Estimating the state of charge in a latent thermal energy storage heat exchanger based on inlet/outlet and surface measurements

Wim Beyne^{a,b}, Kenny Couvreur^{a,b,c}, Ilya T'Jollyn^{a,b}, Steven Lecompte^{a,b} and Michel De Paepe^{a,b}

^a Department of Electromechanical, Systems and Metal Engineering - UGent, Ghent, Belgium, wim.beyne@ugent.be

^b FlandersMake@UGent – Core lab EEDT - MP, Leuven, Belgium, www.flandersmake.be,

^c Research group Thermal energy in industry, Ghent University, Kortrijk, Belgium

Abstract

The performance of latent thermal energy storage (LTES) heat exchangers is related to the stored energy (i.e. state of charge) during the (dis)charging of the energy storage system. Furthermore, methods to correlate performance indicators such as the averaged effectiveness and phase change time are based solely on the latent heat stored. Therefore, measuring the stored energy in the separate components is crucial to understand the behavior of LTES systems and expand the correlation methods for performance indicators. However, technical limitations often do not allow to measure the stored energy. This article presents a LTES heat exchanger where only measurements at the in- and outlet of the heat transfer fluid and on the outer surface of the heat exchanger were possible. Based on this sparse set of measurements, estimators for the stored energy are developed. To test these estimators, a finite volume model of the LTES heat exchanger is made and fitted to experiments. The estimators for the stored energy in the heat transfer fluid, metal and phase change material reach a maximum deviation of respectively 1.9 %, 10 % and 2.1 % with the stored energy predicted by the finite volume model. By analyzing the stored energy as a function of time, four charging phases can be distinguished. The present correlating methods for performance indicators focus on the third latent phase. By estimating stored energy, the other phases can also be understood and modeled which can expand correlating methods for LTES heat exchangers in future work.

Keywords: latent thermal energy storage, state of charge, numerical model, state of charge estimators

Highlights

- Estimators for the total and partial stored energy are developed and validated.
- The estimator for the heat transfer fluid energy is generally applicable.
- A finite volume latent thermal energy storage model is developed and fitted.

1. Introduction

Latent thermal energy storage (LTES) heat exchangers have been intensively studied for a wide variety of applications such as buildings [1-3], grid level energy storage [4, 5] and cold chain transport [6]. This range of applications has sparked a large amount of interest in literature. Besides the development and improvement of phase change materials (PCMs) [7-9], the research has focused on improving heat transfer rate of latent thermal energy storage [10-13], modeling the solid liquid phase change in the heat exchanger [14-17] and the performance of storage systems in specific applications such as district heating systems [18-21], buildings [19] or concentrated solar power [20].

In order to implement LTES heat exchangers, their performance in an energy system must be evaluated. This can be done by implementing the LTES heat exchanger and performing experimental or numerical tests using the heat transfer fluid mass flow rate and inlet temperature provided by the energy system. For example, Gasia et al. [22] compared five performance indicators for four different shell-and-tube heat exchangers. A second possibility is by modeling the LTES heat exchanger using CFD. Colella et al. [18] performed a CFD analysis for a LTES heat exchanger for district heating systems. Several authors combine both CFD and experiments. Another example is the study of Ma et al. [23] in which a LTES heat exchanger is investigated specifically for solar heating in colder climates using both experiments and CFD. However, many of these studies only determine the performance for a small number of operating points. Evaluating the performance of a LTES heat exchanger in a new application with a different operating point requires redoing experimental or numerical tests.

Instead performing tests for each new operating point, a performance indicator can be correlated as a function of the operational point. An often applied performance indicator correlation is the averaged effectiveness number of transfer units (NTU) method. The method correlates the averaged effectiveness during phase change as a function of the mass flow rate and heat transfer surface area. It has been successfully applied to shell and tube [27, 28], packed bed [29], spiral coils in tanks [30] and finned tube in shell [31] LTES heat exchangers. Another correlation method is phase change time. The correlation for phase change time is based on a structure proposed by Raud et al. [32] for a shell and tube heat exchanger. The correlation was expanded for rectangular channels and has good agreement with data sets found in literature [33]. The coefficients for both effectiveness-NTU and phase change time can either be fitted to experiments or determined based on theoretical derivations.

Both the averaged effectiveness and phase change time methods determine an averaged value as performance indicator. To fully characterize the behavior of a LTES heat exchanger, the outlet temperature as a function of time should be predicted. The charging time energy fraction (CTEF) method allows to develop a predictive model for the outlet HTF temperature based on a set of charging experiments [37]. This method links charging time to the internal energy change or stored energy of a LTES heat exchanger. Contrary to the averaged effectiveness and phase change time methods, the coefficients of the CTEF method have to be fitted to experimental results.

There is thus a dilemma in the choice of a correlation method for performance indicators: either correlate an averaged indicator which can be linked to geometry and material properties or correlate the output as a function of time but without the link. The present paper aims to help resolve this dilemma by bridging the gap between the phase change time and average effectiveness method on one side and the CTEF method on the other.

The key difference between the analytical solutions of the phase change time and averaged effectiveness method and the purely experimental CTEF method is the internal energy change which are considered. The analytical solutions only consider latent heat [34, 38], while the CTEF method is linked to the internal energy of HTF, container and PCM [37]. The internal energy change of the container, HTF and PCM thus need to be estimated separately in order to predict the CTEF method coefficients from the phase change time solution. Furthermore, since the CTEF method is an experimental fitting strategy, the energy estimators should be based on experimental measurements and not on numerical modeling.

There is fairly limited research on the internal energy change in HTF, metal and PCM separately. Martinelli et al. [39] studied a tube in tube LTES heat exchanger enhanced with metal foam. The energy of the PCM and metal components was estimated using a grid of temperature measurements. The energy in the HTF was estimated based on the mean HTF temperature. The same method was used by Gasia et al. [40] to estimate heat losses during storage periods. Gasia et al. [41] also used a grid of temperature measurements to estimate the internal energy change of the PCM however the internal energy change of HTF and container was not reported. In another paper, Gasia et al. [40, 42] determined the stored energy in the PCM using a heat balance however the energy change of container and HTF was neglected.

Several authors report the state of charge (SOC), which is equivalent to either the total stored energy (e.g. [43]) or the latent stored energy (e.g. [44-47]). The SOC associated with latent heat is also often reported as a liquid fraction (e.g. [41, 48-53]). Since the measurement techniques for SOC and stored energy are similar, the SOC measurement techniques are further looked into in this section.

According to Zsembinski et al. [54], the sensors for SOC can be categorized according to what SOC definition they measure: total internal energy change or latent energy change. Besides a classification based on SOC definition, measurement techniques for SOC can be categorized to whether the sensor performs a local or a global measurement [54]. Local measurements result in the SOC at a specific location in the LTES, while global measurements result in the overall SOC.

Sensible heat is associated with a temperature change and therefore temperature sensors are appropriate to measure it. Temperature sensors by themselves are local measurements. Therefore, if the temperature differences in the thermal storage system are large, multiple temperature measurements aligned in a grid are required. The temperature grid technique has been applied in research for both lab-scale heat transfer experiments [55-57] as on full LTES heat exchangers [42, 58].

To measure latent heat both local and global measurement techniques are available. Local techniques require a grid of sensors to estimate the global liquid fraction. Sensors based on electrical properties have been tested for ice storage systems. These are based on resistive, capacitive and inductive measurements [59]. Some of these sensors also have commercial applications [60]. Other local measurement techniques are based on the transmission of ultrasonic or light waves [59]. Finally, temperature sensors can be used to estimate the local latent heat, since some PCMs experience a phase change temperature range rather than a single phase change temperature. However, this estimation has inherently a large uncertainty due to the sensor accuracy compared to the phase change range. Furthermore, due to hysteresis, there is no single temperature-enthalpy relation but rather one for cooling and one for heating. Even worse, due to subcooling the enthalpy-temperature curve for solidification is not necessarily invertible. However, a grid of temperature sensors can provide a global estimation of the location of the phase change front in the battery even though the local error of each sensor is large. For example, Zhou et al. [61] used a temperature grid to detect the start of solidification after an initial subcooled state. Barz et al. [44]

developed a nonlinear state observer based on a temperature grid. The application of these local sensors requires multiple measurements distributed throughout the PCM. Such a grid of measurements can be complex or even impossible to construct for many heat exchanger designs.

Global techniques can measure latent heat of an entire PCM volume. Digital cameras have been used to estimate the liquid fraction in lab scale experiments [56]. This method cannot be applied in LTES heat exchangers, if the PCM is not visually accessible. Another category of global measurements is based on the density change during phase change. An innovative technique based on the resulting difference in sound damping techniques was proposed by Steinmaurer et al. [62]. A second method based on volume change is measuring the pressure in an expansion volume. A final method directly measures the PCM level as it expands or contracts during phase change. This method is successfully applied in ice storage systems [45]. All techniques based on the density change require a measurable change in PCM level which is not possible for all LTES heat exchanger geometries.

