container with a 2-3mm wall thickness.

Properties	PlusICE S17	HDPE	
Melting Temperature (deg.C)	17	126	
Latent Heat Capacity (kJ/kg)	155	-	
Volumetric Latent Heat Capacity (MJ/m ³)	236	-	
Specific Heat Capacity (kJ/kg.K)	1.90	1.9	
Density (kg/m ³)	1525	955	
Thermal Conductivity (W/mK)	0.43	0.43	
Maximum Operation Temperature (deg.C)	60	-	
Flat ICE S17 Module Weight	5.4 kg		

Table 1: Thermo-Physical Properties of PlusICE S17 [PCM Products Ltd]

4. Thermal Energy Storage Tank Design

4.1. Tank Configuration

The TES tank has internal dimensions of length 2110mm, width 1038mm and height 1000mm. the internal water column has a height of approximately 900mm, with 100mm spare for experimental data capture cabling. The tank contains a total of 320 FlatICE stacked modules with the tank makeup given in Table 2.

	Total Volume (m ³)	Total Mass (kg)
Water	0.59	596
FlatICE Modules (x320)	1.36	1728

The spatial arrangement of the tank is improved by separating it into 4 quadrants by installing a centralised horizontal and vertical divider; there are 80 modules in each pass section stacked in two columns as shown in Figure 4. This aims to improve the flow path and limit stagnant flow regions.

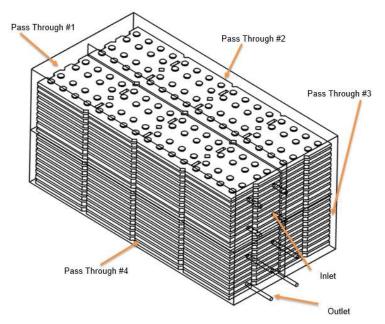


Figure 4: TES Tank arrangement and flow path

The modules are stacked and connected with male, and female 'lego-like' studs with a separation distance of \sim 12mm. The spacing between the modules and nearby wall is equal or less than the distance between the modules, encouraging water to flow uniformly through the modules to maximise heat transfer. There is a 50mm gap at the end of each pass-through section (lengthwise). This allows the water to mix as it flows to the next quadrant.

The tank is supplied via four inlets positioned uniformly on the inlet of pass number 1; four outlets are positioned at the end of pass number 4. Multiple inlets have been chosen to distribute the incoming water across the stacked modules and to promote mixing.

4.1. Tank Insulation

The tank wall is comprised of 12mm polypropylene, 50mm polyurethane and 9mm of polypropylene as shown in Figure 5.

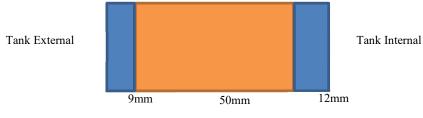


Figure 5: Tank insulation cross-section

The tank is insulated to minimise heat conduction and convection into the tank, reducing the effective heat load. This is important in the experiment so that the effect of heat transfer is not significant, to try and limit the complexity of the computer model. The net heat gain/loss transfer between the tank and the external environment based on the temperature difference has been calculated to inform the modelling. The heat transfer with the surroundings has been estimated using the following equation:

$$Q = U * A * dT$$

Where A is the surface area of the boundary layer, dT is the difference in temperature and U is overall thermal transmittance:

$$U = \frac{1}{(\frac{1}{heat \ transfer \ coefficient(1)} + \frac{thickness(1)}{thermal \ conductivity(1)} + \cdots)}$$

Heat transfer coefficients are assumed to be 50 W/m²K for air boundary and 2000 W/m²K for water. Values for the components of the boundary are shown in Table 3.

