Performance management of EV battery coupled with latent heat jacket at cell level

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# ABSTRACT

This numerical study evaluates the cell level performance management of an Electric Vehicle (EV) battery with Latent Heat (LH) jacket (as passive cooling). In this regard, a battery cell is conjugated with Phase Change Material (PCM) is assessed under continuous cycles of discharging and re-charging. This study is validated with numerical and experimental data with less than 1 % deviation captured from literature for a Panasonic 18650PF Lithium-ion (Li-ion cell). The thermal and electrical performance of key parameters is assessed with and without the existence of a PCM under various climatic conditions including extreme winter -20 °C, winter 0 °C, ambient 25 °C, hot summer 40 °C, and extreme hot/desert 55 °C temperatures. In addition, the choice of PCMs and circumferential jacket thicknesses around the battery (1 mm, 3 mm, 5 mm, and 7 mm) is evaluated in terms of thermal performance for multiple discharge/charge cycles under safe manufacturer operating conditions. Initially the PCM is in a solid state and results indicate that the conjugated thermo-chemical and electrical system is stable whilst LH is active however once fully melted, Sensible Heat (SH) dominates. This study shows, passive cooling maintains the thermal performance of the battery cell for longer, i.e., a 3 mm jacketed PCM as passive cooling results in a 340 % thermal performance improvement in the number of consecutive discharge/charge cycles at ambient weather, 25 °C. At higher ambient temperatures (40 °C and 55 °C) improvement in thermal performances of up to 275 % and 440 % are achieved, respectively. At lower ambient temperatures at -20 °C and 0 °C thermals stability up to 162 % and 160 % with PCM respectively as opposed without for consecutive cycling. It is therefore concluded that efficient passive management is a feasible approach in reducing the harmful effects of overheating, including thermal runaway, thus improving the safety and performance of the electrical energy storage system (EES) in Electric Vehicles (EVs) and Hybrid Electric Vehicles (HEVs).

*Keywords:*

Lithium-ion (Li-ion) battery cell

Passive cooling

Phase change material (PCM)

Computational fluid dynamics (CFD)

Coupled thermal electrical modelling

Transient analysis

Continuous charging discharging

# **Nomenclature**

mushy zone constant () *Greek symbols*

specific heat () thermal diffusivity

inner diameter (mm) expansion coefficient ()

outer diameter (mm) dynamic viscosity ()

friction factor [-] small number

Fourier Number [-] density ()

g gravity acceleration () constant density ()

h sensible enthalpy ) non dimensional term

reference enthalpy ) Electrical conductivity of the passive material (S/m)

H total enthalpy () Electrochemical reaction heat due to electrochemical

reactions

k thermal conductivity () Heat generation rate due to battery internal short-circuit

L latent heat ) Heat generation due to the thermal runaway reactions under

Pressure the thermal abuse condition

SOC State of Charge

source term

t time (s)

T temperature K

Liquid temperature K

operation temperature K

inner surface temperature K

solid temperature

reference temperature K

fluid velocity

# **1 Introduction**

Renewable energy storage is becoming widely acceptable as an alternative source of energy storage and is a viable candidate in the application of zero emission vehicles such as HEVs and EVs. Increased energy demands and consumable resources have albeit dictated the main source of energy in the form of fossil fuels. Unfortunately, industrial processes that employ these sources, have negatively impacted our natural environment in the form of rising worldwide temperatures thus causing a surge in energy demand and rising heat generation. As a result of these global changes there is an ever increasing requirement for renewable energy sources to meet this demand and thus reduce/slow down the impact on our climate [1].

This study seeks to highlight these renewable energy resources in the form of EES [2-5] and Thermal Energy Storage [6-8], they have gained attention in their role of reducing the carbon emissions. Increased attention towards these types of “green” transport as outlined by Kim et al., [9] has driven the capitalization of EV and HEV production in recent years.

According to Meunzel et al., [10], the rechargeable Li-ion battery with its small volume has received great interest due to its high energy density, long life cycles, low self-discharge rate, high voltage and chemical stability when compared with other rechargeable batteries. Studies have shown that when operated at standard ratings, the optimal battery performance is achieved [11]. Li-ion batteries are extremely sensitive to temperature, and it can have an impact on the battery life cycle, stability, and performance as well as operational safety [12-15]. According to [9-10,12-14], deviation from the optimum working temperatures can cause a reduction in the electrical as well as high temperatures causing thermal runaway and potential of fire and explosion.

Even distribution of battery temperature has been found to aid in the thermal and electrical response of the battery [16-17]. Li-ion battery cells operate safely between the temperatures of 20 °C to 40 °C [18-19], this can vary slightly according to the manufacturer and battery type [10]. Fluctuations outside this optimum operating temperature range can cause two types of harmful effects namely: overheating and undercooling. Large temperature gradients from the effects of divergent surface temperature negatively affect the battery performance, therefore maintaining uniform temperature distribution across the battery would aid in its stability [18-20], commonly known as Battery Thermal Management Systems (BTMS) [16-17,21-22]. BTMS is usually focused on active cooling by using a variety of techniques and materials including air [19] and liquid cooling [23-24]. These techniques are required to maintain the optimum battery temperature however they increase the complexity of the EVs and HEVs. There is a significant increase in loading for driving (e.g., fan, pump) and delivering (e.g., channels, pipelines), a cooling medium to and from the batteries. Therefore, if passive cooling alone can provide the cooling capability in the batteries, the BTMS system will be much simpler and lighter, as unnecessary devices and equipment for driving and delivering active cooling medium will be eliminated from the system.