Some LTES heat exchanger geometries do not allow for sufficient internal measurements to apply any of the techniques to estimate SOC described above. However, SOC and stored energy estimates are still required to describe the operation of the LTES heat exchangers. In those cases, two measurement types are still available. The first measurement type is the heat transfer fluid mass flow rate and the heat transfer fluid temperature at the in- and outlet of the LTES heat exchanger. The second measurement type is the surface temperature gradient on the outside of the container.

To the author's knowledge, only a single experimental study exists which develops stored energy estimators for container, PCM and HTF during charging of a LTES heat exchanger [39]. In contrast to the present study, internal measurements of the PCM were possible. The present article discusses developing stored energy estimators for a LTES heat exchanger which only allows measurements on the outside wall of the LTES heat exchanger and at the in- and outlet of the HTF. Based on the available measurements, estimators are developed for the total energy stored and energy stored in the metal, HTF and PCM in the present paper. To validate the estimators, a finite volume model of the heat exchanger is developed. The heat exchanger is described in Section 2 and the energy estimators in Section 3. To validate the energy estimators, the finite volume model of the LTES heat exchanger is developed in Section 4.

The estimators can be normalized to their maximum value, which allows obtaining SOC estimators. The stored energy and SOC are equivalent, to avoid confusion the remainder of the paper discusses the stored energy.

The heat exchanger charging was previously described based on solidification time [34], total charging time [33] and through the charging time energy fraction method [37]. Compared to the previously published papers, a finite volume model of the LTES heat exchanger was constructed and fitted. Furthermore, the energy content of HTF, metal and PCM is estimated using an integral method for the HTF energy, which has not been previously reported.

2. Experimental design

2.1. Experimental setup

The latent thermal energy storage system has been designed for cold chain transport of vaccines. Therefore, a PCM is chosen with a phase change temperature in the vaccine transport range of 2 – 8 °C. Accordingly, the organic PCM RT5HC from the company Rubitherm is chosen [63]. The properties of the

PCM as given by the manufacturer are summarized in Table 1. A Differential Scanning Calorimetry (DSC) analysis was performed to confirm the latent heat provided by the manufacturer [34]. The values provided by the manufacturer were within the error margin of the ones obtained by the DSC analysis.

Property	Value	Unit
Congezing area	6-5	°C
Latent heat $\pm 7.5 \%$	220	kJ/kg
Specific heat capacity	2	kJ/kgK
Solid density (at -15 °C)	880	kg/m ³
Liquid density (at 20 °C)	760	kg/m ³
Thermal conductivity	0.2	W/mK

Table 1: Main parameters of phase change material as provided by the manufacturer [34].

The RT5HC is contained in a heat exchanger which was previously described by Beyne et al. [33, 37] and Tarragona et al. [34]. The heat exchanger is constructed from extruded aluminum profiles as shown on Figure 1. In each profile, aluminum layers create 14 channels. In the seven channels which are labelled with an A, aluminum foam is added after which these channels are welded shut. The six remaining channels (labelled with a B) are left open to allow HTF to flow through the heat exchanger. The channel labelled with a C is used to connect the extruded profiles.

Figure 1: Cross section of the extruded profile [34].

Four extruded profile pieces are welded together side by side as shown in Figure 2. Holes are drilled in the top of the channels labelled with an A. Through these holes, the PCM is added after which the volumes are closed using threaded bolts.

Figure 2: Four profile sections with filling holes for the PCM prior to the installation of the HTF collectors. The blue arrows show the direction of the HTF flow.

Figure 2 shows the direction of the HTF flow through the battery. To distribute, collect and turn the HTF, two collectors are welded on the end of the four conjoined profiles as shown in Figure 3. The collectors are internally divided in five parts connecting each profile with the next one.

Figure 3: The full LTES heat exchanger with numbered profiles and collectors. The red lines show the internal divisions of the collectors.

Table 2 summarizes the main geometric parameters of the latent thermal energy storage heat exchanger.

Property	Value	Unit
Profile length	806	mm
Profile height	50	mm
Profile width	158	mm
Profile wall thickness	2	mm
PCM channel width	10	mm
HTF channel width	8.3	mm
Collector width	28	mm

Table 2: Main geometric parameters of the LTES heat exchanger.

In order to solidify the PCM in the LTES heat exchanger, the inlet HTF temperature has to be below the solidus temperature of RT5HC. In the present setup, the inlet HTF temperature is varied between -15 °C and 0 °C. As HTF, Temper -30°C from the company Climalife [64] is chosen for its low congealing point, non-toxicity and good heat transfer properties. The properties are given by the manufacturer tabulated as a function of the temperature. Similar as in Beyne et al. [33], the tabulated data is fitted to polynomial functions. The order of the polynomial is chosen so the fitting error is in the same order of magnitude as the measurement error. The resulting polynomials with their fitting errors are shown in Table 3.

Property		Correlation	Error	Unit
Specific heat capacity	c	$-2.86 \times 10^{-5} T^2 + 3.00 \times 10^{-3} T + 3.07$	10	kJ/kgK

Viscosity	μ	$-2.00 \times 10^{-8} T^5 + 1.68 \times 10^{-6} T^4$ $- 9.33 \times 10^{-5} T^3$ $+ 4.67 \times 10^{-3} T^2$ $- 1.59 \times 10^{-1} T + 3.96$	10^{-2}	mPa s
Thermal conductivity	k	$1.29 \times 10^{-3} T + 0.46$	10^{-2}	W/mK

Table 3: The polynomial functions determining the Temper -30°C properties in the temperature range 30 °C to -30 °C. The temperature in the correlations is in Celsius.

The HTF is modeled as an incompressible fluid with a constant value of 1184 kg/m³ which is the density at 0 °C.

Since the HTF is assumed to be incompressible, a change in specific internal energy can be determined by integration of the equation for the specific heat capacity. The pressure drop contribution to the specific enthalpy is assumed to be negligible compared to the temperature change. As a result, the specific enthalpy difference between inlet and outlet is equal to the difference in specific internal energy.

The LTES heat exchanger is charged by using a flow of cold Temper -30°C. Initially the heat exchanger is at room temperature. A vessel of Temper -30°C is cooled to a set point temperature between 0°C and -15°C. Once the set point temperature is reached, the chiller is turned off. The vessel is connected to the LTES heat exchanger and cold HTF is pumped through the heat exchanger causing the PCM to solidify. The experiment is ended once there is no significant temperature difference between inlet and outlet temperature. After the initial startup, the mass flow rate supplied to the LTES heat exchanger is constant while the inlet temperature rises slowly due to mixing in the HTF vessel. The pump is turned off once there is no longer a significant temperature difference between inlet and outlet of the HTF.

2.2. Experimental design

As discussed in the introduction, most techniques for measuring total stored energy would require measuring inside the HTF and PCM channels. For the PCM, it is difficult to differentiate between measuring the metal foam and the PCM. Furthermore, the wall thickness of the aluminum container is only 2 mm. Consequently it is difficult to tap threaded holes in the surface and place temperature sensors inside the battery. The accuracy would also suffer from the conductive path formed by the sensor itself. As a result, the stored energy will be estimated using only HTF measurements at in- and outlet and surface metal measurements.

The sensible heat of the metal is estimated by placing temperature sensors on different locations on the surface of the battery. Two groups of sensors are placed on each profile: one at the start of the profile and one group at the end of the profile. In each group, one sensor is placed on top of a PCM channel and one on top of a HTF channel. Secondly three sensors are placed on the intermediate collectors. The sensors placed on the metal surface are T-type stick-on thermocouples. The thermocouples are fixed at their location using aluminum tape and insulated from the ambient using insulating tape.

The HTF temperature is measured by submerging two K-type mineral insulated thermocouples in the HTF flow both at the in- and outlet.

All thermocouples are referenced using an insulated reference junction with Pt100 temperature measurement. The thermocouples and reference junction are calibrated with an accuracy of ± 0.15 °C using a calibrated oven.

The HTF mass flow rate is measured at the inlet by a Krohne Optimass 1400C S25 with an accuracy of $\pm 0.15\%$ of the reading value plus an error of 0.00075 kg/s. The mass flow rates of all the experiments are in the range of 0.25 kg/s to 1.0 kg/s.

Figure 4 schematically shows the location of the sensors on the battery with black sensors being stick-on thermocouples and the red sensors inserted in the HTF flow.

Figure 4: A CAD drawing of the full battery with the location of all sensors. The black sensors are stick-on thermocouples, the red sensors are inserted in the HTF flow.

