Numerical analysis of phase change materials for thermal control of power battery of high power dissipations

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Abstract. Solid-fluid phase change materials have been of increasing interest in various applications due to their high latent heat with minimum volume change. In this work, numerical analysis of phase change materials is carried out for the purpose of thermal control of the cylindrical power battery cells for applications in electric vehicles. Uniform heat density is applied at the battery cell, which is surrounded by phase change material (PCM) of paraffin wax type and contained in a metal housing. A two-dimensional geometry model is considered due to the model symmetry. The effects of power densities, heat transfer coefficients and onset melting temperatures are examined for the battery temperature evolution. Temperature plateaus can be observed from the present numerical analysis for the pure PCM cases, with the temperature level depending on the power densities, heat transfer coefficients, and melting temperatures. In addition, the copper foam of high thermal conductivity is inserted into the copper foam to enhance the heat transfer. In the modeling, the local thermal non-equilibrium between the metal foam and the PCM is taken into account and the temperatures for the metal foam and the PCM are obtained respectively.

1. Introduction

Since the phase change materials (PCMs) can store large amounts of heat with chemical stability and many other advantages [1-3], they have been widely used in various fields such as electronics cooling and battery thermal management. Duan & Natere [4] experimentally studied two types of PCM for thermal management of battery cell for application in electric vehicles. The first type of PCM had a melting temperature 18°C, and the second type had a melting temperature of 50°C. The results showed that the temperature of heater can be better maintained by PCM in comparison with natural convection. Kandasamy et al. [5] investigated the application of PCM package for thermal management of electronic components experimentally. The effects of power input, orientation of package, and various melting/freezing times under cyclic conditions were investigated. The results showed increased power input would accelerate melting rate, but the thermal properties of the package has minimal impact at different orientation to the gravity. Wu et al. [6] prepared a type of phase change material board (PCMB) with thermal storage capacity of 141.74 J/g and thermal conductivity of 7.654 W/(m K). PCMB displayed much better cooling effect in comparison to natural air cooling in their investigation. Compared with natural air cooling and liquid cooling, PCM could keep...
temperature of electronics at a smaller range of temperature swing and minimize the temperature difference among the cells.

The above studies shows that phase change materials have improved performance in heat storage and temperature control at low heating rate. However, PCM would not perform well for applications with high heating rate and narrow temperature range such as power potteries in electric vehicles, due to the disadvantage of low thermal conductivity of the phase change material, which may not dissipate the heat in a timely manner. To solve this problem, the researchers have proposed several methods. [7-11]. Mills et al. [10] combined expanded graphite with paraffin wax, and the results showed the thermal conductivity of this new composite material was two orders of magnitude larger than that of pure paraffin. Fleming et al. [11] fabricated a shell and tube latent heat storage unit using aluminium foam for heat transfer enhancement. The experimental measurements showed that during melting and solidification process of phase change material, the metal foam significantly improved the heat transfer performance. Literature survey showed that the phase change material has excellent performance in thermal management for battery cells, but most of work is focused on experimental studies. Though some numerical study on the thermal enhancement has been conducted for PCM inserted with metal foam, the corresponding numerical studies are still limited for cylindrical batteries, and the local thermal equilibrium is often used for the composite PCM with foam structure.

In this paper, numerical simulation method is applied to study battery thermal management system with phase change material either with or without metal foam enhancement, which is targeted to the application in electric vehicles. The battery was located in the center of a concentric PCM container, dissipating heat to the ambient through the PCM layer and the convection at the outer wall of the container. High power densities are applied of 399223W/m$^3$, 532297W/m$^3$, and 798446W/m$^3$, respectively. Both the heat conduction and natural convection of PCM will be numerically simulated and analyzed based on the battery temperature evolution. Thermal profiling of battery is also studied with the addition of copper metal foam in the phase change material.