A comprehensive review of PCMs [25,26] of low (-20 °C to 5 °C), medium-low (5 °C to 40 °C), medium (40 °C to 80 °C) and high (80 °C to 200 °C) temperatures were analysed on impact of applications. Medium-low and medium temperature PCMs are more directly related to electronic cooling as a heat sink and in some cases a heat source where the low thermal conductivity of the PCM becomes useful for maintaining stable operating temperatures for purely passive cooling [27]. Natural convection melting, volume, and cell-spacing between cell-scale models are all considerations alongside the thermal conductivity that affects the performance of PCMs as a cooling medium for the thermal management of batteries. These also include battery voltages and uniform temperature for experimental and numerical approaches involving multi-scale multi-dimensional physics models, [28-32].

Research has shown that coupled electrochemical battery and thermal PCM systems has stabilised the temperature [17-18,33-44]. In this instance, heat energy produced from the battery is readily absorbed by the PCM to store the energy as LH [24,41]. PCMs store LH during phase changing as the temperature increased and reached its liquidus temperature point. During this phase change, the temperature of the PCM remains constant, which are useful in thermal applications including free cooling, air conditioning (AC), passive cooling, heat recovery systems and solar energy storage systems [23,42-43].

One of the main parameters that influence the performance of the battery is the State of Charge (SOC) [45]. The SOC usually denoted as a percentage of the remaining capacity is constrained between its fully charged position at 100 % and the fully/deep discharged position at 0 % and as an approximation since the State of Health (SoH) and the Remaining Useful Life (RUL) [46-47] should be considered.

The focal point of this study is to evaluate the impact of passive cooling on Panasonic 18650PF Li-ion battery cell (PCM cooling conjugated with an EES) under various conditions with measured thermal and electrical indicators of performance (SOC, Temperature, and Power) applied in EVs and HEVs, which to the best of authors’ knowledge has not previously been investigated. This study focuses on two cases including a single battery cell (with and without PCM) which undergoes cycles of consecutive discharging and recharging under climatic conditions including extreme winter -20 °C, winter 0 °C, ambient 25 °C, hot summer 40 °C, and extreme hot/desert 55 °C temperatures . Notably, this study takes into consideration the safety concerns of these thermally reactive materials and to reduce the possibility of potential hazards such as fire and explosion. As such, temperature safety limits (charging 0 °C to 45 °C, discharging -20 °C to 60 °C) and voltage (2.5 V to 4.2 V) were imposed on all test cases as well as other constraints. Furthermore, an evaluation study on the effect of the PCM jacket thickness around the cell (1 mm, 3 mm, 5 mm, and 7 mm) is investigated to identify the significance of the volume of the storage system and to effectively reduce the added weight. The study also investigates a variation in PCM applicable to the change in ambient weather conditions.

The structure of the study follows a numerical method detailing the models, mathematical and numerical approaches, assumptions and boundary conditions and verification including numerical (special grid, temporal, and mushy zone) and experimental results validation, results and discussion followed by conclusions.

# **2 Numerical Method**

## *2.1 Models*

The schematic domains of the battery cell are displayed in **Fig. 1** for a cylindrical 18650PF Panasonic Li-ion battery cell as well as the geometrical dimensions. Isometric, front, and side views show battery cell with and without a jacketed PCM. The outer walls both cases, with and without PCM, is set to be adiabatic and hence thermally unaffected from the environment. The dimensions show that the outer diameter and length of the active zone for this battery cell is 18 mm and 65 mm respectively, while the outer diameter and height of the tabs is 6.6 mm and 0.2 mm, respectively.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| A picture containing diagram  Description automatically generated | Battery cell WITHout PCM | Battery cell  WITH PCM |  |  |  |
| ISOMETRIC VIEW | A picture containing telescope, microphone  Description automatically generated | A picture containing microphone, light  Description automatically generated | A picture containing text, scale, device  Description automatically generated  PCM | |
| FRONT  VIEW | A picture containing circle  Description automatically generated | Icon  Description automatically generated |
| SIDE VIEW | Shape, background pattern, rectangle  Description automatically generated | Background pattern  Description automatically generated |

Fig. 1. Schematic of cylindrical 18650 battery cell displaying isometric, front, and side views for battery cell without PCM as well as the jacketed battery cell with PCM.

## *2.2 Mathematical and numerical model approach*

For PCM modelling, an enthalpy-porosity formulation was used to solve the fluid flow equations for melting and solidification instead of tracking the melting/liquid-solid front [49-50]. In the cases where the volume of the cell is liquid, a quantity known as liquid fraction was used to correlate these cells based on enthalpy balance evaluated at every iteration. A “pseudo” porous zone known as the mushy zone, was quantified by the liquid fraction with minimum and maximum values of zero at solidification and 1 at melting, respectively. The values of the mushy zone region were associated to the porosity from solidification to fully melted, 0 to 1 and in the case where the full solidification of the material takes place, the porosity as well as velocity are null. Sink terms applied to momentum and turbulence were used to assess the phase change variation of the solid zones [51]. The thermophysical properties of the PCM and walls are listed in **Table 1**.

The numerical approach for modelling the PCM zone for melting and solidification [41] relates to the following:

The energy equation is stated as:

(1)

Where is derived as the sum of sensible enthalpy, , and the latent heat, :

(2)

(3)

and latent heat, , is defined as:

(4)

The liquid fraction, , is derived as

; (5)

is the source term derived from the momentum sink:

(6)

is a number equal to 0.001, to prevent an invalid result when divided by zero

is the mushy zone constant between [24,41,]; was studied for melting process in this analysis (see 2.5.3)

Substituting the Eqns. {2}-{5} into Eq. {1} yields the energy equation as

(7)

Substituting Eq. (6) into (7) gives the momentum equation:

(8)

With the inclusion of the forces due to gravity, buoyancy driven flows known as natural convection flows are caused from the deviation in density due to temperature. The natural convection in this case occurs within an enclosed domain and so the Boussinesq Approximation is valid to initialise faster convergence for a reference density (constant) and temperature as shown:

(9)

Which is a valid approximation when:

(10)

Eq. (8) can be re-written as:

(11)

The governing equation for continuity:

(12)

The non dimensionless numbers = DV, , and (13)

D = 2 (, the energy equation for the non-dimensionless terms are:

(14)

where Fourier Number,

The numerical approach for modelling the battery cell zone:

A coupled thermal-electrical simulation is used to evaluate the heat generation rate for normal operation, the Multi-Scale Multi-Domain method (MSMD) is used. This method uses a multi-domain, multi-physics approach based on the problem definition where the distributed temperature is analysed along the battery length scale.