All measurements are read using a Keithley 2700 multiplexer and acquired using Labview. The maximum sampling time is 5 seconds. The sensors, types and uncertainties are summarized in Table 4.

Sensor	Type	Accuracy
Surface temperature sensor	K-type stick on thermocouple (TC-direct)	$\pm 0.15\text{ }^{\circ}\text{C}$
Inserted temperature sensor	K-type mineral insulated thermocouple (TC-direct)	$\pm 0.15\text{ }^{\circ}\text{C}$
Mass flow rate	Krohne Optimass 1400 C S25	$\pm 0.15\text{ \%} + 0.00075\text{ kg/s}$

Table 4: Used sensors and associated uncertainties.

3. Energy Estimators

In the present section a method is developed to estimate the total energy stored and the energy stored in the HTF, the metal container and the PCM during the charging of the battery. Since the battery does not allow internal measurements, all estimators are based on the HTF temperature measurement at in- and outlet and metal surface temperatures.

The energy estimators are composed from the conservation of energy expressed for a control volume over an adiabatic battery with a single inflow and outflow of HTF (Equation 1). In Equation 1, the internal energy U is split in the internal energy of the HTF U_{HTF} , the PCM U_{PCM} and the metal U_{metal} as these are the three materials constituting the thermal battery.

$$\frac{dU}{dt} = \frac{dU_{HTF}}{dt} + \frac{dU_{PCM}}{dt} + \frac{dU_{metal}}{dt} = \dot{m} (h_{in} - h_{out}) \quad (1)$$

The right hand side of Equation 1 is the total efflux of energy and will be denoted as $\dot{F}$ (Equation 2). It is determined by the HTF mass flow rate and, HTF in- and outlet temperature measurements.

$$\dot{F} = \dot{m} (h_{in} - h_{out}) \quad (2)$$

Equation 1 is integrated as a function of time which results in Equation 3. Determination of the total energy stored $J(t)$ and the energy stored in each of the constituting materials, $J_{HTF}(t)$, $J_{PCM}(t)$ and $J_{metal}(t)$ are the goal for the stored energy estimation.

$$J(t) = J_{HTF}(t) + J_{PCM}(t) + J_{metal}(t) = \int_{t_{start}}^t \dot{F} dt \quad (3)$$

As shown in Equation 1 and described by Zsembinski [54], the total stored energy $J(t)$ can be estimated from the integrated efflux of energy $F(t)$. For this approach to be valid, the heat gains from the thermal battery to the ambient need to be negligible. To check whether this is the case, the energy stored at the end of the experiment $J(t_{end})$ is estimated and compared to the integrated efflux of energy.

If the battery is assumed to be at a constant uniform temperature at the start and end, the stored energy $J(t_{end})$ can be determined as a function of the initial temperature of the battery and the final temperature of the battery respectively T_{start} and T_{end} . The resulting estimated stored energy will be denoted by $\Delta U(T_{start}, T_{end})$ (Equation 4). The initial temperature is estimated as the average HTF outlet temperature during the initial charging phase. The final temperature is estimated as the average HTF inlet and outlet temperature at the end of the experiment. The variation on both the initial temperature estimate and final temperature estimate with the surface temperature measurements is within 0.75 °C. The resulting uncertainty on the estimated stored energy is small compared to the uncertainty on the latent heat of the PCM.

$$\begin{aligned} \Delta U(T_{start}, T_{end}) &= \rho_{HTF} V_{HTF} (u_{HTF}(T_{end}) - u_{HTF}(T_{start})) + m_{metal} c_{metal} (T_{end} - T_{start}) \\ &+ m_{PCM} [c_{PCM} (T_{end} - T_{start}) + h_{lat}] \end{aligned} \quad (4)$$

The estimated stored energy $\Delta U(T_{start}, T_{end})$ should be equal to the total integrated efflux of energy $F(t_{end})$ for the integrated efflux of energy $F(t)$ to be a valid integral estimator of the total stored energy $J(t)$.

The internal energy of the HTF can be determined as a function of the local temperature $T(\vec{x}, t)$, by assuming the HTF to be an incompressible liquid. The total energy of the HTF $U_{HTF}(T(\vec{x}, t))$ can be determined by integrating the specific internal energy over the HTF volume (Equation 5). Note that the local temperature $T(\vec{x}, t)$ describes the local temperature in the entire battery for HTF, PCM and metal. By integrating over only the HTF volume V_{HTF} in Equation 5, the local HTF temperature is selected from Equation 5.

$$U_{HTF}(T(\vec{x}, t)) = \rho_{HTF} \int_{V_{HTF}} u_{HTF}(T(\vec{x}, t)) dV \quad (5)$$

The energy of the metal in the thermal battery can be calculated assuming a constant specific heat for the aluminum c_{metal} by integrating the temperature over the metal mass (Equation 6).

$$U_{metal}(T(\vec{x}, t)) = m_{metal} c_{metal} \int_{m_{metal}} T(\vec{x}, t) dm \quad (6)$$

The energy of the PCM is determined by Equation 7 which requires knowledge of both the local temperature $T(\vec{x}, t)$ and liquid fraction $\lambda(\vec{x}, t)$ in the entire PCM mass.

$$U_{PCM}(T(\vec{x}, t), \lambda(\vec{x}, t)) = m_{PCM} \int_{m_{PCM}} c_{PCM} T(\vec{x}, t) + h_{lat} \lambda(\vec{x}, t) dm \quad (7)$$

The stored energy in each constituting material is determined by taking the difference in internal energy between the start of the experiment and time t .

Determining $J_{HTF}(t)$, $J_{metal}(t)$ and $J_{PCM}(t)$ thus requires measuring the local temperature $T(\vec{x}, t)$ and liquid fraction $\lambda(\vec{x}, t)$. However, internal measurements of temperature and liquid fraction are not possible for the thermal battery under investigation. Therefore, estimations are developed based on the surface temperature, HTF mass flow rate and HTF in- and outlet temperature measurements. These estimations can then be validated by comparing to the stored energy predicted by the results of the finite volume method developed in Section 4.

There are only temperature measurements of the HTF at the inlet and outlet of the battery. These measurements allow determining an upper and a lower estimate of $T(\vec{x}, t)$ which correspond to an upper and a lower limits of the HTF energy U_{HTF} as a function of time, since the specific internal energy is continuously increasing as a function of temperature.

Both the upper and lower limits of the temperature estimation are a function of the time to replace the entire volume of HTF in the battery. Each time instant t_i can be associated with the future time instant at which the present battery HTF mass is replaced $t_{rep}(t_i)$ (Equation 8). In Equation 8, the HTF flow is assumed not to mix with the incoming flow.

$$t_{rep}(t_i) = t_j \text{ for which } V_{HTF} \rho_{HTF} = \int_{t_i}^{t_j} \dot{m} dt \quad (8)$$

The conservation of energy is applied to a control volume encompassing only the HTF in Equation 9. If there is no heat transfer between the HTF and the metal ($\dot{Q}_{HTF-metal} = 0$), the temperature of the HTF mass in the battery is the outlet temperature measured between t_i and $t_{rep}(t_i)$. However there is heat transfer, therefore the temperature of the HTF will actually be lower than the outlet temperature if the local temperature of the battery is higher than the HTF temperature. The energy estimate resulting from this estimate is thus an upper limit for the HTF energy U_{HTF}^u (Equation 10).

$$\frac{dU_{HTF}}{dt} = \dot{m} (h_{in} - h_{out}) + \dot{Q}_{HTF-metal} \quad (9)$$

$$U_{HTF}^u(t_i) = \int_{t_i}^{t_{rep}(t_i)} \dot{m}(t) u_{HTF}(T_{out}(t)) dt \quad (10)$$

Similarly, a time step can be associated with the past time step at which none of the current HTF mass was present in the battery $t_{rep}^{-1}(t_i)$. If there is no heat transfer in this case, the temperature of the HTF mass is the inlet temperature measured between time t_i and $t_{rep}^{-1}(t_i)$. If there is heat transfer, the temperature of the HTF inside the battery is higher. Therefore the resulting energy estimate is a lower limit for the HTF temperature in the battery $U_{HTF}^L(t_i)$ (Equation 11).

$$U_{HTF}^L(t_i) = \int_{t_{rep}^{-1}(t_i)}^{t_i} \dot{m}(t) u_{HTF}(T_{in}(t)) dt \quad (11)$$