2. Numerical model

![Two-dimensional geometrical model](image)

**Figure 1.** The two-dimensional geometrical model in the present study

The physical problem was depicted in Figure 1, which consisted of the battery, the pure paraffin PCM or PCM composite made of paraffin and copper foam (25PPI, 97%porosity), insulation and
cylindrical enclosure. The diameter and height of 18650 lithium ion battery were 18mm and 65mm, respectively. The thickness of insulating spacers, made of polycarbonate, was 1mm, the housing had an inner diameter of 31mm and depth of 66mm, with a wall thickness of 4mm. Due to symmetry, the two-dimensional computational model was developed. The battery generated a constant heat source $q$. The boundary at the bottom surface of the housing was adiabatic. Outer wall surface of cylindrical housing was set to the boundary of constant heat transfer coefficient $h$. The initial temperature of computational domain was $25^\circ C$. Table1 showed thermo-physical properties of PCM, whereas Table2 showed thermo-physical properties of the other materials in the model. Surface area weighted average temperatures of the battery outer wall and the housing outer wall and liquid fraction of PCM were monitored during simulation.

### Table 1. Thermo-physical properties of paraffin PCM

| Parameters                                | Value      |
|-------------------------------------------|------------|
| Density of paraffin ($\text{kg/m}^3$)     | 920        |
| Specific heat capacity ($\text{J/kgK}$)   | 2400       |
| Latent heat of paraffin ($\text{J/kg}$)   | 195000     |
| Melting temperature of paraffin ($^\circ C$) | 47-53      |
| Thermal conductivity of paraffin ($\text{W/mK}$) | 0.2       |
| Thermal expansion coefficient ($K^{-1}$)  | 0.00085    |

### Table2. Thermo-physical properties of aluminum, copper foam and polycarbonate

| Density ($\text{kg/m}^3$) | Thermal conductivity ($\text{W/mK}$) | Specific heat ($\text{J/kgK}$) |
|---------------------------|--------------------------------------|-------------------------------|
| Polycarbonate             | 1200                                 | 0.19                          |
| Copper foam               | 8978                                 | 387.6                         |
| Aluminum                  | 2719                                 | 202.4                         |

The following assumptions were made in the present numerical simulation:

- The liquid paraffin was considered as incompressible Newtonian fluid and the buoyancy was subjected to the Boussinesq approximation.
- The local thermal non-equilibrium was assumed between the copper foam and the PCM.
- The effect of radiation heat transfer was ignored.
- The specific heat and thermal conductivity of battery and PCM were constant.
- The copper foam was assumed homogeneous and isotropic.

Based on the above assumptions, the Darcy-Brinkman-Forcheimer Momentum equations were used in numerical calculations. Two energy equations model was applied to describe the local thermal non-equilibrium between paraffin and copper foam [12].

Continuity equations,

$$\frac{\partial \rho_f}{\partial t} + \frac{\partial (\rho_f \mu)}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \rho_f \mu \right) = 0$$

Momentum equations,

$$\frac{\rho_f}{\varepsilon} \frac{\partial u}{\partial \tau} + \frac{\partial}{\partial z} \left( \frac{\rho_f}{\varepsilon} uu \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\rho_f}{\varepsilon} uu \right) = -\frac{\partial p}{\partial r} + \frac{\partial}{\partial z} \left( \frac{\mu_f}{\varepsilon} \frac{\partial u}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\mu_f}{\varepsilon} \frac{\partial u}{\partial r} \right)$$

$$-\frac{\mu_f \beta^2}{K} \frac{\rho C_{\varepsilon}}{\sqrt{\kappa}} |u|^2 - (1 - \beta^2) A_u u + \rho g \alpha (T_f - T_{ref})$$

(2)
The energy equations are developed with the two-temperature energy model. For paraffin,

\[
\frac{\rho_f}{\varepsilon} \frac{\partial \nabla}{\partial \tau} + \frac{\partial}{\partial \tau} \left( \frac{\rho_f}{\varepsilon} \nabla \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\rho_f}{\varepsilon} \nabla \right) + \frac{\partial}{\partial \tau} \left( \frac{\rho_f}{\varepsilon} \nabla \right) + \frac{\partial}{\partial \tau} \left( \frac{\rho_f}{\varepsilon} \nabla \right) - \frac{\mu_f}{\varepsilon} \frac{\partial}{\partial r} \left( \frac{\mu_f}{\varepsilon} \frac{\partial}{\partial r} \nabla \right) \right] = \frac{\varepsilon}{r^2} \frac{\partial}{\partial r} \frac{\partial}{\partial r} \nabla - \frac{\partial}{\partial r} \frac{\partial}{\partial r} \nabla - \frac{(1 - \beta)^2}{\beta^2 + \delta} A_{nu} \nabla
\]