Layer	Material	Thickness (mm)	Surface Area (m ²)	Thermal Conductivity (W/mK)
Tank	Polypropylene	12	8.88	0.11
Insulation	Polyurethane	50	10.19	0.022
Cladding	Polypropylene	9	10.45	0.11
Lid	Acrylic	12	2.74	0.2

Table 3: Insulation properties

The tank has a calculated overall heat transfer coefficient of approximately $0.4 \text{ W/m}^2\text{K}$. Based on a temperature differential of 10 deg.C between the tank internal and external conditions, there is a thermal transfer of 40W which has a negligible effect on the overall tank thermal performance.

4.2. Tank Thermal Capacity

The theoretical thermal storage capacity as a combination of latent and sensible heat absorption due to a defined temperature rise, can be calculated with the following equation:

$$Q_{s} = \int_{t_{i}}^{t_{m}} m_{p}CpdT + m_{p}fL + \int_{t_{m}}^{t_{f}} m_{p}CpdT + \int_{t_{i}}^{t_{w}f} m_{w}CpdT$$
$$Q_{s} = m_{p}[Cp(t_{m} - t_{i}) + fL + Cp(t_{f} - t_{m})] + m_{w}[Cpw(t_{wf} - t_{i})]$$

Where:

- $Q_s = Thermal Storage Capacity$
- $t_i = Initial Temperature$
- $t_f = Final Temperature$
- $t_m = Phase \ Change \ Temperature$
- $t_{wf} = Final Water Temperature$
- $m_n = Phase \ Change \ Material \ Mass$
- $m_w = Water Mass$
- $f = melt \ fraction$
- L = Latent Heat Capacity PCM
- $C_p = Specific Heat Capacity PCM$
- $C_w = Specific Heat Capacity water$

Based on the thermal properties for PlusICE S17 and water with an initial temperature of 12 deg.C and an end temperature of 20 deg.C (Section 2.1) and assuming a total melt ratio of 1.0, the theoretical thermal storage capacity for the tank is calculated as $Q_s = 320,000 \text{ kJ}$. In reality, this figure is not physically obtainable. This would be the total energy absorbed by the tank if the tank was warmed from 12 to 20 deg.C very slowly, so that it reaches 20 deg.C uniformly throughout the tank and the PCM fully phase transitions. This is effectively the energy absorbed at close to a 0 kW load. The limiting factor for the actual total heat capacity is the PCM melt fraction, which is limited by the thermal conductivity, i.e. the outlet temperature is achieved before all the PCM undergoes a phase transition.

5. Computational Model

5.1. Geometry

The TES tank geometry is modelled in 3D with the tank wall and dividers as surfaces and the PCM blocks as solids as shown in Figure 6. The FlatICE module geometry is simplified to a state that improve the computational efficiency, whilst maintaining the output accuracy; the PCM volume and surface area is maintained. The PCM block thickness does not account for the HDPE wall thickness. The wall thickness and material properties are applied virtually and modelled as thin-walled shell elements to reduce the mesh complexity. The inlet and outlet pipe domains are modelled as 10x diameter to allow the velocity profile to fully develop.

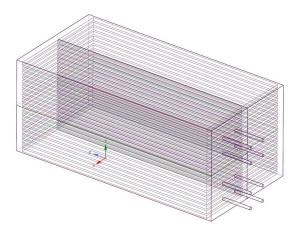


Figure 6: TES Tank model geometry

5.2. Assumptions

The assumptions made during the modelling are:

- 1. The air volume in the tank is considered negligible and not modelled
- 2. Volumetric expansion of the PCM (S17) is considered negligible and not modelled.
- 3. Thermo-physical properties of the PCM and HDPE are independent of the temperature
- 4. Natural convection is considered by the Boussinesq Approximation whereby density is constant
- 5. The melting is transient and unsteady
- 6. No heat generation within the PCM
- 7. External ambient conditions are not considered, external tank walls are modelled as adiabatic

5.3. Mesh Generation

The model is solved by finite volume method using the Fluent Meshing v20R2. The mesh elements allow the mathematical solver to apply governing equations to be solved on predictably shaped and mathematically defined volumes. The shared topology setting is applied to ensure a conformal mesh is created between all intersecting bodies (tank, partitions and PCM modules).