Note that both the upper and lower limit are not defined over the entire measurement time interval: $[t_{start}; t_{end}]$. Before $t_{rep}(t_{start})$ the inverse function t_{rep}^{-1} is not defined. Therefore the lower limit is not defined before $t_{rep}(t_{start})$. Similarly after $t_{rep}^{-1}(t_{end})$, the function t_{rep} is not defined and as a result the upper limit is not defined after $t_{rep}^{-1}(t_{end})$. This does not pose an issue for the upper limit, since the charging cycle is finished well before $t_{rep}^{-1}(t_{end})$. For the lower limit this does however pose an issue since the current definition does not allow to determine the initial energy of the battery. Therefore, the lower limit definition is expanded in the region $[t_{start}; t_{rep}(t_{start})]$ as $U_{HTF}^{L,e}$ (Equation 12). The expanded lower limit is technically only a lower limit after $t_{rep}(t_{start})$.

$$U_{HTF}^{L,e}(t_i) = \begin{cases} \int_{t_{rep}^{-1}(t_i)}^{t_i} \dot{m}(t) u_{HTF}(T_{in}(t)) dt & \text{if } t_i \geq t_{rep}(t_{start}) \\ \int_{t_{start}}^{t_i} \dot{m}(t) u_{HTF}(T_{in}(t)) dt + \int_{t_i}^{t_{rep}(t_i)} \dot{m}(t) u_{HTF}(T_{out}(t)) dt & \text{else} \end{cases} \quad (12)$$

The estimated energy stored in the HTF $\hat{J}_{HTF}(t_i)$ at time t_i is calculated as the average between the upper and lower limit energy limits (Equation 13). The limits provide the upper and lower bounds for this estimator.

$$\hat{J}_{HTF}(t_i) = 0.5 \left(U_{HTF}^{L,e}(t_i) - U_{HTF}^{L,e}(t_{start}) + U_{HTF}^u(t_i) - U_{HTF}^u(t_{start}) \right) \quad (13)$$

Several authors have characterized the heat transfer between the HTF and the metal and PCM in LTES heat exchanger for example through the definition of a time-averaged effectiveness [65-67]. However in most cases, the heat transfer rate between HTF and the metal and PCM cannot be directly measured. These authors therefore have to assume that the measured efflux of energy is the result of heat transfer between HTF and PCM rather than the mass conservation of the HTF.

The heat transfer rate can also be estimated by subtracting the time derivative of the estimated HTF energy from the efflux of energy. Both the estimated HTF energy (Equation 13) and efflux of energy (Equation 2) are solely based on the in- and outlet temperature and the mass flow rate of the HTF. Therefore the heat transfer rate in the LTES heat exchanger can be formally estimated, which will allow to determine the applicable range of methods such as the time-averaged effectiveness method.

The metal mass can be split into three basic components: the profiles, the collectors and the metal foam (see Figure 3). The profiles are the extruded pieces which contain the PCM. The collectors are placed at the front and back of the profiles to collect and direct the HTF through the battery. The metal foam energy will be included in the PCM energy as local thermal equilibrium between metal foam and PCM is assumed. The metal energy estimates will thus be split into an estimate for the profiles and for the collectors.

There are four profiles in total which each have four surface temperature measurements. The two measurements on the inlet and outlet are averaged as T_p^{in} and T_p^{out} . The temperature at the inlet of each profile T_p^{in} will be lower than the temperature at the outlet T_p^{out} due to the lower local HTF temperature and the developing flow at the start of the profile. An estimation based on the measured surface temperatures is thus limited between an upper value obtained from $T_p^{out}: \hat{f}_{p,j}^u(t_i)$ (Equation 14) and a lower value obtained from $T_p^{in}: \hat{f}_{p,j}^l(t_i)$ (Equation 15). The subscript j denotes the number of the profile.

$$\hat{f}_{p,j}^u(t_i) = c_{metal} m_{p,j} (T_{p,j}^{out}(t_i) - T_{p,j}^{out}(t_{start})) \quad \forall j \in \{1,2,3,4\} \quad (14)$$

$$\hat{f}_{p,j}^l(t_i) = c_{metal} m_{p,j} (T_{p,j}^{in}(t_i) - T_{p,j}^{in}(t_{start})) \quad \forall j \in \{1,2,3,4\} \quad (15)$$

Based on Equation 6, the energy of the collectors can be determined by estimating the collector mean temperature. Collector section 1 and 5 are not equipped with a temperature sensor. Therefore, their mean temperature is estimated as respectively the inlet and outlet temperature. This estimator neglects the thermal resistance between the inlet and outlet collectors and the HTF. The other three collectors are equipped with a surface temperature sensor. The resulting energy estimator $\hat{J}_C(t_i)$ is given by Equation 16 with m_C the mass of one of the two collectors.

$$\hat{J}_C(t_i) = c_{metal} m_C \left(\frac{T_{in}(t_i) - T_{in}(t_{start})}{4} + \frac{T_{C,2}(t_i) - T_{C,2}(t_{start})}{2} + \frac{T_{C,3}(t_i) - T_{C,3}(t_{start})}{2} + \frac{T_{C,4}(t_i) - T_{C,4}(t_{start})}{2} + \frac{T_{out}(t_i) - T_{out}(t_{start})}{4} \right) \quad (16)$$

Contrary to the HTF energy and profile energy estimator, there are no upper and lower limits defined for the energy stored in the collectors. The total stored energy in the metal in the collectors is only 9.5 % of the energy stored in all the metal and 2.5 - 3 % of the total stored energy. This is comparable to the effect of the uncertainty of the latent heat. Therefore, the collector energy by itself is not further investigated.

The stored energy in the metal $\hat{J}_{metal}(t_i)$ is determined by sum of the energy stored in the collector $\hat{J}_C(t_i)$ and the average of the upper and lower limit of the stored energy for all four profiles (Equation 17). The upper and lower limit for the metal energy are determined by replacing the average in Equation 17 by respectively the upper and lower limit (Equation 14 and 15).

$$\hat{J}_{metal}(t_i) = \hat{J}_C(t_i) + \sum_{j=1}^4 0.5 (\hat{f}_{p,j}^u(t_i) + \hat{f}_{p,j}^l(t_i)) \quad (17)$$

The upper and lower limit for profile energy are limits to estimators which can be constructed from averaging the two surface temperature measurements. These are not limits to the actual energy of the profiles since the surface might not be the maximum or minimum temperature of the profiles. The limits should thus be regarded as limits on estimators which can be constructed by combining these specific measurements.

The energy stored in the metal foam enhanced PCM is not directly measured. Therefore the energy is estimated using Equation 1. If the heat losses can be neglected, the energy stored in the enhanced PCM is estimated by Equation 18.

$$\hat{J}_{PCM}(t_i) = F(t) - \hat{J}_{HTF}(t_i) - \hat{J}_{metal}(t_i) \quad (18)$$

Errors on the estimators presented above are determined based on the error on the thermocouples, the mass flow rate sensors and the properties and masses of the HTF and metal using the method described by Taylor et al. [68].

4. Finite volume model

A finite volume method resolving the conservation of energy in the thermal battery results in a discretized version of the local temperature $T(\vec{x}, t)$ and liquid fraction $\lambda(\vec{x}, t)$. Therefore, the predictions of the finite volume model can be used to validate the energy estimators expressed by Equation 13, 17 and 18. The present section deals with the development of the finite volume model which is implemented in Python.

4.1. Finite volume model development

The battery is modeled by expressing the conservation of mass and energy and discretizing the battery to solve these conservation laws. The model consists of two modular building blocks: the profiles which contain the PCM and the collectors which only contain HTF and metal. The profiles are further split which results in a cross section containing three components: HTF, metal and metal foam enhanced PCM (see Figure 5).

By connecting the models of the collectors and profile cross sections in series, a model for the full cold storage is made. The profile cross sections and collectors are assumed to interact only with the HTF flow. This simplification allows calculating the profile cross sections and collectors without upstream coupling which greatly reduces calculation time.

In both the collectors and profile cross sections, the HTF is discretized in a single control volume. The heat transfer is estimated using an experimentally correlated heat transfer coefficient which reduces computational complexity compared to discretizing and resolving the fluid flow.

Similar to the HTF, the metal is discretized in a single control volume in both the collector and profile cross section. The metal only contributes about 15 % to the total internal energy change for a charging cycle between 20 °C and -10 °C. Furthermore, it has a high conductivity which limits the temperature difference in the metal.

The metal foam enhanced PCM can be modelled on pore scale [69], however this is computationally expensive [70]. Therefore, volume-averaging theory (VAT) has been used to successfully model metal foam enhanced PCM [14, 71-74]. Volume-averaging theory (VAT) averages the metal foam and fluid in representative fluid volumes [75] which require less elements to achieve grid convergence. Therefore, VAT will form the basis of the model for the metal foam enhanced PCM.

