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Fast and experimentally validated model of a latent thermal energy storage device for system level simulations

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Abstract

Latent storages utilising phase change materials (PCM) to store thermal energy offer a considerably higher energy density at a nearly constant temperature level in comparison to sensible storage systems. Despite this advantage, only a few companies have successfully incorporated latent storage technologies into their product range. This may be due several engineering challenges and in particular the lack of a computationally fast and accurate mathematical model to facilitate the optimal incorporation of latent heat storages into an energy system. The presented study fills this gap and proposes a new, fast and experimentally validated mathematical modelling approach for latent heat storage units.

The modelling approach is based on a 1-dimensional finite volume discretisation of the governing energy equation applied to the storage unit. The phase change is modelled using an effective heat capacity of the PCM. A source term is introduced, which accounts for the thermal input and output to and from the heat exchanger. The rate of heat transfer is calculated using analytical heat transfer equations for the given heat exchanger geometry. Effective thermal conductivities are applied to describe the heat transfer from the phase change material to the heat transfer fluid and vice versa.

To calibrate and validate the model, a comprehensive experimental campaign was performed using two different commercial latent storage units supplied by Sunamp Ltd. with a phase change temperatures of 34°C and of 58°C. Both units use a salt hydrate based phase change material in combination with a fin-tube heat exchanger. A comparison between experimental and model generated data showed excellent agreement. The averaged heat transfer outlet temperature deviation between model and experiment for a given inlet temperature profile and mass flow rate for two different subsequent charging and discharging cycles amounts to less than 1.2 K for both storage units. Furthermore, it could be demonstrated that the model can be used with analytic equations for the effective thermal conductivity and hence does not require a calibration if used for other PCMs or HEX geometries. Due to its low computational burden and its physical modelling approach, the proposed model may be used for both fast system level performance investigations as well as latent storage design for a given application. It may therefore be implemented in commercial software packages such as TRNSYS [1] or Simulink [2].
1. Introduction

According to the International Energy Agency in 2014, heat accounted for a third of the world energy consumption in the year 2011. Around three-quarters of final energy use for heat was provided by fossil fuels [3]. As penetration of fluctuating renewable energy sources increases, energy storage is of paramount importance to solve the mismatch between supply and demand. Since final energy consumption of heat is much larger than electricity, especially in domestic dwellings [4], the end user's flexibility and self-consumption of renewables may be significantly increased using thermal energy storage. Thermal energy storage systems are hence regarded as a key technology for enabling increased share of renewable energy in the supply system [5].

Latent heat storage systems offer the ability to store a considerable amount of heat at an almost constant temperature. To enhance the heat transfer between the phase change material and the heat transfer fluid (HTF), the heat exchanger surface is usually extended e.g. by the usage of fins [6]. Latent heat storage systems incorporating phase change material (PCM) surrounded heat exchangers have been investigated in many applications. They can be integrated in the space heating systems [7] or used to store thermal energy for domestic hot water supply 'cite Campos-Celador [8]–[10]. The high volumetric energy density may also allow an increased self-consumption of photovoltaic power using PV-driven heat sources (heat pump or direct electrical). Furthermore, PCM based storage can be used to absorb heat from solar thermal collectors and provide it when needed, thus increasing their overall solar fraction [11]. PCM surrounded heat exchangers have further been investigated in solar cooling applications [12] or for waste heat recovery [13]. Other studies used the technology as buffer storage in air-conditioning or heat pump systems where the ability to store heat at an almost constant temperature level is a very attractive feature. It could be shown that PCM based storages have beneficial effects on the efficiency of the defrosting of air/refrigerant heat exchangers in heat pumps systems[14], in heat pump water heaters [15] and in air conditioning systems [16].

It appears that research in the field of latent storage technology mainly focuses on the enhancement of the heat transfer or the optimization of phase change material properties. However, a remaining challenge which has been rarely addressed in literature is the optimal integration of latent storages into an energy systems which requires an analysis of interactions between the storage and connected system components. The optimal dimensioning and integration, however, is a key requirement to fully exploit the potential advantages of latent storage systems regarding cost and energy savings. Dynamic computer models are a promising approach to tackle this challenge.

It is therefore the scope of this work to propose a model that is capable to predict the behaviour of the latent heat storage and its integration into the overall energy system. It is particularly of interest that the model allows to conduct long term system simulation (e.g. on a yearly basis) dependent on changing boundary conditions. Low computational effort what results in short simulation times is a crucial necessity.

In this study, “Heat Batteries” manufactured by Sunamp Ltd. [17] were used for model calibration and validation. These Heat Batteries are salt hydrate based latent storage units. They are equipped with a fin-tube heat exchanger (HEX), which transfers heat from a heat transfer fluid to the PCM surrounding the HEX and vice versa. With such systems relying on a multitude of interconnected physicaland thermal processes, the availability of computationally fast and accurate mathematical models are of great importance to determine the sensitivity of each process on the heat transfer rate, to optimise their design, and to investigate the performance of whole energy systems.

In the following sections, the modelling approaches for the design and dimensioning of latent heat storage systems will be discussed.
1.1 Numerical modelling approaches

The modelling of latent storage systems is based on a mathematical formulation of the solid/liquid phase change. The analysis of the heat transfer in phase change processes is complex due to the nonlinearity of the solid/liquid interface.

The numerical methods applied in research to describe phase changes can be divided in adaptive grid and fixed grid methods. Using the adaptive grid methods, the exact location of the solid/liquid interface is evaluated on every grid point for each time step and thus the grid has to be adopted for every timestep. Fixed grid methods do not require an explicit treatment of the solid/liquid interface, instead the position is estimated by the calculated temperatures. However, fixed grid methods require a scheme able to cope with strong nonlinearities. The major advantage of fixed grid methods is that mass- momentum and energy equations may be applied independent on the present phase of the material. Accordingly, the mathematical calculation of the phase change can be achieved through simple modifications of existing heat transfer numerical methods [18].