Surface Mesh

The following settings are applied for the surface mesh:

- 1. Global Settings
 - i. Minimum face size: 4mm
 - ii. Maximum face size: 60mm
 - iii. Growth rate: 1.2
- 2. Local sizing (Tank & Dividers)
 - i. Face size: 60mm
 - ii. Growth rate: 1.2
- 3. Local size (PCM Modules)
 - i. Face size: 5.8mm
 - ii. Growth rate: 1.2

Inflation Boundary Layer

Inflation layers are assigned to the boundary walls for the PCM modules and inlet and outlet pipes. Inflation layers improve the accuracy in modelling the velocity flow gradient at the wall boundary; this is particularly important when calculating heat transfer within the boundary layer on the PCM module surfaces as demonstrated in a literature [Ruzicka, 2018]. If the boundary layer is lacking resolution the correct rate of heat transfer is not modelled and the model will not accurately predict the cooling potential of the tank.

The k-Omega SST turbulence model used for the analysis, a y+ value of <1 is recommended for this model to take advantage of the low-Reynolds number formulation at the wall boundary. The y+ value is a non-dimensional distance and is used in turbulence modelling to determine the correct size of the cells near domain walls.

The PCM module boundary layer first cell height is calculated to achieve a y+ value of 1.

$$\Delta y = L \cdot y^+ \cdot \sqrt{74} \cdot Re^{-\frac{13}{14}}$$

Where:

- 1. $\Delta y =$ First cell layer height
- 2. Flow length scale, 29 mm (shortest length on PCM Block)
- 3. $y^+ = 1$
- 4. Reynolds Number Re

The Reynolds number is calculated by the hydraulic diameter method.

$$Re = \frac{VD_H}{v} = \frac{0.016 \cdot 0.031}{1e - 6} = 510$$

Where:

- 1. Bulk flow velocity, V = 0.0164 m/s
- 2. Hydraulic diameter, $D_H = 0.031$ m
- 3. Kinematic viscosity of water at 20 deg.C, v = 1e-6 m2/s

Therefore, the first layer thickness is given as:

$$\Delta y = 0.029 \cdot 1 \cdot \sqrt{74} \cdot 510^{-\frac{13}{14}} = 7.63e - 4m$$

The maximum first layer thickness to achieve a y+ of 1 is therefore 0.76mm.

The inflation layer settings applied to the PCM surface:

- 1. Inflation method: Uniform
- 2. First layer height 5e-4m
- 3. Number of layers, 10
- 4. Growth rate 1.05

An inflation is also applied to the inlet and outlet pipes with following settings:

- 1. Inflation method: Uniform
- 2. First layer height 5e-4m
- 3. Number of layers, 6
- 4. Growth rate 1.05

Figure 7 demonstrates the resultant inflation layer for the PCM surface. An inflation layer has not been added to the internal surface due to the solid phase and the local velocity being negligible during the liquid phase.

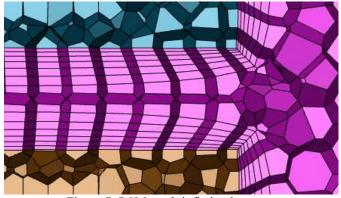


Figure 7: PCM mesh inflation layer

Volume Mesh

The Poly-Hexcore method is used to generate the volume mesh; this creates hexahedron elements in the bulk regions and isotropic poly-prisms in the boundary layer connection zones. This method results in a high-quality mesh whilst minimising element count. The maximum cell length was set to 18mm, the resultant mesh is shown in Figure 8 and comprises of 35 million cells.

The mesh quality is evaluated against the ANSYS Fluent recommended values, with all being good or above, orthogonal quality of 0.45, maximum aspect ratio 40.2, skewness 0.55.