The PCM undergoes solidification during which convection is less important than in melting except in the initial stages when the PCM is still liquid [76]. Furthermore, the metal foam suppresses the natural convection in the PCM [77]. Therefore, natural convection is neglected. As a result, the conservation of mass and momentum equations do not need to be resolved for the PCM.

With the above simplifications, the metal foam enhanced PCM is modelled by two equations describing the conservation of energy: one for the metal foam and one for the PCM. If local thermal equilibrium between metal foam and PCM is assumed, the VAT model can be further simplified to a single energy

equation describing both metal foam and PCM [71]. Several authors found that the assumption of local thermal equilibrium does not lead to large discrepancies in overall liquid fraction between single equation and two equation VAT models [71, 78]. Therefore, local thermal equilibrium is assumed and the metal foam enhanced PCM is modeled by a single equation.

Since natural convection is neglected, the only reason for the phase change front to be two dimensional are the aluminum top and bottom of the PCM channels acting as fins. This aluminum top and bottom is only 2 mm thick and therefore their effect on the heat conduction is neglected. As a result, the PCM in the cross section can be discretized into a one-dimensional structure of metal foam enhanced PCM layers.

The discretization resulting from the discussion above is shown schematically on Figure 5.

Figure 5: Schematic representation of the thermal battery discretization.

With the profiles discretized, the conservation of mass and energy can be applied to the HTF, metal and PCM control volumes. The control volumes will be numbered with the index i from 1 to n_x in the flow direction and for the PCM with the index j from 1 to n_y away from the heat transferring wall. Figure 6 shows a schematic representation of the control volumes for the i^{th} profile cross section.

Figure 6: Schematic representation of the i^{th} cross section for a discretization with 3 control volumes in the PCM ($n_y=3$).

The metal and PCM mass are fixed in the construction, so only the HTF mass changes during the charging of the battery.

The density change of the HTF is neglected (0.8 % between 20 °C and -10 °C) as well as the volume change of the battery due to thermal expansion (~ 0.2 % between 20 °C and -10 °C). The conservation of mass applied to any control volume with one inlet and one outlet results in an equal in- and outgoing mass flow rate $\dot{m}$.

The conservation of energy is expressed for the i^{th} HTF control volume as Equation 19 by neglecting the change in kinetic and potential energy of the HTF. Since the pressure drop is neglected, both the specific internal energy of the HTF u_{HTF} and the specific enthalpy h_{HTF} can be estimated from the specific heat given by the manufacturer.

$$m_{HTF}^i \frac{du_{HTF}^i}{dt} = \dot{m}(h_{in}^i - h_{HTF}^i) + UA_{HTF-metal}^i (T_{metal}^i - T_{HTF}^i) \quad (19)$$

The mass of the i^{th} HTF control volume is the total mass of HTF in the profile divided by the number of control volumes along the flow length n_x .

$$m_{HTF}^i = \frac{z_P L_P w_{HTF} n_{HTF} \rho_{HTF}}{n_x} \quad (20)$$

The overall heat transfer coefficient between metal and HTF $UA_{HTF-metal}^i$ consists of the thermal resistance of the metal and the convective resistance of the HTF (Equation 21). The heat transfer surface A is the total heat transfer surface between the HTF and metal without the top and bottom of the profiles.

$$UA_{HTF-metal}^i = \left(\frac{1}{h^i A} + \frac{d_{metal}}{2k_{metal}A} \right)^{-1} \text{ with } A = \frac{2z_P L_P n_{HTF}}{n_x} \quad (21)$$

The convective heat transfer coefficient in the i^{th} control volume h^i is estimated using a correlation by Muzychka and Yovanovich [79] where the mean Nusselt number in the control volume is taken (Equations 22-26). The characteristic length in this correlation is the square root of the through flow surface area. AR is the aspect ratio of the channel.

$$Nu_{\sqrt{A_f}}(x^*) = \left[\left(\frac{2 f(Pr)}{\sqrt{x^*}} \right)^m + \left(\left\{ 0.6135 \frac{f Re \sqrt{A_f}}{x^*} \right\}^5 + \left\{ 3.24 \frac{f Re \sqrt{A_f}}{8\sqrt{\pi} AR^{0.1}} \right\}^5 \right)^{m/5} \right]^{1/m} \quad (22)$$

$$f(Pr) = \frac{0.564}{[1 + (1.664 Pr^{1/6})^{9/2}]^{2/9}} \quad (23)$$

$$m = 2.27 + 1.65 Pr^{1/3} \quad (24)$$

$$f Re \sqrt{A_f} = \frac{12}{\sqrt{AR}(1 + AR) \left[1 - \frac{192 AR}{\pi^5} \tanh\left(\frac{\pi}{2 AR}\right) \right]} \text{ with } AR = w_{HTF}/z_P \quad (25)$$

$$x^* = \frac{x}{\sqrt{A_f} Re \sqrt{A_f} Pr} \text{ with } A_f = z_P L_P \quad (26)$$

In Equation 19, h_{in}^i is the specific enthalpy of the incoming HTF mass which is equal to the enthalpy in the upstream HTF control volume h_{HTF}^{i-1} .

The conservation of energy is applied to the metal control volume in Equation 27. The control volume is in contact with the first PCM control volume as well as with the HTF.

$$m_{metal}^i c_{metal} \frac{dT_{metal}^i}{dt} = UA_{HTF-metal}^i (T_{HTF}^i - T_{metal}^i) + UA_{PCM-metal} (T_{PCM}^{i,0} - T_{metal}^i) \quad (27)$$

The mass of the metal control volume m_{metal}^i is the total metal mass of the profile divided by the number of control volumes in the flow direction n_x .

The overall heat transfer coefficient between the metal and PCM is given by Equation 28 with n_y the number of control volumes in the PCM cross section.

$$UA_{PCM-metal} = \left(\frac{w_{PCM}}{4 k_{eff} A n_y} + \frac{d_{metal}}{2 k_{metal} A} \right)^{-1} \text{ with } A = \frac{2 h_P L_P n_{HTF}}{n_x} \quad (28)$$

k_{eff} is the effective thermal conductivity of the metal foam enhanced PCM. Calmidi and Mahajan [80] and Bhattacharya et al. [81] provided a correlation for the effective conductivity fitted to their experiments. These correlations together with the analytical solution provided by Mesalhy et al. [82] are compared for aluminum foam and a fluid with a thermal conductivity of 0.2 W/mk. The effective conductivity for a porosity of 0.96 is estimated between 3-3.4 W/mK depending on the correlation used. This value is in the range of experimentally measured values for the combination of aluminum foam and paraffin wax [39].

The specific internal energy of the PCM u_{PCM} consists of sensible and latent heat. The PCM is assumed to be incompressible, therefore the sensible heat only depends on the PCM temperature. The sensible heat capacity c_{PCM} is assumed to be constant. The latent heat depends on the liquid fraction in the PCM control

volume λ or the ratio of the mass of PCM which is liquid to the total PCM mass. By taking 0 K as reference temperature, the specific internal energy of the PCM can thus be written as Equation 29 where h_{lat} is the specific enthalpy of phase change.

$$u_{PCM} = c_{PCM} T_{PCM} + \lambda h_{lat} \quad (29)$$

The PCM does not undergo an isothermal phase change but rather solidifies between 6-4 °C. The liquid fraction is therefore determined as a linear function between these temperature limits (Equation 30).

$$\begin{aligned} \lambda &= \frac{T_{PCM} - 4^{\circ}C}{2^{\circ}C} \text{ if } 4^{\circ}C < T_{PCM} < 6^{\circ}C \\ &= 0 \text{ if } T_{PCM} < 4^{\circ}C \\ &= 1 \text{ if } 6^{\circ}C < T_{PCM} \end{aligned} \quad (30)$$

The specific internal energy of the PCM is thus only a function of the temperature. However, the specific internal energy as a function of temperature is strongly non-linear which destabilizes the numerical solution of the conservation of energy equation. This problem can be solved by treating the latent heat as a separate source term: λh_{lat} and updating this source term according to the method of Völler and Prakash [83].