The fixed grid approaches can be further categorised into the enthalpy method and the effective heat capacity method [19]. Governing equations are introduced that are applied for both, the discretised solid and the liquid phase. Using the enthalpy-based method the enthalpy is described as a temperature dependent algebraic expression [20]. A phase change temperature range (the so-called mushy zone) is defined in which the phase change enthalpy is added or subtracted to the specific temperature dependent enthalphy of the PCM. Thus, the solid/liquid interface is not explicitly tracked but its location is defined by the mushy zone. In the effective heat capacity method, the latent heat is approximated by a large heat in sensible form over the phase change temperature interval [18]. Measurements (e.g. Differential Scanning Calorimetry DCS) may be used for both methods [19], [21].

Neglecting natural convection, the governing energy equation reads

\[ \rho \cdot \frac{\delta h}{\delta t} = \nabla \cdot (\lambda \nabla T) \]  

Eq.(1)

for the enthalpy formulation and employs or uses \( \rho, \lambda \) and \( h \) as the temperature dependent density, thermal conductivity and enthalpy of the PCM and \( T \) as the PCM temperature. The effective heat capacity method is based on the following equation:

\[ \rho \cdot c_{p,\text{eff}} \cdot \frac{\delta T}{\delta t} = \nabla \cdot (\lambda \nabla T) \]  

Eq.(2)

Here, \( c_{p,\text{eff}} \) is the temperature dependent effective heat capacity of the PCM. The advantages of the enthalpy method is the better numerical stability, however, interims steps to calculate the temperature field are required. Contrary, the effective heat capacity method calculates the temperature field directly[21]. For both approaches, the finite volume method (FVM) as well as the finite element method (FEM) can be applied to facilitate the analysis of complex geometries such as finned heat exchangers. Both, the enthalpy and the effective heat capacity method are introduced in commercially available computational heat transfer codes [22], hence they have been extensively used in the past to investigate the heat transfer in latent heat storages using fin-tube heat exchangers in several studies.

Velray et. al [41] studied the solidification process of a tube heat exchanger with internal fins. A 2-dimensional enthalpy-based model was used. Experimental data of temperatures at fixed positions were compared to the numerical data. The comparison showed good agreement. Similar work was performed by Jmal et al. [24]. A numerical study of PCM solidification in a finned tube heat exchanger including natural convection was performed in their work. The 2-dimensional model, based on the enthalpy method, was validated with experimental data. Therefore, temperatures at fixed positions are compared in this work. Khalifa et al. [25] published a numerical and experimental study on solidification around axially finned heat pipes. The enthalpy-based method was used and again the 2-dimensional model was validated using temperatures measurement at fixed positions.
Neumann et al. [26] combined a complex 3-dimensional model based on the effective heat capacity method with a 1-dimensional model to investigate the heat transfer in a latent storage using a fin and tube heat exchanger. Within the former model, half a fin and a fin gap filled with PCM was modelled and the 1-dimensional model was then used to model the entire heat exchanger pipe. Using this approach, the computational burden could be considerably reduced. However, the computational time required was still around 30min on a recent workstation for a charging process. Zauner et al. [27] modelled a discharging process of a finned tube latent heat storage unit using effective heat capacities. To reduce the computational effort, they exploited the rotational symmetry of the heat exchanger geometry.

The computational efficiency for a small 2-dimensional domain of a latent storage geometry was comprehensively investigated by Pointner et al. in [28]. Both, the enthalpy and the effective heat capacity method were investigated. The study showed that for a mesh size of 20x21, the computational time highly depends on the algorithm used but remains in any case considerable because of the relatively high number of elements resulting from the 2-dimensional geometry. A 1-dimensional model can lead to a considerable reduction of the computational time. However, the heat transfer between PCM and heat transfer fluid has to be described analytically in this case. Using effective heat conductivities for the PCM/fin compound appears to be a promising method to tackle this challenge.

To the best knowledge of the authors, no numerical model of a fin-tube latent storage exists in literature, which is suitable for system simulations over an extended period of time with low computational effort and high accuracy.
2. Methods

This chapter is divided into two parts. The first section deals with the numerical model developed in the study. In the second section, the experimental apparatus developed by Heriot-Watt University and the experimental procedure are described.

2.1 Numerical modelling approach

2.1.1 Governing equation and discretisation

The basis of the numerical approach applied in the present study is a 1-dimensional energy governing equation for conductive heat transfer. Convective effects are tackled using an effective thermal conductivity of the material. The 1-dimensional governing equation is given in Eq.3.

\[ C_{tot} \frac{dT}{dt} = A_{cs} \cdot \lambda_{eff} \cdot \frac{dT}{dx} + (\dot{Q}_{HEX} - \dot{Q}_{Loss}) \quad \text{Eq.}(3) \]

\( A_{cs} \) is the cross-section area of the storage unit and \( \lambda_{eff} \) the effective thermal conductivity of the PCM heat exchanger compound. \( C_{tot} \) is the lumped or total heat capacity of the node which is calculated based on the mass and heat capacity of the heat exchanger \( m_{HEX} \) and \( c_{p,HEX} \) as well as mass and effective heat capacity of the PCM \( m_{pcm} \) and \( c_{p,pcm,eff} \) respectively. The lumped heat capacity of the considered slice \( C_{tot,i} \) is:

\[ C_{tot,i} = \frac{m_{HEX} c_{p,HEX} + m_{pcm} c_{p,pcm,eff}(T_i)}{N} \quad \text{Eq.}(4) \]

The heat capacity of the heat exchanger is assumed to be constant. For the PCM, the effective heat capacity method is applied. Therefore, the capacity during phase change is considerably higher than in the completely liquid or solid phase. Data obtained through three-layer calorimetry [29] for the effective heat capacity \( c_{p,PCM,eff} \) was used for both PCMs. Between all measured data points, a cubic interpolation was performed. A plot of the two measured heat capacities is shown in Figure 1.