The thermal and electrical fields are calculated using the following differential equations:

(15)

Where and are the effective conductivities for the positive and negative electrodes, and are phase potentials for the positive and negative electrodes, is the electrochemical reaction heat due to electrochemical reactions, is the heat generation rate due to battery internal short-circuit and is the heat generation due to the thermal runaway reactions under the thermal abuse condition. For normal operation and no internal short circuit, and are set to zero.

The Equivalent Circuit Model (ECM) in **Fig. 2** replicates the battery electrical behaviour in an equivalent circuit and engages six parameters based on the work from [53] that monitors the electrical performance of the battery during cycles.

Diagram

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Fig. 2. Schematic of electric circuit corresponding to the ECM.

The electric circuit equations corresponding to the voltage-current correlation is given by:

(16)

(17)

(18)

(19)

Where is the battery cell voltage that can obtained either from the circuit solution in in **Fig. 2 using** the Circuit Network solution method or calculated as from the MSMD solution method. For a given battery, the open circuit voltage, resistors’ resistances, and capacitors’ capacitances are functions of the battery state of charge (SOC) and temperature. The functions are defined as fifth order polynomial forms (Equations 20 – 25) used for derivation of the coefficients of the discharging and recharging.

(20)

(21)

(22)

(23)

(24)

(25)

The source terms corresponding to Equation 15 are derived as:

(26)

(27)

Where is the current, and is the open circuit voltage.

Table 1: Thermophysical properties of battery cell (active zone), PCMs and insulation walls [54-55].

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | 18650 Battery cell | Pos Tab | Neg Tab | PCM  (N-octadecane) | PCM  (RT44HC) | PCM  (Stearic acid) | Plexiglass  (insulation) |
| Density () | 2092 | 2719 | 8978 | 770 | 700 | 1150 | 1190 |
| Cp (Specific Heat) () | 678 | 871 | 381 | 2196 | 2000 | 2830 | 1470 |
| Thermal Conductivity () | 18.2 | 202.4 | 387.6 | 0.148 | 0.2 | 0.29 | 0.19 |
| Viscosity () |  |  |  | 0.003 | 0.0033 | 0.0078 |  |
| Thermal Expansion Coefficient () |  |  |  | 0.00091 | 0.00076 | 0.0008 |  |
| Pure Solving Melting Heat () |  |  |  | 243500 | 250000 | 186500 |  |
| Solidus Temperature (K) |  |  |  | 298.15 | 314.15 | 327.5 |  |
| Liquidus Temperature (K) |  |  |  | 302.15 | 317.15 | 337.1 |  |

## *2.3 Assumptions*

To analyse the numerical models presented in **Fig. 1**,the following assumptions are made:

* The battery cell is initially fully charged
* All physical properties of the battery cell are constant
* A transient laminar fluid flow analysis applied for the discharging and recharging of the battery including viscous and incompressible flows
* Heat transfer in the battery cell is due to conduction
* ECM model parameters affecting the electrochemical and thermal properties of the battery are due to the discharging and charging coefficients for the fifth order polynomial form data type
* Gravitational acceleration of 9.81 m/s2 acts downward in the negative y-direction including Boussinesq approximation due to natural convection heat transfer and modelling of the PCM melting and solidification
* Excluding density, all PCM properties are constant
* Molten PCM fluid flow is laminar, incompressible, and viscous.

### *Safety Constraints*

Safety limits were imposed in this study that influenced the battery voltage and temperature during charging and discharging to prevent degradation of the battery, overcharging, thermal runaway, fire, and explosion. In that regard, following restrictions are imposed or battery charging and discharging in the simulations experimental work:

* Simulation cut-off voltage (Maximum/Minimum voltage limits) is set to 4.2 V and 2.5 V, respectively.
* Simulation cut-off temperature (maximum temperature limits) is set at 45 °C and 60 °C, respectively. I.E., in the simulation cut-off is imposed where any further increase in temperature will compromise the integrity of the battery leading to hazardous situations.

## *2.5 Initial and boundary conditions*

To analyse the numerical models presented in **Fig. 1**,the following initial and boundary conditions are considered:

* Adiabatic (zero heat flux) outer circumferential walls applied for all models (outer battery walls and PCM walls for the cases with and without PCM) to prevent heat loss to the environment. In other words, the proposed systems are isolated
* Adiabatic (zero heat flux) walls applied to battery tabs
* Battery cell and PCM thermophysical properties and insulation material are listed in Table 1
* Initial PCM temperature is set to solidus temperature for the models with PCM, and battery cell temperature set to ambient temperature specified (extreme winter weather -20 °C, winter weather 0 °C, ambient weather 25 °C, hot summer weather 40 °C, and extreme hot/desert weather 55 °C).

## *2.6 Verification study*

### *2.6.1 Special grid independence study (mesh)*

The special grid independence analysis ensures that the cases studied were independent of the grid sizes. An analysis of grid independence was performed using the meshing feature that created a structured meshing including quadrilateral cells results. The analysis compared the different grid sizes ranging between coarse, selected and fine defining larger to smaller cells, respectively. The comparison with and without PCM showed little deviation (less than 1 %) between the different grids. An adequate number of elements was chosen for the battery cell with (86877 elements) and (84801 elements) without PCM had high average Orthogonal Quality (greater than 0.95) and low Skewness (less than 0.25).