Conservation of energy can now be applied to the PCM control volumes which results in Equation 31 for the control volume adjacent to the metal, Equation 32 for a middle control volume and Equation 33 for the last control volume.

$$\begin{aligned} m_{PCM}^{i,1} c_{PCM} \frac{dT_{PCM}^{i,1}}{dt} &= UA_{PCM-metal} (T_{PCM}^{i,1} - T_{metal}^i) + UA_{PCM} (T_{PCM}^{i,2} - T_{PCM}^{i,1}) + \frac{d\lambda^{i,1}}{dt} m_{PCM}^{i,1} h_{lat} \end{aligned} \quad (31)$$

$$m_{PCM}^{i,j} c_{PCM} \frac{dT_{PCM}^{i,j}}{dt} = UA_{PCM} (T_{PCM}^{i,j-1} + T_{PCM}^{i,j+1} - 2 T_{PCM}^{i,j}) + \frac{d\lambda^{i,j}}{dt} m_{PCM}^{i,j} h_{lat} \quad (32)$$

$$m_{PCM}^{i,n_y} c_{PCM} \frac{dT_{PCM}^{i,n_y}}{dt} = UA_{PCM} (T_{PCM}^{i,n_y-1} - T_{PCM}^{i,n_y}) + \frac{d\lambda^{i,n_y}}{dt} m_{PCM}^{i,n_y} h_{lat} \quad (33)$$

The mass of a PCM control volume $m_{PCM}^{i,j}$ is the total PCM mass in the profile divided by the number of control volumes along the flow length n_x and the number of control volumes in the PCM cross section n_y . The heat transfer coefficient between the PCM control volumes UA_{PCM} is given by Equation 34.

$$UA_{PCM} = \frac{2 k_{eff} A n_y}{t_{PCM}} \text{ with } A = \frac{2 h_P L_P n_{HTF}}{n_x} \quad (34)$$

Equations 19 to 34 define a model for the profiles.

The conservation of energy for the collector has the same form as for the profiles (Equation 19) with a difference in the mass of the control volume and the overall heat transfer coefficient between the HTF and metal. The mass of the control volume is the total volume of the collector multiplied with the density of the HTF. There are no correlations to determine the heat transfer coefficient in the collectors. Therefore, the heat transfer coefficient is estimated by fitting the estimated collector temperature to the measured temperature. This method is not very accurate, however the metal in the collectors only

contributes to 0.6 % of the total stored energy. As such, the inaccuracy will have little impact on the simulation result.

The conservation of energy for the metal control volume in the collectors is expressed as Equation 35.

$$m_{metal}c_{metal}\frac{dT_{metal}}{dt} = UA_{HTF-metal}(T_{HTF} - T_{metal}) \quad (35)$$

Equations 19 to 35 are integrated in time using a Crank-Nicholson scheme with an adaptive time step of maximum 1 s. The time step is reduced when the number of iterations per time step increase above a preset level which depends on the number of control volumes.

Grid convergence is checked by comparing three grids: $(n_x = 5, n_y = 5)$, $(n_x = 10, n_y = 10)$ and $(n_x = 20, n_y = 20)$, using the method of Roache [84]. The coarsest grid is found to give satisfactory results compared to the experimental results. For more information, the reader is referred to Appendix A.

The finite volume model is developed using several assumptions and simplifications. For clarity these assumptions are listed below.

- Collectors and profile cross sections are only coupled through HTF flow.
- Profile cross sections can be modelled as a single HTF and PCM channel.
- Metal can be modelled in a single control volume.
- Metal foam enhanced PCM:
 - o VAT modeling is appropriate.
 - o Natural convection is negligible.
 - o Local thermal equilibrium is assumed between metal foam and PCM.
 - o Liquid fraction is described by Equation 30.
- HTF and PCM are incompressible.
- LTES thermal expansion is negligible.

4.2. Finite volume model fitting

The finite volume model is developed under several simplifying assumptions and the factors determining the heat transfer (k_{eff} and h) are subject to experimental uncertainty. The effective conductivity k_{eff} differs between 3 and 3.4 W/mK depending on the used correlation. Furthermore, thermal contact resistance between metal foam and container can be important and is difficult to estimate. With regards to the convective heat transfer coefficient, Muzychka et al. [79] propose an uncertainty of $\pm 15\%$ for the correlation of the convective heat transfer coefficient. As a result of the assumptions made and uncertainty, the finite volume model requires fitting to match the experimental results.

To fit the model to the experiments, an objective function quantifying the deviation between the model prediction and experiments is required. The deviation is quantified using the average integrated temperature difference between the measured and modeled HTF outlet temperature $I_{\Delta T}$ (Equation 36). In Equation 36, t_c is the total charging time of the experiment. Equation 36 is calculated for each experiment. The objective function is given by the sum of the average integrated temperature difference for all experiments.

$$I_{\Delta T} = \frac{1}{t_c} \sum_{i=1}^{n_t} |T_{out,exp}^i - T_{out,model}^i| (t_{i+1} - t_i) \quad (36)$$

The fitting strategy adjusts the conductive heat transfer resistance by directly altering the effective conductivity of the metal foam enhanced PCM k_{eff} . The convective heat transfer coefficient is fitted by multiplying the convective heat transfer coefficient by a fitting factor C_f . By not directly fitting the convective heat transfer coefficient itself, the correlation by Muzychka et al. [79] still allows to include entrance effects on the convective heat transfer coefficient.

The minimization of the objective function is performed using the methods programmed in the method *minimize* from the *SciPy.optimize* Python package [85]. The Constraints By Linear Approximation (COBYLA) algorithm is selected to minimize the objective function since it does not require gradient information and can deal with constrained optimization.

The deviation between experiment and model prediction is minimized for all experiments separately. The resulting optimal pairs of k_{eff} and C_f are shown in Figure 7. Since every experiment obtains a different optimal solution and the difference between the optimal solutions is large, an alternative fitting strategy is required.

Figure 7: Fitting variables which minimize the objective function for each of the experiments.

The effective thermal conductivity lumps several physical phenomena and assumptions. Of these phenomena, only the convection in liquid PCM is a function of the inlet HTF temperature or mass flow rate. However, the natural convection probably only has a minor role. Therefore, the effective thermal conductivity should not depend on operating conditions and should be constant for all experiments.

A second round of optimizations is conducted where the effective thermal conductivity is fixed as 1.3 W/mK and the correction factor C_f is used to fit the result. The product of the correction factor C_f and the modelled average convective heat transfer coefficient h_{avg} as a function of the Reynolds number is plotted in Figure 8. The correction factor shows an approximately linear relation with the Reynolds number.

Figure 8: Product of the fitting coefficient C_f and the average heat transfer coefficient h_{avg} as a function of Reynolds number which minimizes the deviation between experiment and simulation with a fixed effective thermal conductivity of 1.3 W/mK.

A final round of optimizations is performed where all experiments are optimized simultaneously. The first fitting variable is the effective thermal conductivity k_{eff} which is equal for all experiments. The convection correction factor is determined by Equation 37 which defines the two other fitting variables s_c and s_i .

$$C_f = \frac{1}{h} (s_c Re + s_i) \quad (37)$$

The result of the optimization algorithm is summarized in Table 5.

Name	Symbol	Value	Units
Effective thermal conductivity	k_{eff}	1.297	W/m K
Slope for convective correction factor	s_c	0.3115	W/m ² K
Intercept for convective correction factor	s_i	311.7	W/m ² K
Average integrated temperature difference	-	0.2	K

Table 5 : The result of fitting the model to the experiments.

The fitted coefficients are used to simulate all performed experiments and compare them to the measured values. The resulting integrated average temperature differences are shown in Figure 9. The errors are generally below 0.15 K which corresponds to the thermocouple error. The error is the largest for high temperature differences ($1/\Delta T$) and the highest mass flow rate.

Figure 9: Integrated absolute average temperature difference between simulated and measured outlet temperature for all performed experiments as function of $1/\Delta T$ and average mass flow rate.

The sensitivity of the model output to the fitting parameters is tested by varying the effective thermal conductivity k_{eff} and convective correction factor C_f by $\pm 5\%$. The maximum deviation of the outlet temperatures is 0.3 K and 0.48 K for the 10 % variation of respectively k_{eff} and C_f while the time averaged absolute temperature difference is 0.2 K and 0.09 K.

Figure 10 shows the measurement and finite volume model predictions for an experiment with a mass flow rate of 0.5 kg/s and an inlet temperature of about -7°C . The yellow dashed line shows the predicted outlet temperature. The prediction is within the error margin for the outlet temperature for the majority of the experiment with an integrated absolute average temperature difference of 0.1 K. Figure 11 shows the same experiment but with the y-axis scale between -9°C and -2°C .

Figure 10: Comparison between outlet temperature prediction by the finite volume method and the measured inlet and outlet temperature, and the mass flow rate.

Figure 11: Comparison between outlet temperature prediction by the finite volume method and the measured inlet and outlet temperature, and the mass flow rate: zoomed version of Figure 10.

5. Estimator validation

Figure 12 shows the integrated efflux of energy F , the stored battery energy $\Delta U(T_{start}, T_{end})$ and the stored energy $J(t)$ predicted by the finite volume model. The integrated efflux of energy and stored energy are not significantly different at the end of the charging process. Therefore, the integrated efflux of energy can be used as an estimate of the stored energy as a function of time.