![Figure 1: Effective heat capacity values based on three-layer calorimetry measurements for (a) the SU34 and (b) the SU58 PCM. To prevent numerical instabilities in the model presented here, the data is interpolated with a cubic polynomial between all points.](image)

As shown in Figure 2, the storage unit is spatially discretised into \( N \) nodes of equivalent height \( \Delta h = \frac{h}{N} \) with \( h \) as the total height of the storage unit. Two source terms are introduced which account for the storage losses in node \( i \) \( \dot{Q}_{Loss,i} \) as well as the enthalpy exchanged by the heat exchanger \( \dot{Q}_{HEX,i} \). The resulting differential equation describes the temperature evolution within a storage node \( i \):

\[ C_{tot,i} \frac{dT_i}{dt} = A_{cs} \cdot \lambda_{eff} \cdot \frac{dT_i}{dx} + (\dot{Q}_{HEX,i} - \dot{Q}_{Loss,i}) \]
\[ C_{\text{tot},i} \frac{dT_i}{dt} = A_{Cs} \left( \lambda_{\text{eff},i+1} \cdot \frac{(T_{i+1}-T_i)}{\Delta h} + \lambda_{\text{eff},i-1} \cdot \frac{(T_{i-1}-T_i)}{\Delta h} \right) + \left( \dot{Q}_{\text{HEX},i} - \dot{Q}_{\text{Loss},i} \right) \quad \text{Eq. (3)} \]

Where \( A_{Cs} \) is the cross-section area of the storage unit and \( \lambda_{\text{eff},i+1} \) as well as \( \lambda_{\text{eff},i-1} \) are the averaged effective thermal conductivity values of the PCM heat exchanger compound between node \( i \) and \( i-1 \) respectively node \( i \) and \( i+1 \).

The following assumptions are the foundation of the developed model:

- The temperature is constant within one slice.
- The heat exchanger (fins and tube coils) has the same temperature as the PCM within a node.
- The thermal inertia of the HTF within the HEX tubes is neglected and the HTF acts as a heat source only.
- To calculate the heat transfer from the HTF to the PCM, stationary conditions are assumed within a single time step, which lead to the application of simple, analytic equations to describe the heat transfer.
- Phase transition kinetics, such as supercooling during solidification, are neglected. Due to the large PCM volume (approx. 17L) and the utilisation of nucleating agents, this assumption appears to be reasonable.
- A constant, temperature independent effective thermal conductivity exists for both, the solid and the liquid phase of the PCM.

Finally, at the boundaries (node 1 and N), a zero-gradient condition is defined since losses to the environment are considered as a source term in the governing equation.

2.1.2 Description of the source terms in the heat transfer equation

**Losses**

The heat losses from node \( i \) to the environment are estimated with an overall heat transfer coefficient between the PCM and the ambient. The storage modules are insulated with vacuum insulation panels. Due to the high thermal resistance between of the vacuum panels \( R_{\text{ins}} = 20 \text{mm} \) and a conductivity of \( \lambda_{\text{ins}} = 0.004 \text{ W/(mK)} \), \( R_{\text{ins}} = 8.8 \text{K/W} \), free convection at both boundaries of the storage.
tank wall is neglected to the losses ($R_{conv}=0.09 K/W$ assuming 20 W/(m²K) free convection heat transfer coefficient). The resulting equation for steady-state heat conduction reads:

$$Q_{loss,i} = A_{amb,i} \cdot \frac{\lambda_{ins}}{l_{ins}} (T_{PCM,i} - T_{amb}) \quad \text{Eq.(5)}$$

where $A_{amb,i}$ is the surface area between the PCM and ambient of node i. Furthermore, $\lambda_{ins}$ and $l_{ins}$ are the thermal conductivity and thickness of the insulation (cf. Section 2.2.1 for details).

**HEX input and output**

The heat exchanger input and output $Q_{HEX,i}$ is calculated based on an energy balance for the heat transfer fluid applied on node i, hence,

$$Q_{HEX,i} = m_{HTF} \cdot c_{p,HTF} \cdot (T_{HTF,in,i} - T_{HTF,out,i}) \quad \text{Eq.(6)}$$

where $m_{HTF}$ is the mass flow rate of the heat transfer fluid (here water) and $c_{p,HTF}$ the specific heat capacity of the heat transfer fluid, assumed to be constant. A simple upstream scheme is used for the calculation of the HTF inlet temperature of the node, thus, for instance, the inlet temperature of node i corresponds to the outlet temperature of node i-1. For the first node, $T_{in,1}$ corresponds to the storage inlet temperature. The outlet temperature of each node is calculated using the logarithmic temperature difference $\Delta T_n$, between the heat transfer fluid and the PCM [30]. The resulting heat flow rate from the PCM to the HTF is calculated using Eq.(7):

$$Q_{HEX,i} = A \cdot U_i \cdot \Delta T_{in,i} \quad \text{Eq.(7)}$$

Where $A$ is the inner tube wall area within node i and $U_i$ the overall heat transfer coefficient from HTF to PCM which is explained below. The resulting heat transfer rate based on equation (7) must fulfil the HTF energy balance defined in equation (5). The resulting system of equations is solved to obtain the HTF outlet temperature of node i.