(3)

The energy equations are developed with the two-temperature energy model. For paraffin,

\[
\varphi_f \left( \epsilon_j + H \frac{d \beta}{d T_f} \right) \frac{\partial T_f}{\partial \tau} + \rho_f \epsilon_j \left( \mu \frac{\partial T_f}{\partial z} + 1 \frac{\partial}{\partial r} (\nu T_f) \right) = \left( k_u + k_v \right) \nabla^2 T_f + h_{sf} a_{sf} \left( T_s - T_f \right)
\]

(4)

For copper foam,

\[
(1 - \epsilon) \rho_s c_s \frac{\partial T_s}{\partial \tau} = k_{ se} \nabla^2 T_s - h_{sf} a_{sf} \left( T_s - T_f \right)
\]

(5)

\[
\beta = \begin{cases} 
0, & T_f < T_{m1} \\
(T_f - T_{m1})/(T_{m2} - T_{m1}), & T_{m1} \leq T_f \leq T_{m2} \\
1, & T_f > T_{m2}
\end{cases}
\]

(6)

In the numerical investigation, the liquid fraction \( \beta \) for the PCM was denoted in the followings. \( \beta = 0 \) represents the solid phase, \( \beta = 1 \) represents the liquid phase and \( \beta = 0 \sim 1 \) represents that the paraffin was in the mushy region. \( T_{m1} \) and \( T_{m2} \) were the onset melting temperature (MT) and the peak temperature of the PCM according to the DSC test curve.

Permeability \( K \) and inertial coefficient \( C \) were determined by the following equations,

\[
K = \frac{\epsilon^2 d_f^2}{36 \chi (\chi - 1)}
\]

(7)

\[
C = \frac{0.00212 (1 - \epsilon)^{0.132} \left( d_f / d_p \right)^{-1.63}}{\sqrt{K}}
\]

(8)

Where \( \chi \) was the tortuosity coefficient of the copper foam relating to the porosity,

\[
\chi = 2 + 2 \cos \left( \frac{4 \pi}{3} + \frac{1}{3} \cos^{-1} (2 \epsilon - 1) \right)
\]

(9)

The interfacial surface area, \( a_{sf} \), can be determined by,

\[
a_{sf} = \frac{3 \pi d_f}{d_p^2}
\]

(10)

The interfacial heat transfer coefficient, \( h_{sf} \), was formulated as,

\[
h_{sf} = \begin{cases} 
0.76 Re^{0.4} Pr^{0.37} k_f / d_f, & 0 < Re \leq 40 \\
0.52 Re^{0.5} Pr^{0.37} k_f / d_f, & 40 < Re \leq 1000 \\
0.26 Re^{0.6} Pr^{0.37} k_f / d_f, & 1000 < Re \leq 20000
\end{cases}
\]

(11)
3. Numerical method

The commercial computational fluid dynamics software Ansys Fluent was used as the solver in the present study. Due to symmetry, the two-dimensional geometry was considered, which could reduce the number of grids and decrease computing cost. Quadrilateral surface mesh was utilized. To better capture internal characteristics of paraffin during melting, refined grids were applied at the PCM zone. In total 17260 grids was applied, and the time step of 0.1s were used to balance the accuracy of results and the computational time. The second-order-upwind scheme was used to compute convection term and pressure-implicit with splitting of operation (PISO) algorithm for pressure-velocity coupling, and PRESTO for pressure correction. Since the dynamic viscosity of liquid paraffin was sensitive to temperature [13], it was determined by the following equation,

\[ \mu = 0.11994 \times 10^{-4}T + 9 \times 10^{-7}T^2 \]  

The other thermo-physical parameters of paraffin wax have been shown in Table 1.

4. Results and discussion

4.1. Effects of battery power density

Figure 2 showed the numerical results of the temperature distributions of pure paraffin at different time steps \( \tau = 500s, 1000s, 1500s \) and 2000s, respectively. At \( \tau = 500s \), temperature distribution decreased from the battery on the left to the right almost uniformly in paraffin zone. At this time, heat dissipation of battery was mainly through heat conduction, because paraffin just began to melt as showed in Fig. 3. Temperature distribution of paraffin was no longer uniform as the heating time evolved. Temperature was higher at the upper left corner and lower at the lower right corner since the melted paraffin, heated by the battery, moved to the upper left region under the effect of buoyancy. Paraffin remains the solid phase or mushy phase at the lower right corner and the heat transfer thereof was mainly by heat conduction.