The predictions of the finite volume model closely match the experimental results in Figure 12. Since the model is fitted to predict the measured outlet temperature, the integrated efflux of energy should match. Furthermore, heat gains are neglected in the finite volume model. Therefore, the model predictions have to match the measured integrated efflux of energy.

The integrated efflux of energy shows an initial phase, a fast increase after which the rate of change decreases, stabilizes and finally drops. The initial phase consists of a mass flow rate increase from 0 to its set point value where the inlet temperature drops from room temperature to the set point (see Figure 10). During the fast increase mass conservation of the HTF is dominant over the heat transfer to the metal. Once the HTF inside the battery is displaced, the heat transfer to the metal and PCM determines the curve of the integrated efflux of energy. As the battery cools down, the rate of change of the integrated efflux of energy decreases. Once the PCM temperature is reduced to the solidification temperature, the efflux of energy stabilizes. Only at this point, the LTES heat exchanger behaves like a latent storage system. Once the PCM is fully solidified, the battery temperature drops from the solidification temperature and the integrated efflux of energy reaches the total stored energy.

Figure 12: Integrated efflux of energy F , stored energy $\Delta U(T_{start}, T_{end})$ and finite volume stored energy predictions estimates for the experiment shown on Figure 10.

Figure 13 shows the HTF energy estimates as well as the limit estimates for the energy and the finite volume model prediction. The energy stored in the HTF determined by the finite volume model is between the upper and lower limit estimate for the total HTF energy stored during the entire experiment. Furthermore, the HTF stored energy estimate $\hat{J}_{HTF}$ is within the error margins of the finite volume prediction. The limit estimators proposed in Equation 10 and 12 and the stored energy estimator proposed in Equation 13 are thus valid estimators.

The energy stored in the HTF amounts to almost 1 MJ, which is almost 27 % of the total stored energy in the battery. About 80 % of the HTF energy is stored in the initial 50 seconds of the experiment, after 100 seconds this has increased to about 96 %. The majority of the HTF energy is thus stored in the initial stage of charging. The fraction of the energy stored in the HTF is about double of the fraction found by Martinelli et al. [39], however this can be explained by the different heat exchanger design. Martinelli et al. [39] also found that the majority of the internal energy change of the HTF occurs in the initial stages of the experiment.

The estimator for HTF energy proposed by Martinelli et al. [39] is determined using the average temperature between in- and outlet. As is evident from the good agreement between estimator and finite volume model, the estimator presented in this study provides a high level of accuracy based on the same set of measurements used by Martinelli et al. [39].

Figure 13: HTF energy estimates $\hat{J}_{HTF}$, limits and the finite volume model predictions for the experiment shown in Figure 10.

The initial rise of the HTF rate of energy change is caused by an increasing mass flow rate and a decreasing inlet temperature. If the inlet temperature and mass flow rate changed instantaneously to the set point, the rate of change of the HTF energy would instantaneously change to the maximum value and hold this value.

The gradual drop in the HTF energy rate of change can be explained by the incoming HTF mixing with the residual HTF in the battery. If the HTF in the battery did not mix with the incoming flow, the HTF temperature would decrease sharply once the residual HTF is replaced. On the other hand, if the HTF in the battery was perfectly mixed, the outlet temperature would decrease from the onset of the flow. This is not the case, since the outlet temperature remains constant at the start of the experiment.

The energy stored in the metal $\hat{J}_{metal}(t_i)$ is estimated by the sum of the collector energy and the average of the upper and lower limit for the profiles (Equation 17). Figure 14 shows the energy estimators for the profiles. The total stored energy is almost 0.40 MJ or 10 % of the total energy. The finite volume prediction falls within the error margin for the metal energy for the entirety of the process. The estimator is thus sufficient for analyzing the energy stored in the metal. Martinelli et al. [39] found a similar container energy fraction and time behavior.

Figure 14: Metal stored energy estimator $\hat{J}_{metal}$, limits and finite volume model predictor for the experiment shown on Figure 10.

Similar to the HTF energy, the stored energy in the metal experiences a startup phase at the beginning of the experiment. In this initial phase, the warm HTF fluid is being replaced by cold HTF fluid. As more and more of the profiles come into contact with the cold HTF, the local temperature difference between the metal and the HTF increases. As a result, the heat transfer to the metal increases which results in a fast increase in metal stored energy. Once the local metal temperature is dropping as fast as the local HTF temperature, the rate of change reaches a maximum.

The stored metal energy stabilizes between 50 and 200 seconds in two distinct phases. Between 50 seconds and 100 seconds, the local HTF temperature is still changing significantly resulting in a higher heat transfer rate. After 100 seconds, the local HTF temperature remains constant leading to a lower heat transfer rate to the metal. Between 100 and 200 seconds the rate of change drop is the compounded response of the locally decreasing metal temperatures.

Around 200 seconds the stored energy stabilizes. The PCM is solidifying at near constant temperature. As a result, the metal temperature drops less rapidly.

Finally from 400 seconds onward, the rate of change experiences a second albeit much smaller peak. Locally, some parts of the battery are completely solidified. The heat transfer rate from the PCM to the metal is decreased and the metal temperature can decrease at a faster rate.

The stored energy in the enhanced PCM is shown in Figure 15. The total stored energy in the PCM is 2.24 MJ which constitutes 61 % of the total stored energy. It contains both sensible and the latent heat of phase change. The finite volume model predictions are close to the energy estimator based on the measurements except in the initial phase of charging. The limits represent this inaccuracy in the initial phase with a large margin between upper and lower estimator limit. However, the PCM estimator is close to the model predictions once the heat transfer to the PCM becomes the dominant influence in the total stored energy. Martinelli et al. [39] found a similar behavior for the energy stored in the PCM with a delayed start after which the PCM internal energy change dominates the total stored energy.

Figure 15: PCM stored energy estimator $\hat{f}_{PCM}$, limits and finite volume model predictor for the experiment shown on Figure 10.

The PCM energy estimator in the initial phases is not smooth due to the numerical differentiation of the experimental measurements. There is also a large variation between the upper and lower limit estimates for the PCM energy. However, on average the energy rate of change rises in the first 100 seconds and reaches a maximum around 100 seconds.

The energy rate of change rise can be explained by the same mechanism as for the rate of change of the metal energy. Both the local metal temperature and PCM temperature drop. The compound effect is an increasing heat transfer rate to the PCM which lags the rate of change of the metal's energy.

The maximum PCM energy rate of change curve is not as sharp as for the curve for the rate of change of the HTF and metal energy. Once the PCM reaches the upper temperature of the solidification range at the PCM-metal interface, the heat capacity of the PCM increases sharply.

After the maximum value, the rate of change drops steadily until about 400 seconds after which the rate of change drops slightly faster. The higher capacity of the PCM results in a lower time constant for the rate of change response.

At 400 seconds, the rate of change starts to drop more rapidly. Parts of the battery are completely solidified reducing the local capacity. This phenomena causes the increase in rate of change of stored metal energy after 400 seconds.

Based on the energy estimators, the charging process can be divided into four phases. In the first phase from about 0-40 s or 7 % of the total charging time, the HTF energy rate of change contributes about 70 %. The HTF energy rate of change is determined by the HTF mass conservation. The second phase ranges between 40 s and 100 s for 10 % of the total charging time. In this phase, the heat transfer to the metal and PCM increases in importance as the HTF contribution drops. Both the heat transfer to metal and PCM are determined by sensible cooling. The PCM contribution dominates in the third phase. This part is determined by the solidification of the PCM and ranges to about 400 s which results in 50 % of the charging time. In the final phase, the heat transfer rate to the PCM drops as the PCM is solid during about 33 % of the total charging time. Both sensible and latent cooling play an important role in this part.

The two common correlating methods for performance indicators focus on the third phase of charging which constitutes about 50 % of the total charging time. This finding clearly indicates a gap in the research

on the separate phases of charging and the connection between these phases which would allow to correlate performance indicators throughout the charging of a LTES heat exchanger.

Table 6 lists the maximum and integrated average deviations between the energy estimators and the results of the finite volume model. Both the maximum and integrated average percentage deviation is the largest for the metal energy estimator with respectively 9.7 % and 3.9% while the deviation for both the HTF and PCM is around 2 % and 0.5 % for the maximum and integrated average deviation respectively.

The deviation between the efflux of energy determined by the finite volume model and the experimental measurements is minimized by the fitting of the heat transfer coefficients. Therefore, the deviation of the efflux of energy is not included as a validation of an energy estimator but rather as a reference for the estimator deviation. The internal energy change of the HTF, metal and PCM are not minimized by the fitting and are usable to validate the energy estimators.