The overall heat transfer coefficient from the phase change material to the heat transfer fluid $U_i$ is calculated using analytical equations which describe the heat transfer in the given geometry. In the present case, a fin-tube heat exchanger of the supplier, Sunamp Ltd. was utilised. A simplified schematic of a part of the HEX geometry is shown in Figure 3. The geometry is composed of a cylindrical copper tube surrounded by the PCM. To enhance the heat transfer, metallic fins are used as illustrated in Figure 3 (b). The heat transfer from the HTF to the outer tube wall may be analytically described using the first two terms in the denominator of Eq. (8). For a more complex fin geometry, however, no simple analytic solution exists. Furthermore, during the phase change, the liquid/solid interface is time varying which continually alters the coefficients. In the current study, a simple, computationally efficient method related to the effective medium approach introduced by Lamberg et al. [31], is applied. Thus, the finned HEX geometry is modelled using an analytical description for a cylinder in combination with an effective conductivity $\lambda_{eff}$ which accounts for the presence of the fins and additional physical effects, e.g. convection. The resulting overall heat transfer coefficient $U_{HTF}$ between the PCM and the HTF with respect to the inner radius of the tube coil yields:

$$U_{HTF} = \frac{1}{\frac{1}{U_{HTF}} + \frac{1}{U_{in}} \ln \left( \frac{r_{TC,in}}{r_{TC,in}} \right) + \frac{1}{U_{out}} \ln \left( \frac{r_{TC,out}}{r_{TC,out}} \right)} \quad \text{Eq.(8)}$$

where $U_{HTF}$ is the convective heat transfer coefficient from the HTF to the inner tube wall, $r_{TC,in}$ and $r_{TC,out}$ the inner and outer tube wall radius respectively, $\lambda_{TC}$ the thermal conductivity of the tube coil. $\lambda_{eff}$ depends on the state of the PCM and accounts for physical effects present in each phase.
Figure 3: Simplified part of the heat exchanger geometry: (a) cut through a heat exchanger coil and (b) corresponding side view.

In this study, it is assumed that a constant, temperature independent effective thermal conductivity exists for both, the solid and the liquid phase of the PCM. In the solid phase, the effective conductivity accounts for the effects of the fins as well as the thermal contact resistance. In the liquid phase, the effects of free convection are considered in the lumped coefficient. In the two-phase region, the transfer coefficient is linearly interpolated between the effective conductivity of the two phases according to the liquid fraction. Mathematically, the approach may be described as follows:

$$\lambda_{\text{eff}} = \begin{cases} 
\lambda_{\text{eff},s} & \text{if } T_{\text{PCM}} < T_{\text{PC,s}} \\
\phi \cdot \lambda_{\text{eff},l} + (1 - \phi) \cdot \lambda_{\text{eff},s} & \text{if } T_{\text{PC,s}} < T_{\text{PCM}} < T_{\text{PC,l}} \\
\lambda_{\text{eff},l} & \text{if } T_{\text{PCM}} > T_{\text{PC,l}} 
\end{cases} \quad \text{Eq.(9)}$$

$T_{\text{PC,s}}$ is the temperature where the PCM is fully solid and at $T_{\text{PC,l}}$ the material is fully liquid. The liquid fraction $\phi$ is a function of the material temperature and is calculated using equation 10.

$$\phi = \frac{\int_{T_{\text{PC,s}}}^{T_{\text{PC,l}}} c_p \cdot \lambda_{\text{eff}}(T) \, dT - \Delta h_{\text{PC}}}{\Delta h_{\text{PC}}} \quad \text{Eq.(10)}$$

where $\Delta h_{\text{PC}}$ is the total phase change enthalpy. Finally, to calculate the convective heat transfer coefficient between the heat transfer fluid and the inner tube wall $\alpha_{\text{HTF}}$, an empirical correlation for flow regimes in the transition zone between laminar and turbulence introduced by Gnielinski [32] is applied. The correlation uses a linear interpolation between laminar and turbulent convective heat transfer coefficients depending on the Reynolds number in the transition zone. At the investigated operating conditions, the flow regime is likely to be in the metastable transition zone. As summarised in Table 3 and Table 4, the Reynolds number at a temperature of 40°C is between 1125 and 3750 for the given HTF mass flow rates.

2.1.3 Numerical procedure

The resulting system of differential equations based on Eq. (3) is solved using an adaptive Runge-Kutta scheme implemented in commercial code Matlab. To determine the source terms, Eq. (10) to Eq. (5) are subsequently solved for each node, starting with node 1. It is worth mentioning that the HEX source term depends on the HTF inlet temperature and mass flow rate which act as a model input and could be time dependent, i.e. the model can be used for time varying input.

2.2 Experimental
Laboratory experiments were conducted in this study to calibrate and validate the developed numerical model. Calibration and validation were performed with independent datasets. The experiments were performed at Heriot Watt University, School of Engineering & Physical Sciences, located in Edinburgh, Scotland.

2.2.1 Experimental apparatus

A schematic of the apparatus used is shown in Figure 4. An electric cartridge heating element rated at 3kW was installed with a bespoke power supply unit marked as PSU in Figure 6. The electric heating element is immersed in the fluid (water) and circulated using pump P01 making a closed loop as typically found with an indirect style solar thermal system or a heat pump system without direct condensation in the storage unit. Heat is transferred to the fluid in the second loop (water) via a brazed plate heat exchanger marked as PHEX in Figure 6 and circulated using pump P02 through two series connected heat exchangers filled with SU34 (Calcium Bromide Hexahydrate plus additives) and SU58 (Sodium Acetate Trihydrate plus additives) with a nominal phase change temperature of 34°C and 58°C respectively. The latent heat storage units manufactured commercially by Sunamp Ltd, are shown with the designators SU34 and SU58 in Figure 4. The material properties of the phase change materials used in the units are provided in Table 1. The heat exchanger made by Sunamp Ltd is a metallic fin and tube type design. Copper tubes are used in both units. The fins are made of copper in the SU34 device and aluminium in the SU58 Heat Battery. The PCM, in liquid form is poured into the storage container surrounding the heat exchanger during the manufacturing process and allowed to solidify as it cools. From Figure 6, the rig allows both the charging and discharging of a single unit or alternatively for the two units to be connected in series Both units were insulated using vacuum insulation panels of manufacturer Kevothermal [33] with thickness \( d_{\text{ins}} = 20 \) mm and a conductivity of \( \lambda_{\text{ins}} = 0.004 \) W/(mK) (value taken from datasheet). Each Sunamp PCM storage unit is rated to store approximately 2.5 kWh of thermal energy. Therefore, the total capacity of the thermal energy storage system tested is around 5 kWh. This capacity is sufficient to heat 100L of water up by 40°C.