### *2.6.2 Temporal independence study (time-step)*

Atemporal independency study (time-step) with the influence of the time-step size on the Temperature for the first discharge of the battery cell at an ambient temperature of 25 °C was performed at fixed time-step size at 10 s, 50 s, 100 s (selected), and 150 s for the battery cell without PCM. For this case, the percentage deviation was less than 0.1 % for the selected time-step size of 100 s and was seen as sufficient to conduct the study. For the other case where the battery cell is jacketed with a PCM, a manual adaptive type of time-step size was used to achieve converged results. This ensured that the movement of the melting front and the mushy zone region was accurately captured to effectively evaluate the heat transfer effects due to conduction, convection, and natural convection.

### *2.6.3 Mushy zone constant independence study*

The mesh independency study was performed to understand the impact of the mushy zone constant values, from 1e4 to 1e8 on the melting of the PCM N-octadecane due to the thermal influence generated from the battery cell. In this case, the ambient battery temperature was 25 °C and was deep discharged at 1C rate. Results had little to no impact on the temperature as well as the PCM liquid fraction (approximately 1 %). This can be attributed to the small volume (5973 mm3) of PCM (3 mm circumferential diameter) used in this analysis, as larger volumes of PCM can significantly impact the natural convection [1]. It is during this phase of convection heat transfer which is associated with the rate at which the PCM melts. This study has only incorporated the melting phenomenon of the PCM and does not take the solidification into consideration. In solidification the mushy zone constant would be overlooked since conduction heat transfer would be the dominant heat transfer mechanism. It is noted that ~ 65 % of the PCM was melted at the end of the first discharge, which indicates that the majority of the PCM was liquid with percentage deviation ~1 % for all cases compared to the selected case (1e5).

## *2.7 Computational model setup*

ANSYS Fluent 2021 R1 is used to numerically simulate all cases including discharging and recharging of the battery cell, as well as melting of the PCM using a pressure-based solver adequate for laminar viscous model flows. A transient time analysis was used with implemented Pressure Implicit Splitting Operator (PISO) scheme for the pressure-velocity coupling. Momentum and Energy equations were analysed using second order upwind, while for pressure, PRESTO! was used in the spatial discretization. The under-relaxation factors for pressure, density, momentum, energy, and liquid fraction were set to 0.3, 1, 0.7, 1 and 1, respectively. The convergence criteria were set to 1 micro for each timestep.

# **3 Results and discussion**

## *3.1 Validation*

**Fig. 3A and B** displays the results of the validation of PCM melting and battery cell discharge respectively, captured from literature [41,48,56-58] with less than 0.1 % deviation compared with the present study. Using the captured data for the Panasonic battery cell seen in [48], the coefficients of the fifth order polynomial form were calculated as seen in equations (20-25) and used as the inputs for the MSMD ECM model. Following the insertion of the assumptions and boundary conditions, the cell was discharged from an ambient temperature at 25 °C at a rate of 1C and heat transfer coefficient at 7 (W/m2K) with adiabatic outer walls. The PCM assessed in the validation case was N-eicosane [41] which showed close agreement with the melting of the PCM and the phase change over time. This PCM validation study is shown to predict the melting front movement with close accuracy and a similar analysis is conveyed in this present study with the most suitable PCM.

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Fig. 3. Validation study results: A) Validation of the PCM melting for liquid fraction versus Fourier Number () for the present study compared with numerical data from literature [57,58]; B) Validation of the battery cell thermal analysis for Temperature (°C) versus Time (s) for the present study compared with numerical and experimental data from literature [48,56] at reference ambient temperature of

25 °C.

## *3.2 Coupled Thermo-chemical and electrical results*

The results of the combined thermo-chemical and electrical study of the battery cell in the presence and absence of PCM for the following investigations are presented in this section and sub-sections:

* Investigation on impact of PCM on the battery cell performance under charging and discharging cycles to ascertain its suitability to be considered as a thermal management system for battery cells.
* Investigation on impact of PCM circumferential thickness (1 mm, 3 mm, 5 mm, and 7 mm) on battery performance to determine the most appropriate size for thermal management of batteries.
* Investigation on impact of ambient weather conditions on PCM effectiveness for the thermal performance of batteries to design batteries with a lengthened stability in the process of discharging and recharging cycles even in extreme weather conditions.

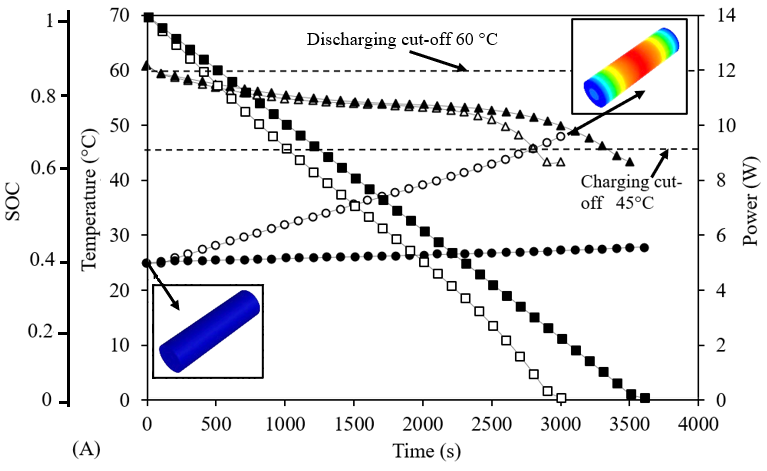
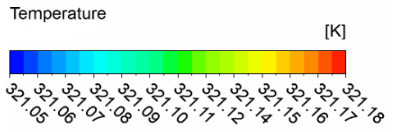
### *3.2.1 Impact of PCM on battery performance under charging and discharging cycles*

The objective of this study was to ascertain whether adding PCM as passive cooling is a suitable solution to enhance the battery performance under charging and discharging cycles. Results of the coupled thermo-electrochemical impact on the battery cell with jacketed PCM is displayed in **Fig. 4**.