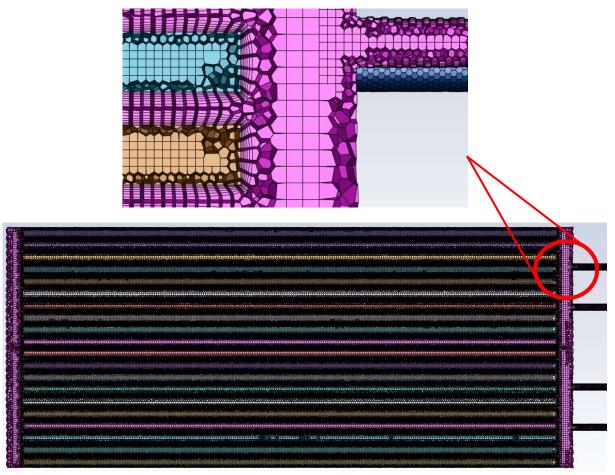


Figure 8: TES tank volumetric mesh with magnified section

5.1. Simulation Physics and Approach

The energy equation is applied to account for heat transfer; Fluent solves the total enthalpy form of the energy equation for a material as the sum of the sensible and latent heat. The solidification and melting model is applied to solve the phase change process across a defined temperature range.

The k-Omega Shear Stress Transport (SST) turbulence model is applied. This model is classified as a Reynolds-averaged Navier Stokes (RANS) model where all the effects of turbulence are modelled. This model is reliable at capturing the boundary layer when taking advantage of a fine near-wall mesh. It is well used in industry due to the high accuracy to computational expense ratio.

The size and complexity of the model means it is important to take an approach that minimises the simulation time. The Reynolds numbers in the bulk flow is calculated as laminar and the water flow rate is assumed constant during operation. The model is first initialised as steady state with the flow and turbulence equation active. After convergence is achieved, the model is continued as a transient simulation by enabling the energy equation only. The transient simulation has a time step of 10 seconds.

The pressure velocity coupling method for the steady state component is SIMPLEC and PISO for the transient component. The spatial discretization settings for pressure, momentum and energy are Second Order Upwind. Under relaxation factors are left as default.

A custom convergence criterion is applied based on the integral of the total surface heat flux across the PCM module surfaces at 10^{-4} .

The recirculation inlet and outlet boundary conditions are used. This replicates the experimental setup so that a fixed thermal load (kW) is continuously applied to the tank. The inlet and outlet temperature differential is set to 2.5 deg.C, 5.1 deg.C and 7.6 deg.C for the 12 kW, 24 kW and 36 kW load cycles, respectively.

6. Results and Discussions

The model was simulated against the three heating load cycles achievable in the experimental setup, 12 kW, 24 kW and 36 kW. It was challenging getting the model to run within a feasible time frame due to the intense computational demands. All simulations were performed on a desktop PC with an Intel Xeon 5120 processor, NVIDIA Quadro P6000 video card and 256 GB of RAM. Several issues occurred in trying to achieve a suitable level of convergence to ensure heat transfer was accurately modelled. It was found the mesh inflation layer settings have a significant impact on the overall rate of heat transfer and subsequent tank utilisation time; various settings were tested in order to achieve a converged result, Figure 9 shows the converged heat flux rate across the PCM surface.

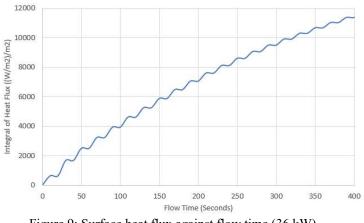


Figure 9: Surface heat flux against flow time (36 kW)

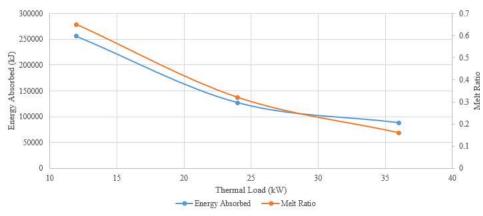
The surface wall y+ value was exported from Fluent having an average value of 0.67 and a maximum of 0.95, indicating the inflation settings are sufficient for capturing the velocity profile in the boundary layer with a y+ <1.