	Maximum		Integrated average	
	Value [kJ]	%	Value [kJ]	%
Efflux of energy, F	50.1	1.4	10.3	0.3
Internal energy change HTF, J_{HTF}	19.1	1.9	4.6	0.5
Internal energy change metal, J_{metal}	42.3	9.7	16.8	3.9
Internal energy change PCM, J_{PCM}	47.0	2.1	13.4	0.6

Table 6: Maximum and integrated average deviation between stored energy estimates and finite volume results.

The estimators developed in Section 3 provide accurate estimates of the energy stored in HTF, metal and PCM for the presented LTES heat exchanger geometry. Furthermore, the estimator for the internal energy change of the HTF only depends on measurements at the inlet and outlet of the LTES heat exchanger. Therefore, it could be applied to other LTES geometries as well. The estimator for the internal energy change of the metal requires small temperature deviations between the metal parts' outer surface and inner volume. In geometries such as e.g. shell and tube LTES heat exchangers, this might not be the case. Finally, the accuracy of the estimator for the internal energy of the PCM depends on the accuracy of the estimator for HTF, metal and the stored energy which additionally requires negligible heat losses.

6. Conclusion

The stored energy or state of charge as a function of time is an important parameter in characterizing the charging of a LTES heat exchanger. Furthermore, the distribution of the stored energy to each of the heat exchanger's components is interesting for understanding and predicting charging cycles. However, obtaining an accurate measurement of the stored energy is often based on measurements inside the LTES heat exchanger which can be impossible to obtain due to the heat exchanger geometry.

The LTES heat exchanger in the present article only allows surface metal temperature measurements and HTF measurement at the inlet and outlet. The total stored energy is estimated by the integrated efflux of energy, which can be validated by checking the energy balance of a charging cycle. The estimator for the stored energy in the HTF, metal and PCM however cannot be validated via an energy balance. Therefore, a finite volume model is developed and fitted to performed experiments.

The finite volume model is based on the solution of the conservation of energy in the thermal battery. To avoid excessive computation time, the conservation of mass and momentum are not resolved in the HTF

and the PCM is modeled as a one dimensional layer. As a result, the convective heat transfer coefficient and effective conductivity need to be fitted. Accordingly, a fitting strategy based on the HTF temperature at the outlet is devised and the model is fitted to 36 performed measurements.

The stored energy estimators are validated using the predictions of the finite volume model. All estimators obtained a good agreement which allowed identifying the fraction of the energy stored in the PCM as a function of time.

The estimator for the energy stored in the HTF depends only on measurements of the HTF temperature at inlet and outlet and the mass flow rate, while the estimator for the metal and PCM energy also depend on surface temperature measurements. Therefore, the developed indicator for the HTF energy in this paper can be applied to all LTES heat exchangers while the indicator for metal and PCM depends on whether surface metal temperatures are representative of the metal temperature inside the thermal battery.

The estimator developed for the HTF can be combined with the efflux of energy measurement to estimate the heat transfer between HTF and the storage materials (PCM and metal). The estimators allow to identify four phases during the charging cycle. Common methods for correlating performance indicators such as the averaged effectiveness and phase change time method only take into account the third phase in which the phase change occurs. By investigating the energy stored in HTF, container and PCM separately, the other phases can be studied as well as the transition between these phases.

Appendix A Grid convergence of the finite volume model

The model is discretized in two dimensions with n_x control volumes in the flow direction and n_y control volumes for the PCM in the cross section. The grid convergence is checked using the method of Roache [84].

To test the grid convergence, a numerical experiment is performed for sequentially finer grids with the same initial state and input signal. For this grid convergence study, the battery is initialized at 20 °C at the start of the mass flow rate of the HTF is increased to 0.25 kg/s with a constant inlet temperature of -10 °C.

The grid convergence is done in two steps. In the first step, the grid convergence along the x and y direction are checked separately by comparing results for $n=5, 10$ and 20 with the other direction fixed at $n=5$. In the second step the grid convergence is checked in both directions with grids of $(n_x = 5, n_y = 5)$, $(n_x = 10, n_y = 10)$ and $(n_x = 20, n_y = 20)$. The results for each grid will be designated with a subscript 1, 2 or 3 in increasing number of control volumes. In both steps the grid refinement ratio r is equal to 2.

The grid convergence of a simulation is expressed in terms of a quantitative measure of the deviation between the simulation results. The simulation will be used to further investigate the impact of design parameters on the charging time energy fraction model which is derived from the HTF temperature at the inlet and outlet and the mass flow rate. The mass flow rate and inlet temperature is the same for each experiment, so the quantitative measure is based on the outlet temperature. Therefore, the integrated outlet temperature difference is used as defined by Equation 38 where the 1000 s are about the time required to reach 99 % of the total charged energy for the tested inlet conditions.

$$I_{\Delta T;kl} = \frac{1}{1000 \text{ s}} \sum_{i=1}^{n_t} |T_{out,k}^i - T_{out,l}^i| (t_{i+1} - t_i) \quad (38)$$

The order of convergence p can be determined based on the deviation between the consecutive grids, $I_{\Delta T;12}$ and $I_{\Delta T;23}$, and the grid refinement ratio r (Equation 39).

$$p = \frac{\ln(I_{\Delta T;23}/I_{\Delta T;12})}{\ln(r)} \quad (39)$$

The grid convergence index for two consecutive grids GCI_{kl} is determined as Equation 40 where a safety factor of 1.25 is taken since three grids are compared.

$$GCI_{kl} = 1.25 I_{\Delta T;12} \frac{r^p}{r^p - 1} \quad (40)$$

The results of the grid convergence analysis are summarized in Table 7. A grid of ($n_x = 5, n_y = 5$) in each profile obtains satisfactory results with acceptable calculation time.

	$I_{\Delta T;12} [mK]$	$I_{\Delta T;23} [mK]$	p	$GCI_{12} [mK]$	$GCI_{23} [mK]$
n_x	27	7	1.96	45.3	11.7
n_y	42	24	0.83	119.6	67.3
$2D$	48	19	1.32	99.2	39.8

Table 7: The results of the grid convergence analysis according to the method of Roache [84].

Nomenclature

Roman symbols

A	Area	$[m^2]$
A_f	Through flow area	$[m^2]$
c	Specific heat capacity	$[J/kgK]$
d_{metal}	Metal wall thickness	$[m]$
F	Integrated efflux of energy	$[J]$
$\dot{F}$	Efflux of energy	$[W]$
h	Specific enthalpy	$[J/kg]$
	Convective heat transfer coefficient	$[W/m^2K]$
h_{lat}	Specific latent heat	$[J/kg]$
$I_{\Delta T}$	Integrated averaged temperature difference	$[K]$
J	Stored energy	$[J]$
k	Thermal conductivity	$[W/mK]$
k_{eff}	Effective thermal conductivity	$[W/mK]$
L_p	Profile length	$[m]$
m	Mass	$[kg]$
$\dot{m}$	Mass flow rate	$[kg/s]$
n_{HTF}	Number of HTF channels in a profile	$[-]$
n_x	Number of HTF control volumes in each profile	$[-]$
n_y	Number of PCM control volumes per HTF control volume	$[-]$
$Nu_{\sqrt{A_f}}$	Nusselt number based on square root of through flow area.	$[-]$

p	Order of convergence	[-]
Pr	Prandtl number	[-]
$\dot{Q}$	Heat transfer rate	[W]
$Re_{\sqrt{A_f}}$	Reynolds number based on square root of through flow area.	[-]
t	Time	[s]
t_{rep}	Time required to replace heat transfer fluid in battery	[s]
t_{rep}^{-1}	Inverse function of t_{rep}	[s]
T	Temperature	[°C]
u	Specific internal energy	[J/kg]
U	Internal energy	[J]
UA	Overall heat transfer coefficient	[W/K]
V	Volume	[m ³]
w_{HTF}	Width of the HTF channel in the profile	[m]
w_{PCM}	Width of the PCM channels in the profile	[m]
x	Distance from inlet of the profile	[m]
$\vec{x}$	Location	[m,m,m]
z_p	Profile height	[m]

Greek symbols

μ	Dynamic viscosity	[Pa s]
ρ	Density	[m ³ /kg]
λ	Liquid fraction	[-]

Acronyms

CTEF	Charging time energy fraction	
DSC	Differential Scanning Calorimetry	
GCI	Grid Convergence Index	[K]
HTF	Heat Transfer Fluid	
LTES	Latent Thermal Energy Storage	
PCM	Phase Change Materials	
SOC	State Of Charge	

Scripts

C	Collector
end	End of the charging cycle
i	Index in time or space
in	Inlet of the heat transfer fluid
j	Index in time or space
L	Lower limit estimate
out	Outlet of the heat transfer fluid
P	Profile
start	Start of the charging cycle
u	Upper limit estimate
u,e	Extended upper limit estimate
^	Estimator

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