The results show the three indicators of battery performance used in this study namely, State of Charge (SOC), Temperature and Power at the initial temperature of 25 °C at the fully charged state. **Fig. 4 (A)** displays a zoomed image with the complete discharge at a rate of 1C of the battery from initial SOC at 1 for both cases of the battery cell with (shaded symbols) and without (unshaded symbols) PCM. From the initial fully charged position, the battery temperature increased linearly during the first discharge until it reached a temperature of approximately 48 °C (in the absence of PCM). It must be noted that the safe operating temperature range for this type of battery cell is within -20 °C to 60 °C during discharge. This meant that in the absence of the PCM, the battery cell temperature was safely within this range. As shown in this Figure, during this first discharge, the SOC for both cases (with and without PCM) linearly decrease from the initial fully charged position at 1 and was fully/deep discharged at 0. Power drops from maximum power (~12W to ~8W) since there was a drop in the voltage of the battery as it discharged. The addition of the PCM jacket around the battery cell (3 mm circumferential diameter), kept the temperature constant and well within the optimum working temperature range (20 °C to 40 °C), showing that the thermal performance of the battery had improved due to the LH available from the PCM. This in turn extended the battery life cycle by a further 20 % (~600 s) in comparison to the standalone battery cell as shown by the electrical performance captured (SOC and Power).

During the process of discharging, the PCM absorbed the heat generated from the battery cell by conduction heat transfer and the PCM began to melt as the liquidus temperature had been reached. At this stage, the liquid fraction of the PCM (molten PCM) was ~64 %, which indicated that there was still solid PCM with available LH capacity. To better understand the impact of PCM on temperature distribution of a battery, in **Fig. 4 (A)** a localized temperature contour layover is plotted at the initial and final conditions for the battery cell without PCM. Please note, as in the presence of PCM the battery temperature did not change significantly, the contour has been excluded in this Figure. Also note, to display maximum temperature, the lower and upper limit of colour bar varies between 321.05 K to 321.18 K, respectively, therefore a reader can better indicate the location of maximum temperature of battery in the overlayed contour. As shown in overlayed contour, the highest temperature is accumulated at the core of the battery and decreases as it moves towards the battery tabs. This showed that the heat generated is at the centre of the battery where the focus of the LH material should be applied. The indication of highest temperature zone was particularly useful for the designation of surrounding PCM. This initial discharging gave insight into the practicality of combining PCM with a constant volume for a single discharge with the applied assumptions and boundary conditions.

Moreover, a supplementary study (extended version of **Fig. 4 (A)**)seen in **Fig. 4 (B)**, analysed the effects PCM on the electrical and thermal performance of the battery involving continuous cycles of discharge and recharge, to ascertain a timespan, that the proposed model operated safely within its limits as discussed in section 2.4. In this case, the PCM enveloped the core of the battery only excluding the tabs (see **Fig. 1**). Like **Fig. 4 (A)**, the boundary conditions and assumptions remained the same with the initial SOC at 1, temperature at 25 °C and a discharge rate of 1C. It is noteworthy that, as discussed in section 2.4, the discharging (60 °C) and charging (45 °C) cut-off temperature limits and voltage limits between 2.5 V and 4.2 V, a continuous cycle of discharge and recharge was performed (see **Fig 4 (B)**). In the absence of the PCM, as previously pointed out, the temperature of the battery cell reached ~48 °C after the first deep discharge, and well within the discharge temperature safety cut-off limit (60 °C). However, a further continuous recharge could not be completed since the battery temperature was above the charging safety limit (45 °C) for the upcoming process of charging, therefore in practice the battery had to be cooled before the charging started. However, as seen in **Fig. 4 (B)**, further continuous charge and discharge cycles were valid for the case with PCM. After the first discharge, the battery temperature was not significantly increased from its initial temperature of 25 °C since LH was still available from the PCM (36 %) to perform further cycles. Immediately after the first discharge (at 3600 s), a first charging was initialised. During this cycle, the battery cell temperature was still relatively constant with a minimal increase in temperature until the PCM had fully melted at 30 °C indicated by a liquid fraction of 1 (at 5300 s). Since the volume of the PCM was completely molten, all the LH capacity available was used up and there was a transition to Sensible Heat (SH) where no further change in phase can occur, but the temperature of the material continued to rise. In this case, the battery cell temperature started to rise sharply (see **Fig. 4 (B)**) almost mid-way through the charging until the end of the first charging (at 7300 s). At this stage, the temperature had reached ~40 °C and was still reasonably within the safe operating temperature range as the PCM contributed significantly to this. The SOC at the end of this cycle did not fully reach the initial starting charge at 100 % since there was a restriction in the maximum voltage (4.2 V), as discussed in section 2.4. Nonetheless, since at this stage in the cycling, the battery cell temperature was ~40 °C and well below the discharging cut-off limit (60 °C), it means that the process could continue safely into another discharge. At the end of this second discharge (at 10305 s), the temperature was at 54 °C and notably beyond the charging cut-off limit (45 °C) and therefore was unable to proceed to the second charge. By considering a complete cycle to include complete discharging followed by recharging, the introduction of the PCM extended the battery life cycle up to one ½ cycles or 3.4 times in comparison to that without a PCM, based on the conditions previously specified.



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Fig. 4. Comparison of battery cell performance including SOC, Temperature (°C), and Power (W) versus Time (s), in absence and presence of 3mm jacketed PCM at 25 °C ambient temperature; A) during a single battery discharge with overlayed localized temperature contours; B) Consecutive cycles of battery discharge and recharge.