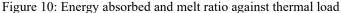
The results from the load cycles are shown in Table 4. The operating time is the period until the tank outlet temperature reaches 20 deg.C. The results demonstrates that a suitably sized TES tank is able to provide a significant amount of cooling for a defined period. Although the outlet temperature has been achieved, the average melt ratio shows that the PCM mass has not been fully utilised, this becomes more apparent as the thermal load (temperature difference) increases.

Tabl	le 4:	TES	tank	model	result
l'ab!	le 4:	TES	tank	model	result

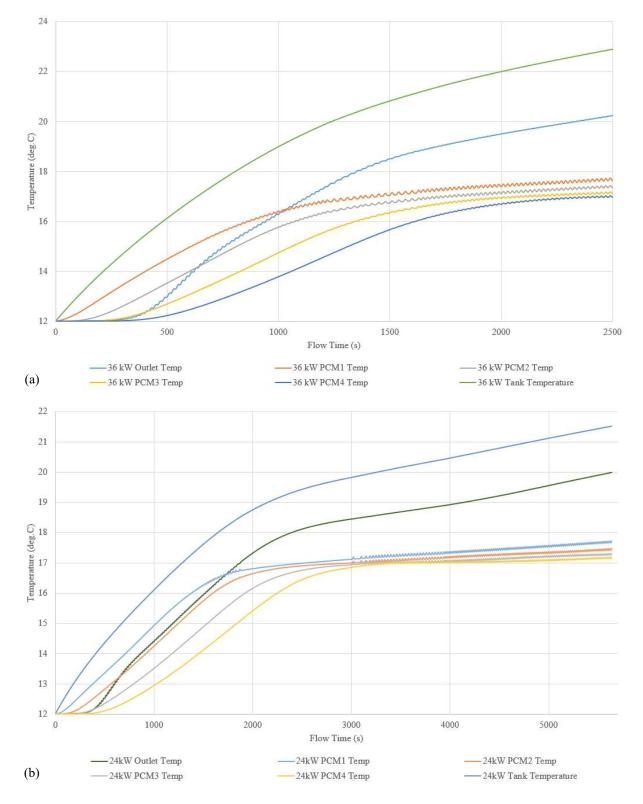
Load	Operating Time	PCM Temperature	Tank Melt Ratio (%)	Energy Absorbed
(kW)	(Seconds)	(deg.C) (Average)		(kJ)
12	18860	18.6	0.77	256092
24	5640	17.4	0.32	126930
36	2340	17.2	0.16	87957

A lower thermal load corresponds to a greater amount of energy absorption, as discussed in Section 4.2 and shown in Figure 10. As expected, the melt ratio is also shown as having a strong correlation to the energy absorbed.





The predicted temperature plots for each cycle are shown in Figure 11. The graphs share a similar profile, all with a linear increase in temperature at the start indicating sensible heating until around 16 deg.C. As the PCM temperature approaches 17deg.C it begins to plateau, evidence of latent heating. The temperature change is subtle due to the large amount of energy required. This corresponds to a reduction in outlet temperature, indicating the PCM is absorbing more energy from the inlet stream. This effect is less apparent at a higher thermal load as the rate of heat transfer within each module is not enough to keep pace with the warming tank.