To achieve the desired mass flow rate in loop two, a second pump marked as P02 in Figure 4 was installed. In addition to the components discussed, additional sensors were installed including thermocouples for temperature measurement (marked as TXX, Figure 4) and flow meters (marked as FXX, Figure 4). All thermocouples were mineral insulated k-type with a probe diameter of 3 mm and inserted into the fluid at the point of measurement. Flowmeters FM-01 and FM-02 were turbine and manufactured from brass by OMEGA instruments (UK). Due to the hydraulic configuration shown, check valves were installed to ensure mains pressure water did not circulate incorrectly within the system as per the recommendations given by the manufacturer. Finally, a digitally actuated solenoid valve (DSV-01) was also included to allow the digital control of the thermal discharge phase.
Figure 4: Schematic of the experimental apparatus used for this study with location of all thermocouples (TXX), flow meters (FXX) pumps (PXX), and power supply unit (PSU).

All sensors (thermocouples, pressure sensors, flow meters), output devices (pumps, PSU, and solenoid valve) were electrically connected to a National Instruments data acquisition system with a four-slot chassis (model: NI-CompactDAQ-9074) and the required modules for reading and controlling the instruments discussed. The measurement accuracy of the used sensors is documented in Table 1. It is assumed that the tolerance of the sensors is uniformly distributed, hence, it is converted into a normal distribution to for the uncertainty analysis. The expanded uncertainty shown in the results plots is based on the 95.5% confidence interval (coverage factor k=2).

<table>
<thead>
<tr>
<th>Sensors</th>
<th>Tolerance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermocouples TXX</td>
<td>± 1.5 K between -40°C and 750°C</td>
</tr>
<tr>
<td>Flowmeter FXX</td>
<td>± 0.4 L/min</td>
</tr>
</tbody>
</table>

A photo of the apparatus built and installed at Heriot-Watt University is shown in Figure 5.
Figure 5: A photo of the experimental test setup.

Thermal input to the system, provided by the 3kW electric cartridge heating element was varied using the power supply unit (PSU) from 0-2000W. How this was varied for the different experiments will be discussed in Section 2.2.2.

The Grundfos Solar PM pumps installed (P01 and P02, Figure 4) accepted a pulse width modulated signal (PWM) to allow the flow rate in both loops to be adjusted. For the heating loop (loop 1), the desired flow rate was governed by the desired temperature rise across the heating element as a typical solar thermal controller or heat pump would do so where a fixed temperature rise is typically sought.

Table 2: Thermophysical properties of the used phase change materials in this study.

<table>
<thead>
<tr>
<th>Storage unit in rig</th>
<th>SU34</th>
<th>SU58</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manufacturer</td>
<td>Sunamp Ltd (United Kingdom)</td>
<td>Sunamp Ltd (United Kingdom)</td>
</tr>
<tr>
<td>Composition</td>
<td>Calcium bromide hexahydrate + additives</td>
<td>Sodium acetate trihydrate + additives</td>
</tr>
<tr>
<td>Phase change temperature</td>
<td>34°C</td>
<td>58°C</td>
</tr>
<tr>
<td>Density</td>
<td>1.96 kg/litre (liquid 75°C)</td>
<td>1.28 kg/litre (liquid 75°C)</td>
</tr>
<tr>
<td></td>
<td>2.19 kg/litre (Solid 20°C)</td>
<td>1.44 kg/litre (Solid 20°C)</td>
</tr>
<tr>
<td>Heat of fusion</td>
<td>110 kJ/kg</td>
<td>226 kJ/kg</td>
</tr>
<tr>
<td>Specific heat capacity</td>
<td>1.3 kJ/kg/K (Solid 20°C)</td>
<td>2.8 kJ/kg/K (Solid 20°C)</td>
</tr>
<tr>
<td></td>
<td>2 kJ/kg/K (liquid 75°C)</td>
<td>3.5 kJ/kg/K (liquid 75°C)</td>
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<tr>
<td>Thermal conductivity solid</td>
<td>1.2 W/(mK)</td>
<td>N.A.</td>
</tr>
<tr>
<td>Thermal conductivity liquid</td>
<td>N.A.</td>
<td>N.A.</td>
</tr>
</tbody>
</table>

2.2.2 Experimental model calibration and validation

The experimental campaign can be divided into two parts: (i) experiments performed to calibrate the model and (ii) experiments used for the model validation. The model calibration deals with the determination of the effective thermal conductivities for the liquid and solid phase utilised in the model. The value of the two parameters were estimated based on a parametric study comparing experimental and simulated water outlet temperatures for measured inlet temperatures and mass flow rates. Hence, the measured water mass flow rate and inlet temperature were used as an input to the model starting with equivalent initial conditions as the experiment.