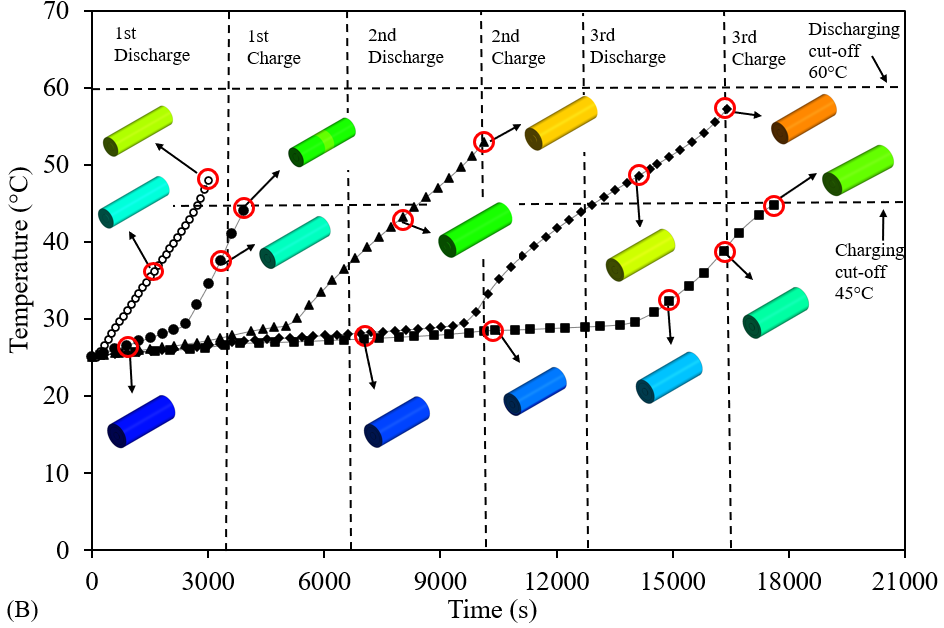
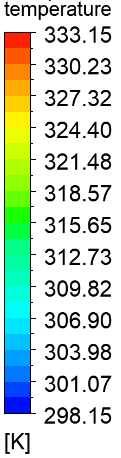
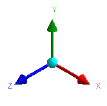
### *3.2.2 Impact of PCM circumferential thickness on battery performance*

As the introduction of PCM proved itself as a promising passive cooling technique, a complimentary study was implemented to ascertain the most suitable PCM size for battery performance. The study analysed the PCM jackets with 1 mm, 3 mm, 5 mm, and 7 mm thicknesses whilst considering N-octadecane as PCM material. **Fig. 5** presents the results of the proposed complementary study. In **Fig. 5 (A)**, a single battery cell underwent deep discharge at the initial temperature of 25 °C at a rate of 1C is displayed with a comparison of the battery cell without (unshaded symbols) and with (shaded symbols) PCM of varying thicknesses. PCM thicknesses of 3 mm, 5 mm and 7 mm performed similarly showing constant temperature. However, the 1 mm thickness of was completely molten at ~2400 s after which a sharp increase in the temperature was observed until the battery was completely discharged (3900 s). This represented a change in the jacket from LH to SH where no further change in phase occurred, but rather, the temperature continued to rise. This can be thought of intuitively, as the greater the volume of PCM, the greater amount of LH available.

This study was further extended into **Fig. 5 (B)**, where continuous cycles of discharge followed by recharge was performed for all the cases for varying thickness of PCM. As seen for the 1 mm PCM thickness, the SH was dominant up to ~2400 s after initialisation. As with the battery cell without PCM, the temperature was beyond the charging cut-off (45 °C) and was unable to proceed to the next cycle (at 3000 s). As seen for the 3 mm, 5 mm, and 7 mm PCM thickness, further cycles were performed. For all cases, the temperature remained constant for a longer time if there was LH present in the PCM (not fully liquid). As previously stated, when the PCM was fully molten, the LH was used up and so SH was dominant, and the temperature started to rise sharply. It shows that as the PCM thickness surrounding the battery cell increased, the battery was able to endure more discharge/recharge cycles. In this case, the 3 mm PCM lasted for 1 ½ cycles, 5 mm for 2 ½ cycles and the 7 mm lasted for 3 cycles whilst taking into consideration the discharging and charging cut-off temperature limits and voltage limits that affect the electrical performance of the battery. The figure also displays the overlayed battery temperature contours in the absence and presence of PCM with varying thicknesses.These contours illustrate the variation of temperature in the cell at different instances. In terms of selecting the optimum volume of PCM to provide the best improvement in thermal performance, the 3 mm jacket PCM thickness around the 18650 cylindrical battery cell was sufficient to illustrate that thermal performance can be prolonged, if the electrical performance was also stable within the limits. When considering jacketing the battery cell with PCM, the available space and volume surrounding the cell must be taken into consideration, as ideally the weight of the BTMS should be kept to a minimum.

Chart

Description automatically generated



Diagram

Description automatically generated

Fig. 5. Impact of jacket PCM thickness: A) Comparison of battery cell Temperature in presence and absence of various circumferential PCM Jacket thicknesses at ambient temperature of 25 °C during single battery discharge; B) Temperature (°C) versus Time (s) in consecutive cycles of battery discharge and recharge with temperature contours at specific instances; C) Liquid fraction versus Time for the melting of the PCM N-octadecane for the battery cell consecutive cycles with liquid fraction contours at specified instances.

**Fig. 5C** shows the liquid fraction versus time for the various sizes of PCM N-octadecane, melting during the consecutive discharging and recharging cycles. The circumferential thickness of PCM was significantly affected by the heat generated, showing that the larger volume liquifies much slower. Liquid fraction contours at front views display the percentage of PCM fully melted at specific times. The battery cell with 1 mm and 3 mm PCM was fully melted after 6000 s and the natural convection is not clearly shown due to small volume sizes. However, for the battery cell with 5 mm and 7 mm PCM, the natural convection during melting is illustrated with a greater volume of solid PCM near the bottom as opposed to the top as shown by the coloured legend. In this case, the volume of PCM could be further increased to prolong the thermal efficiency of the battery. However, considerations towards the weight of the BTMS must be acknowledged as this can have a negative impact on the performance of the vehicle. Based on this study, 3 mm PCM was considered sufficient to extend the thermal performance without having a significant impact on the volume and weight of the system.