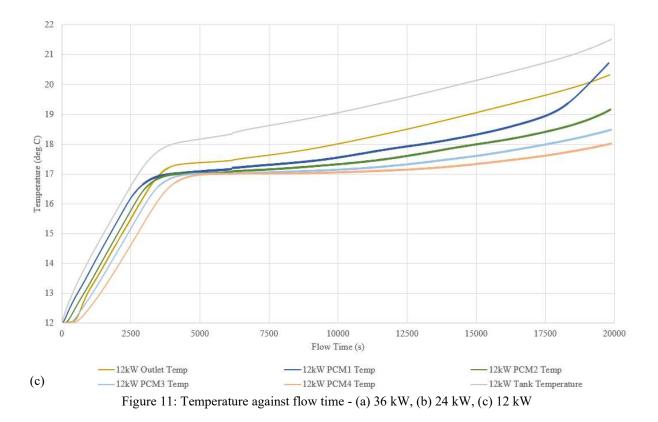


Figure 12 shows contour plots for the melt ratio through a cross section at passes 1 and 4 against 12 kW at varying time intervals.

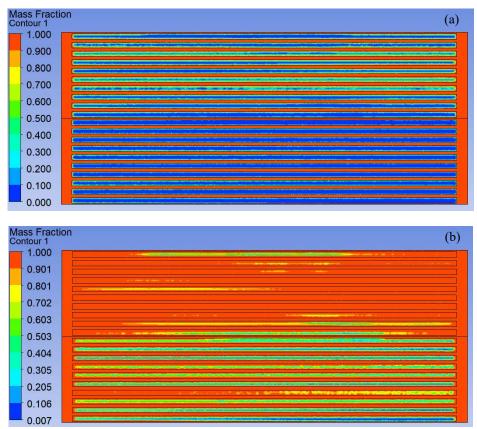
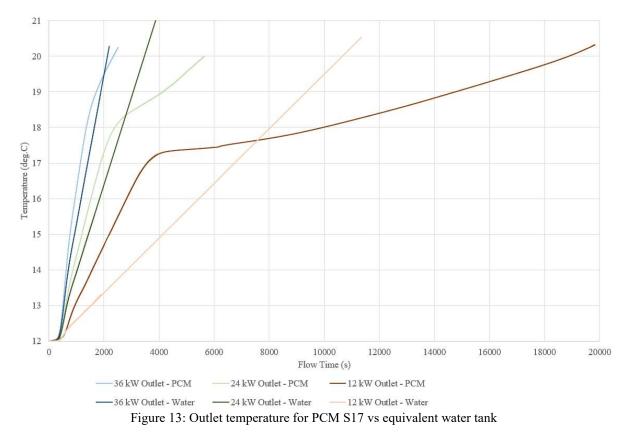


Figure 12: Liquid fraction contour plot - (a) 10,000 seconds, (b) 20,000 seconds

The PCM volume was replaced by liquid water and simulated to provide an equivalent comparison between the two. The results are shown in Figure 13. The outlet temperature gradient is lower for the water model due to the increased thermal characteristics compared to hydrated salts. The graphs for water show a linear profile due to all heating being sensible. At higher thermal loads, the PCM does not have a significant advantage as the rate of heat transfer to the PCM does not keep pace with the warming tank. At lower thermal loads, the PCM melt ratio increases which results in a significantly increased operational time compared to water. For example, at 12 kW, the total energy absorbed is 127,920 kJ for water and 256,092 kJ for the PCM, a 100% increase.



7. Conclusion

This paper has shown the modelling process and key considerations in the development of a computational model for a thermal energy storage tank that replicates an experimental setup.

The model results show the huge potential of a latent heat thermal energy storage system at being able to provide a stored capacity of cooling that can be utilised when required. It has shown that the utilisation of the PCM during the phase transition is linked to the temperature differential. However, the PCM thermal conductivity needs to be greatly enhanced to speed up the process of energy storage.

The next step for the project is to conduct the experiment and compare the findings with the computational model. Further research and testing will be focused on investigating methods for improved heat transfer, optimising the tank configuration flow path, control equipment and designing around additional Naval equipment heat loads (i.e. HVAC). This will ultimately conclude with a potential system that can utilise the diurnal cycle of a ships CW loading cycle to sustain systems during the day and be recharged during periods of low demand.

8. Acknowledgement

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