The root mean square (RMS) deviation between the measured and simulated water outlet temperature was used as the key metric to quantify the disparity between the experimental and model data. Due to the high time variation of the considered charging and discharging cycles, an RMS-deviation based on the state of charge (SOC) of the storage unit instead of an RMS-deviation in time is introduced. The SOC for the parameter estimation is calculated based on the energy balance of the storage system, assuming a fully charged system at the end time $t_{end}$ of the charging cycle. Mathematically, the SOC may be formulate as:

$$SOC(t_c) = \frac{\int_0^{t_c} \dot{Q}_{HTF}(t) - \dot{Q}_{loss}(t) \, dt}{\int_{t_{end}}^{t_{end}} \dot{Q}_{HTF}(t) - \dot{Q}_{loss}(t) \, dt} + SOC_{init} \quad Eq.(11)$$

Where $\dot{Q}_{HTF}(t)$ is the time dependent heat flow rate from the HTF to the PCM during charging which can be calculated based on the HTF inlet and outlet temperature and mass flow rate. Furthermore, $SOC_{init}$ is the initial state of charge which is zero for the performed charging cycles and one for the discharging processes. The storage losses were considered and calculated using Eq. (3) as previously described.
The resulting SOC-based root mean squared deviation for equally spaced measurements $\Delta T_{RMS,SOC}$ reads:

$$\Delta T_{RMS,SOC} = \sqrt{\frac{\sum_{i=1}^{K} (T_{HTF,Exp,out,i} - T_{HTF,Sim,out,i})^2}{K}}$$  \hspace{1cm} Eq.(12)

Where $T_{HTF,Exp,out,i}$ is the SOC-based experimentally obtained HTF outlet temperature at data point i and $T_{HTF,Sim,out,i}$ the simulated and SOC-based outlet temperature of data point i. K is the total number of data points and hence the SOC-difference between two data points amounts to $\Delta SOC = 1/K$.

All charging sequences for calibration and validation were performed with initially completely discharged latent storages with a PCM temperature of approximately 12°C, corresponding to the cold supply water temperature. The storages were charged until the water outlet temperature reached 65°C. For model calibration, a high and low level of magnitude was defined for both the heating rate and mass flow rate of the water during charging. The values were chosen based on heating and mass flow rates which may be expected in domestic applications such as heat pump water heaters [34]. After charging, the storage vessel was discharged with cold supply water of around 12°C temperature with a mass flow rate of 0.12 kg/s until the water outlet temperature reached 15°C. An overview of the charging sequences performed to gain experimental data for the modelling calibration is given in Table 3. The cycles were independently performed for both the SU34 and SU58 storage units. During all experiments, the storage inlet and outlet temperatures, ambient temperature as well as water mass flow rate were measured with a sampling rate of 1 Hz.

<table>
<thead>
<tr>
<th>Nr.</th>
<th>Set heating rate during charging $Q_{Set}$</th>
<th>Set mass flow rate during charging $m_{Set}$</th>
<th>Storage config.</th>
<th>Reynolds number at 40°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.5 kW</td>
<td>0.1 kg/s</td>
<td>Single unit</td>
<td>3750</td>
</tr>
<tr>
<td>2</td>
<td>0.5 kW</td>
<td>0.03 kg/s</td>
<td>Single unit</td>
<td>1125</td>
</tr>
<tr>
<td>3</td>
<td>2 kW</td>
<td>0.1 kg/s</td>
<td>Single unit</td>
<td>3750</td>
</tr>
<tr>
<td>4</td>
<td>2 kW</td>
<td>0.03 kg/s</td>
<td>Single unit</td>
<td>1125</td>
</tr>
</tbody>
</table>

To validate the developed latent storage model, two additional experiments with charging rates and mass flow rates laying within the range of the values chosen for model calibration were performed. The first experiment was again conducted for both heat batteries independently. The experiment contained two charging sequence specified in Table 3. Finally, an experiment with one charging cycle for an SU34 and SU58 heat battery connected in series was carried out and the resulting outlet temperature of the second unit compared with the simulation results. The specifications of this experiment can be found in Table 5.

<table>
<thead>
<tr>
<th>Nr.</th>
<th>Set heating rate during charging $Q_{Set}$</th>
<th>Set mass flow rate during charging $m_{Set}$</th>
<th>Storage config.</th>
<th>Reynolds number at 40°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1 kW</td>
<td>0.05 kg/s</td>
<td>Single unit</td>
<td>1875</td>
</tr>
<tr>
<td>2</td>
<td>1.5 kW</td>
<td>0.09 kg/s</td>
<td>Single unit</td>
<td>3375</td>
</tr>
</tbody>
</table>
Table 5: Charging sequence performed for model validation using the SU58 and SU34 heat battery connected in series.

<table>
<thead>
<tr>
<th>Nr.</th>
<th>Set heating rate during charging ( \dot{Q}_{\text{Set}} )</th>
<th>Set mass flow rate during charging ( \dot{m}_{\text{Set}} )</th>
<th>Storage config.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2 kW</td>
<td>0.08 kg/s</td>
<td>Two units in series, starting with SU34 unit for charging and discharging.</td>
</tr>
</tbody>
</table>
3. Results and Discussion

3.1.1 Model calibration

In Figure 6, the experimentally obtained inlet temperature (dashed blue line), outlet temperature (black solid line), simulated outlet temperature (dashed-dotted red line) as well as the measured mass flow rate of the water (solid red line) are compared. The data corresponds to the four documented charging cycles in Table 3. The previously mentioned variation of charging and discharging sequence duration is observable. Furthermore, the characteristic behaviour of a latent storage unit in terms of temperature development during charging can be recognised. As marked for the second charging cycle, the charging sequence may be divided into three parts: (i) an initial sensible sequence when the PCM is solid, (ii) a temperature plateau during the phase change and (iii) a second sensible sequence when the PCM is entirely melted. The temperature plateau of the outlet temperature is at a level of around 58°C which corresponds to the phase change temperature of SU58. In

![Figure 6: Experimentally determined and simulated water outlet temperatures versus time for the four charging and discharging cycles documented in Table 3 for the SU58 storage unit using $\lambda_{eff,s} = 3.25\text{W/(m\text{K})}$ and $\lambda_{eff,l} = 8.75\text{W/(m\text{K})}$.