### *3.2.3 Impact of ambient weather conditions on effectiveness PCM jacket for thermal management of battery cell even under extreme weather conditions*

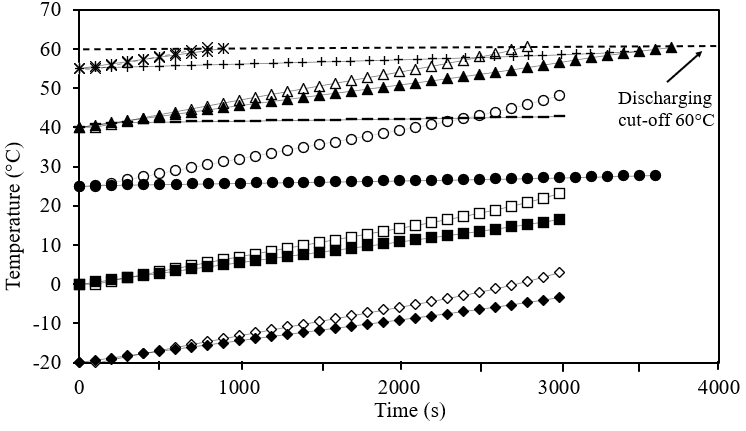
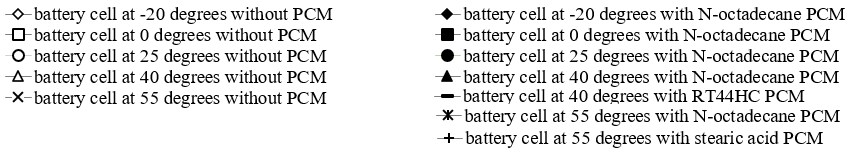


Fig. 6. Comparison of all cases for battery cell discharge with and without PCM N-octadecane at varying initial ambient temperatures of -20 °C, 0 °C, 25 °C, 40 °C and 55 °C

Furthermore, a study performed on the impact of ambient weather conditions from normal to extreme conditions investigated the effectiveness of PCM for thermal management. For this study, varying the ambient temperature conditions for a test case for a single cell battery include -20 °C (extreme winter weather), 0 °C (winter weather), 25 °C (regular ambient weather), 40 °C (hot summer weather) and 55 °C (extreme hot/desert weather). It should be noted that at extremely low temperatures, such as -20 °C, there is an increase in internal resistance and consequently cold start of the battery which was not taken into consideration in this study but could be useful for further investigations. With decreased temperatures, the internal resistance of the battery cell increases, and capacity drops due to slower chemical reactions. **Fig. 6** displays the comparison of all the cases with and without PCM N-octadecane under the various ambient weather conditions after a deep discharge as used previously in this study along with RT44HC and Stearic acid.

At 25 °C, no linear increase is seen as time passes, since the PCM is already molten and the PCM acts as an LH system. Below 25 °C, the ambient temperature weather conditions did not reach the liquidus temperature of the PCM N-octadecane and so the PCM temperature would increase linearly (as the SH is active) until it reaches that melting point (the system acts as LH). For these low temperatures, the N-octadecane (PCM) takes longer to liquify and can undergo further cycles of discharging and recharging until it is fully molten, and the LH returns to SH. For the hot temperatures outlined (40 °C and 55 °C), the PCM N-octadecane was fully molten (at 100 s) and so the LH already turned to SH, since there was no further change in phase. The battery temperature reached the discharging cut-off limit of 60 °C at 2,800 s and 700 s for 40 °C and 55 °C, respectively. In this case, only ½ cycle could be performed whilst safety limits taking into consideration.

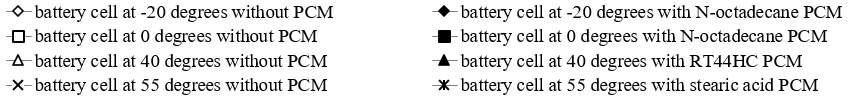
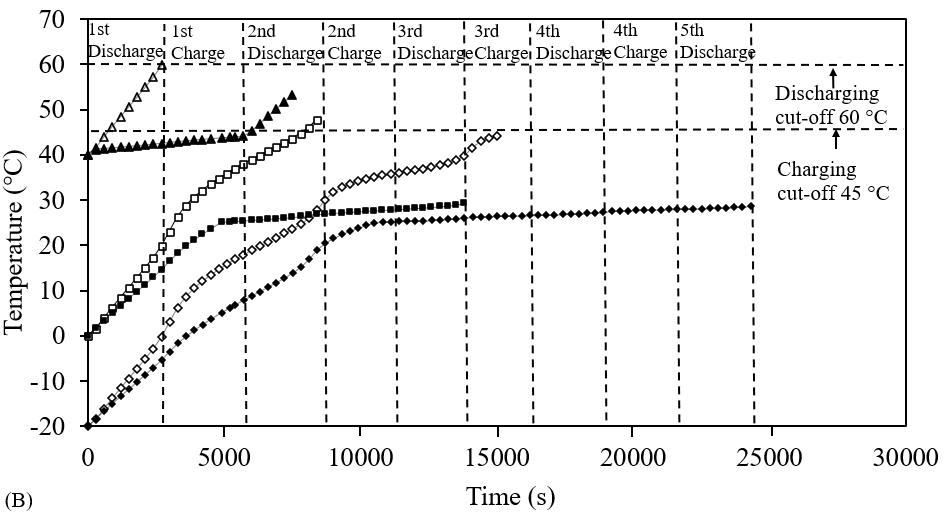


Fig. 7 Comparison of battery cell with (shaded symbols) and without (unshaded symbols) PCM showing the coupled electrochemical and thermal results of Temperature (°C) versus Time (s) at varying initial ambient temperatures of -20 °C, 0 °C, 40 °C and 55 °C for consecutive cycles of battery discharge and recharge.