![Figure 2. Temperature distributions for pure PCM at different time steps](image)
Figure 3. Liquid fraction distributions for pure PCM at different time steps

Figure 4. Velocity fields for pure PCM at different time steps

Figure 3 showed the numerical results of evolution of the solid liquid interface of pure paraffin at the time steps of 500s, 1000s, 1500s and 2000s, respectively, at the power density of 399223 W/m², the heat transfer coefficient of the housing outer wall 4 W/m²K, and the onset melting temperature of paraffin wax was 47°C. The red-colour area denoted the liquid phase, blue-colour area was the solid phase and the mushy region had the colour between red and blue. Solid liquid interface of pure paraffin became inclined, as indicated in liquid fraction contour from 500s to 1000s since the density of liquid paraffin decreased with the increasing temperature, which generated buoyancy force and thereby resulted in natural convection as showed in Fig. 4. At first, liquid paraffin near the high temperature battery wall flowed upward to the top of the paraffin zone due to the buoyancy effect and then moved downward along the solid liquid interface as a result of heat absorbing of PCM at the melting front. The induced natural convection of the liquid paraffin accelerated the heat transfer, which would maintain the battery temperature near a constant level of temperature plateau. As the time evolves, the natural convection was intensified as indicated in the velocity fields in Fig. 4. Thus the heat transfer was also intensified on the upper part of the paraffin zone, further melting the PCM.
Figure 5 showed the numerical results of the battery wall temperature variation at the power density of 399223 W/m$^3$, 532297 W/m$^3$, and 798446 W/m$^3$, respectively. Here the heat transfer coefficient of housing outer wall was 4 W/m$^2$K, and the onset melting temperature of paraffin wax was 47°C. It can be seen that paraffin entered stage of phase change when the battery temperature reached melting point, the battery temperature curves began to level off, forming temperature plateaus. With the maximum temperatures of 62.4°C, 66.2°C, and 73.3°C, respectively for the three different power densities 399223 W/m$^3$, 532297 W/m$^3$, and 798446 W/m$^3$. It was also noted that the battery temperature reduced by about 1.2°C, 0.8°C and 1.4°C at the end of the plateau. This was mainly because the liquid paraffin began to contact the top inner wall of the metallic housing during the melting process, so heat transfer between paraffin and housing was through solid phase heat conduction as well as the convection heat transfer.

4.2. Effects of the convective heat transfer coefficient of housing wall

Figure 6. Battery temperature profile at different h in W/m$^2$K
The convective heat transfer coefficient had an impact on the battery temperature in battery thermal management. Here the convective heat transfer coefficient of the housing outer wall of $4 \text{W/m}^2\text{K}$, $15 \text{W/m}^2\text{K}$, $40 \text{W/m}^2\text{K}$ were considered, the onset melting temperature of paraffin wax was $47^\circ\text{C}$, and power density was $399223 \text{W/m}^3$. Fig.6 shows the numerical results of simulate battery wall temperature variation. The temperature evolutions of battery outer wall before 2000s were basically the same with the improvement of convective heat transfer coefficient. The plateau temperatures formed owing to natural convection in PCM at around $63^\circ\text{C}$ for different heat transfer coefficients. However, there was a great difference in the time points required for paraffin fully melted, which were 2244s and 3064s, when convective heat transfer coefficient of the housing outer wall was $4 \text{W/m}^2\text{K}$ and $15 \text{W/m}^2\text{K}$. At the highest heat transfer coefficient $h=40 \text{W/m}^2\text{K}$, the melting of paraffin wax was not completed even after 6000s elapsed. It demonstrated that an enhancement of the convective heat transfer coefficient would maintain the battery around plateau temperature for a longer time.

4.3. Effects of onset melting temperatures of paraffin

Figure 7. The evolution of the battery temperature with different onset melting temperatures (MT).