In Figure 7, the RMS-deviation for the SU34 storage unit (a) and the SU58 unit (b) are plotted as a function of the solid and liquid effective thermal conductivities. The deviation for both storage units is larger than 5K for conductivities lower than 2 W/(mK). However, as illustrated, the aberration decreases remarkably with increasing liquid effective conductivity.

![Figure 7: Normalised RMS-Deviation as a function of the liquid and solid effective thermal conductivity for the SU34 storage unit (a) and the SU58 unit (b).]
The minimal deviation determined for both heat batteries and the corresponding values for the effective conductivities in the liquid and solid phase are documented in Table 6. For both latent storage units, the SOC-based RMS-deviation for all four charging and discharging cycles was less than 1.3 K which is an excellent agreement between experimental and simulated data considering the large range of heating and mass flow rates during charging. The obtained effective conductivities are reasonable based on expected the physical phenomena in each phase. When the PCM is a completely solid, contact thermal resistance between the HEX and PCM may exist which inhibits the heat transfer and hence leads to a lower effective thermal conductivity [35]. When the PCM is liquid, free convection can be expected due to the temperature dependent density of the PCM. This density difference driven convection enhances the heat transfer and is according to several studies the dominant heat transfer mechanism during melting [36]–[38]. Hence, a higher effective conductivity results in the liquid phase.

<table>
<thead>
<tr>
<th></th>
<th>$\lambda_{eff,s}$</th>
<th>$\lambda_{eff,l}$</th>
<th>$\Delta T_{RMS,SOC}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SU34</td>
<td>2.75 W/(mK)</td>
<td>7.75 W/(mK)</td>
<td>1.27 K</td>
</tr>
<tr>
<td>SU58</td>
<td>3.25 W/(mK)</td>
<td>8.75 W/(mK)</td>
<td>1.28</td>
</tr>
</tbody>
</table>

Finally, a discretisation convergence study was performed to determine influence of the discretisation on the model accuracy. The investigation showed that the deviation between the simulated outlet temperatures between a model with N and N+1 nodes is less than 1% for more than 5 nodes. It is therefore recommended to use at least five nodes. If fewer nodes are used, the model accuracy drops significantly.

### 3.1.2 Model validation

Based on the previously mentioned convergence study, the model validation was performed using a model with six nodes and the effective thermal conductivities documented in Table 6. In Figure 8, the simulated and experimentally measured outlet temperatures for the measured inlet HTF mass flow rate and temperature are plotted versus the state of charge. The corresponding experimental configuration was documented in Table 4. As mentioned, the heating as well as the HTF mass flow rate differ from the experiments performed to estimate the model parameters to guarantee an independent model validation. The simulated and experimental outlet temperature are in good agreement. As shown in Table 7 the SOC-based deviations are less than 1K and 1.2K for the SU58 and SU34 storage unit respectively.

<table>
<thead>
<tr>
<th></th>
<th>$\Delta T_{RMS,SOC}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SU34</td>
<td>1.19 K</td>
</tr>
<tr>
<td>SU58</td>
<td>0.96 K</td>
</tr>
</tbody>
</table>

Most of the simulated data points lay within 95.5% confidence interval of the used thermocouples. A small deviation can be observed during the initial phase of the discharging process. This deviation may be caused by the fact that the thermal inertia of the water, as well as the piping system is not modelled which may have the highest impact on the system behaviour when switching from charging to discharging.
Figure 8: Model validation using data independent from model calibration: Model generated and experimentally determined outlet temperature against the state of charge (SOC) of the SU34 storage unit (a) and the SU58 unit (b).

Finally, in Figure 9, the simulated and measured storage outlet temperatures are plotted versus time for the 2 kW charging cycle described in Table 5. In general, again, an excellent agreement between experimental and numerical data can be observed. During discharging, the model however seems to overestimate the heat flow rate between the PCM and the HTF which results in a higher HTF outlet temperature. This is especially the case for the second storage unit (plot (b)). A possible explanation is the presence of supercooling in the SU58 unit during discharge. The fact that the HTF inlet temperature is relatively high (around 30°C) due to the preheating in the first unit supports this theory since the nucleation rate strongly increases with decreased temperature [39].

Nevertheless, as shown in Table 8, the obtained RMS-deviations for both outlet temperatures amount to approximately 1 K which proves a good agreement between the model and experimental data. It is worth mentioning that in this case, an analysis of the deviation based on a temporal scale appears to be reasonable since only one charging cycle with constant heating rate was considered.
Figure 9: Simulated and experimental HTF outlet temperature of the SU34 unit (a) and the SU58 (b) plotted against time.

Table 8: Determined time-based RMS-deviation $\Delta T_{RMS,t}$ between the outlet temperature of the second unit during charging and discharging for two serially connected Heat Batteries.

<table>
<thead>
<tr>
<th></th>
<th>$\Delta T_{RMS,t}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SU34</td>
<td>1.00 K</td>
</tr>
<tr>
<td>SU58</td>
<td>1.03 K</td>
</tr>
</tbody>
</table>

3.1.1 Verification of effective thermal conductivity

To verify the suitability of the proposed modelling approach, the estimated effective thermal conductivities of the PCM/fin compound are compared with values obtained from analytic models. In literature, a large variety of models and correlations can be found. A comprehensive review on composite PCMs was performed by Zang et al. in [40]. A simple analytic equation for the effective thermal conductivity of a parallel PCM and foam network, as it is the case in the present fin-tube HEX, reads:

$$\lambda_{eff,analytic} = \epsilon \cdot \lambda_{PCM} + (1 - \epsilon) \cdot \lambda_{fin}$$  \hspace{1cm} Eq. (13)

$\epsilon$ is in this case the PCM volume fraction in the PCM/fin compound and $\lambda_{fin}$ the thermal conductivity of the fins ($\lambda_{fin}=204$ W/(mK) for the SU58 heat battery (Al) and $\lambda_{fin}=386$ W/(mK) for the SU34 unit (Cu)).