It can be concluded from **Fig. 6,** thatthe PCM N-octadecane (see properties in **Table 1**) were sufficient up to 25 °C (from extreme cold to ambient weather conditions), due to its solidus and liquidus temperatures. However, the thermophysical properties of PCM N-octadecane is not sufficient for t temperatures higher than 25 °C. This study shows based the geographical weather on the aiming market manufacturers can design enhanced batteries with PCM based on. As the thermal properties of the PCM N-octadecane was inadequate at keeping battery temperature stable for extreme hot weather conditions, another complimentary study was conducted to investigate the impact of different PCM types on the thermal management of the battery. To alleviate the drawback of PCM N-octadecane in the hot weather conditions, two different PCMs were considered for the hot summer weather at 40 °C (RT44HC) and the extreme hot/desert weather at 55 °C (Stearic acid) (see **Table 1**).

**Fig. 7** shows the impact of the variation of PCM for consecutive discharge and recharge cycles. For the cases below 25 °C, SH was still dominant during the first discharge as the liquidus temperature of the PCM N-octadecane had not been reached as previously seen in **Fig. 6**. Unfortunately, due to the extremely high temperature of 55 °C, only a single discharge was performed (see **Fig. 6**)since the temperature was beyond the discharging cut-off limit (60 °C). However, there was still 440 % improvement in the thermal performance of the battery to maintain constant temperature at the end of deep discharge (~4.4x longer). It must be noted that these high temperatures are uncommon, but it is complementary to the results of the possibility of practically using PCM as a passive cooling approach for BTMS designs.

Consecutive discharge and recharge cycles were performed, and the results are shown in **Fig. 7**. For the hot summer weather at 40 °C, the battery cell without PCM could only undergo the 1st discharge before reaching the cut-off temperature (at 2800 s), however, when the PCM was introduced, the battery underwent consecutive charging and was still below the charging cut-off temperature (at 6000 s) and so finally a 2nd discharge was completed (at 7,700 s). LH was active for the first complete cycle of discharge and recharge, however, after this stage, the PCM was fully molten, and SH was active resulting in the sharp increase in temperature during the 2nd discharge. Both cases for 0 °C and -20 °C without PCMs completed consecutive discharge and recharging cycles (1 ½ and 3 cycles respectively) with a steady increase in the temperature until the safety cut-off limit was reached. Similarly, the cases of 0 °C and -20 °C with PCM completed multiple cycles with steady increases in temperature until the PCM started to melt and LH was active. At this region, the battery cell temperature remained constant even up to and after three consecutive cycles for the 0 °C case and up to fifth discharge for -20 °C. This was significant as the battery operated at the optimum temperature up to 2 ½ full cycles and 4 ½ full cycles for the 0 °C case and -20 °C, respectively. After these cycles (at 13,800 s for 0 °C and at 24,300 s for -20 °C), SH was active and no further cycling was performed. The results show that once the most appropriate PCM was chosen based on thermal properties and the ambient conditions, the combined PCM and battery model can maintain its optimum operating conditions for longer.

# **4 Conclusions**

In this study, a 18650 Li-ion cylindrical battery cell was conjugated with PCM to analyse the effects of passive cooling on the thermal performance under consecutive cycles of charging and discharging in varying ambient weather conditions including extreme winter weather -20 °C, winter weather 0 °C, ambient weather 25 °C, hot summer weather 40 °C, and extreme hot/desert weather 55 °C. Variation of circumferential PCM thicknesses including 1 mm, 3 mm, 5 mm, and 7 mm were analysed for the most appropriate PCM thickness and includes variation of PCM for the changing weather conditions. Two cases were analysed one with PCM and one without so that all the heat generated by the battery directly transferred to the PCM. The conclusions from the study are:

* The results of the validation study showed less than 0.1 % deviation from literature with the study results and verification study for the special grid (mesh), temporal (time-step) and mushy zone variations showed that the selected values were sufficiently independent.
* The impact of PCM for regular ambient weather condition at 25 °C, prolonged the thermal performance of the battery cell by 20 % after a single discharge and was effective at maintaining constant temperature for multiple cycles with a total extension of 3.4x (340 % performance improvement). In this first case study, results were positive in the direction of PCM-based thermal-balanced cooling (passive cooling) that provided steady battery temperature control and can function as a standalone BTMS based on the conditions set in this work.
* The impact of circumferential thickness compared PCM jacket sizes of 1 mm, 3 mm, 5 mm, and 7 mm thickness whilst considering N-octadecane as PCM, showed that 3 mm was sufficient for extending the thermal performance.
* Appropriate PCMs chosen for higher temperatures at 40 °C and 55 °C with initial results of discharging, showed constant battery temperature. However, at 55 °C temperature only achieved a single discharge since it reached the cut-off limit, but there was still 440 % improvement (4.4x) in the thermal performance. This temperature is not common but complimentary to the study. Similarly, the 40 °C weather condition without the PCM only underwent a single discharge before reaching the safety cut-off limit, but the addition of the PCM further extended the thermal performance up to 1 ½ cycles.
* For lower temperatures (-20 °C and 0 °C) only SH was observed since the PCM was not at the melting temperature. Consecutive cycles for the 0 °C and -20 °C with PCM remained constant even up to and after 2 ½ and 4 ½ consecutive cycles, respectively displaying 160 % and 162 % thermal performance improvement.

The results show the choice of PCM -based passive cooling on thermal properties and the ambient conditions, can maintain the optimum battery operating conditions for longer.

### **CRediT author statement**

**M. Yang:** Conceptualization, Methodology, Writing – Original Draft, Writing – Review & Editing; **R. A. Nicholls:** Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Writing – Original Draft. **M.A. Moghimi:** Methodology, Software, Validation, Formal analysis, Investigation, Writing – Original Draft, Writing – Review & Editing, Supervision, Project administration, Funding acquisition, management. **A. L. Griffiths:** Writing – Original Draft, Writing – Review & Editing, Supervision.

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