The previously estimated effective conductivities based on model calibration, the PCM volume fraction for both units and the resulting effective conductivity based on Eq. 13 are given in Table 7. $\lambda_{eff,analytic}$ was calculated using the thermal conductivity of the PCM in the solid phase provided by supplier Sunamp (see Table 2, liquid conductivity is not available) and the bulk porosity given in Table 7. It can be seen that the derived values for $\lambda_{eff,analytic}$ deviate less than 5% from the liquid phase effective conductivity obtained from model calibration. This result is valid if the conductivity of the PCMs in the liquid phase does not differ considerably from the conductivity in the liquid phase. For most salt hydrates with known conductivities, the liquid phase conductivity similar or for some salt hydrates up to 50% lower than the conductivity in the solid phase [41]. In this case, the agreement between the model estimated conductivity and the value obtained with Eq. 13 would be even better.

The calibrated conductivities in the solid phase are up to 7 W/(mK) lower than the analytically derived effective conductivity based on Eq. 13. As previously mentioned, this deviation may occur due to thermal contact resistance between the solid PCM and the HEX geometry which is not accounted for in the analytic calculation.

Table 9: Optimal values for the effective thermal conductivities for both storage units with the corresponding SOC based deviation.

<table>
<thead>
<tr>
<th></th>
<th>$\lambda_{eff,x}$</th>
<th>$\lambda_{eff,l}$</th>
<th>$\epsilon$</th>
<th>$\lambda_{eff,analytic}$ (solid)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SU34</td>
<td>2.75 W/(mK)</td>
<td>7.75 W/(mK)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Based the analytic equation for the effective thermal conductivity, the presented modelling approach can be applied without conducting the relatively time-consuming and equipment-intensive calibration process. Following approach is proposed to do so:

1. Calculate \( \lambda_{\text{eff,i}} \) based on Eq.13, PCM material data and the PCM volume fraction in the PCM/fin.
2. Use following analytic equation for 1-dimensional serial heat transfer to calculate the effective conductivity in the solid phase and account for the contact resistances present.

\[
\lambda_{\text{eff,s}} = \frac{1}{\lambda_{\text{eff,i}}} + \lambda_r \tag{14}
\]

In Eq.14, \( \lambda_r \) is the conductivity resulting from contact resistances. Based on the model calibration, an average value for \( \lambda_r \) of XX was obtained which is recommended to be used in Eq.14. Alternatively, a constant effective conductivity may be applied. In Figure DFA, a comparison between experimental data and model generated HTF outlet temperatures with the calibrated model and variable conductivities as well as a constant effective conductivity of 9.1 W/(mK) are shown. In plot (a) the two subsequent charging and discharging cycles for model calibration and in plot (b) a more detailed plot of the first discharging cycle is illustrated. The results indicate that still a high accuracy can be achieved without an experimental model calibration and applying constant effective conductivities in both phases. During discharging, however, the mode reacts more sensitive due to the higher temperature differences between HTF and PCM. Nevertheless, the SOC-based RMS-deviation for both charging and discharging cycles is still only 1.36 K.

![Figure 10](image)

Figure 10: Comparison between experimental and model generated data for two subsequent charging cycles with the calibrated model and constant effective conductivities derived with analytic equations, material and HEX properties.

The results presented in this subsection clearly indicate that the model still provides a high accuracy applying the documented methodology to derive the effective conductivities. Hence, it can be applied for other materials and heat exchanger geometries with high reliability.
3.1.3 Computational effort

The calculation of the four subsequent charging cycles which a duration of approximately 26.5 h took less than 3 s. The model was implemented in Matlab/Simulink and the simulations were performed on a commercial laptop with an Intel (R) Core(TM) i7-7500U CPU with 2.70GHz and a physical memory (RAM) of 16Gb.

The validation confirms the suitability of the proposed modelling approach for accurate and fast predictions of the storage behaviour. It therefore can be used within the considered heating and HTF mass flow rates with high reliability and accuracy. The good results obtained using two units in series furthermore supports the suitability of the proposed model for system level simulations.
4. Conclusions

In the presented study, an accurate model of a fin-tube latent thermal storage unit with very low computational effort is presented. The model is based on a 1-dimensional finite volume discretisation using a heat transfer fluid temperature based source term to calculate the thermal in- and output of the heat exchanger. Two different commercial latent storage units of the British supplier Sunamp Ltd. with two different salt-hydrate based PCMs were used to experimentally calibrate and validate the proposed model. The state of charge-based root mean square deviation between experimentally determined and simulated water outlet temperature is less than 1.2 K for both investigated storage units. Furthermore, a validation with two different storage units connected in series showed excellent agreement between experiment and simulation which proves the applicability of the model for energy system simulations. Due to its low computational effort, the model can be used in annual system simulations. It could moreover be demonstrated that a high accuracy can be achieved using analytic equations to determine the effective conductivities of the phase change material/fin compound. Hence, the model may be used with high reliability without the necessity of an experimental calibration.

It may therefore be implemented in commercial software such as TRNSYS [1] or Simulink [2]. This allows system performance investigations on different combinations of energy sources such as heat pumps or thermal solar collectors with latent heat storages. Moreover, due to its physical approach, the model may be used as a designer tool for the determination of the basic heat exchanger concept in latent storage systems. It is in a next step possible to adapt the HEX source term and investigate the performance of systems using other heat transfer fluids, such as condensing or evaporating refrigerant. It is worth mentioning, that this approach would be applicable for investigations regarding the efficiency of heat pump or air conditioning systems in connection with latent storages. Further studies are recommended to determine the model accuracy and reliability for partially charged states since they may appear in annual system simulations. Experimental data for partially charged systems should therefore be collected and compared with model generated data using the methodology presented in this study.

Acknowledgments

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References