In this section, the effect of the onset melting temperatures of the PCM was examined. Three onset melting temperature (MT) $27^\circ\text{C}$, $37^\circ\text{C}$ and $47^\circ\text{C}$, were considered with the power density of $399223 \text{W/m}^3$. The heat transfer coefficient was fixed to be $4 \text{W/m}^2\text{K}$ for the housing outer wall. The numerical results of the battery wall temperature were illustrated in Fig.7. The time required for onset melting of paraffin wax become shorter with the decrease of the onset melting point of paraffin wax. The paraffin with the lowest melting point of $27^\circ\text{C}$ first began to melt and then entered the stage of temperature plateau, at which the temperature of battery wall was kept around $42^\circ\text{C}$. The paraffin fully melted at $\tau=1468\text{s}$. The paraffin of higher melting points exhibited similar trends, though the plateau temperatures were higher, around $52^\circ\text{C}$ for the onset melting temperature of $37^\circ\text{C}$ and $62^\circ\text{C}$ for the onset temperature of $47^\circ\text{C}$. It is seen that the temperature difference of battery and the onset melting temperature remains almost constant in spite of different onset melting temperature.

4.4. Heat transfer characteristics of pure paraffin and paraffin/metal foam composite
Figure 8. Liquid fraction distribution for paraffin/copper foam composite

Figure 8 showed the liquid fraction distribution for paraffin/copper foam composite. Comparing the liquid fraction of pure paraffin and paraffin/copper foam composite shown in Fig. 3 and Fig. 8, it can be found that the slope of solid liquid interface of PCM composite was much smaller than that in pure paraffin. This was due to the existence of metal foam, so that the liquid paraffin flow was hampered by the ligaments of copper foam. But at \( \tau = 1200 \text{s} \), the majority of the solid phase paraffin had changed into the mushy region, which was quite different from pure paraffin. This was due to the fact that the metal foam composite had a much higher high thermal conductivity and can spread the heat more rapidly within the paraffin. Therefore most of paraffin became mushy before it was fully melted into the liquid. The generation of liquid paraffin in the left PCM area was due to the fact that paraffin in this area was heated by both battery wall and metal foam simultaneously.

Figure 9. Temperature profile at simulate battery wall for pure PCM and paraffin/copper foam composite
The battery temperature evolutions were exhibited in Figure 9 for both the pure PCM and PCM-copper foam composite materials. It was seen that the overall temperature levels of the PCM composites were much lower than the pure PCM case. At the onset of the melting, the temperature difference between the pure PCM and PCM composite reached the highest temperature, which was up to $4.8^\circ C, 7.4^\circ C$ for the heat density $399223 W/m^3, 532297 W/m^3$. The temperature difference between the two heat densities reduced to the minimum when the PCM was fully melted. In comparison, the temperature plateau was more obviously seen in the pure PCM case which helped maintain the battery temperature at a constant level. For the PCM composite case, the addition of copper foam suppressed the natural convection but enhanced the heat conduction greatly, which exhibited a slight slope in the battery temperature evolution.

Figure 10. Velocity field of the numerical simulation for (a) pure PCM; (b) paraffin/copper foam composite

Figure 10 compared the velocity field of the numerical simulation for pure PCM (left) and paraffin/copper foam composite (right) recorded at the heat density, $399223 W/m^3$, and heating time of 1500s. In the pure paraffin case, stronger velocity magnitude was found at the upper left part of the liquid paraffin region. This was due to the high temperature wall surface of the battery continued to heat up the paraffin in its vicinities. In comparison, the velocity magnitude in PCM composite was two orders of magnitude lower. This mainly resulted from the effects of viscous and inertial resistance due to the existence of the ligament of copper foam, which suppressed the natural convection in the PCM composite. Another difference was the mushy regions. As shown in the case of pure paraffin, there were still large portions of solid phase (Figure 3). However, in the case of paraffin/copper foam, due to the high thermal conductivity and volumetric heating effects of the copper foam, all the regions had the velocity magnitude of similar levels (Figure 8). Through the present numerical analysis, the fluid flow and heat transfer for the pure PCM and PCM composite can be well understood.

5. Conclusions
A numerical study had been carried out in using PCM for thermal control of the Lithium ion battery power battery cell. The conclusions can be drawn as follows.

- The temperature plateau phenomena were observed for all the heating power densities. Nonetheless, the plateau temperatures were higher than the maximum melting temperature of
PCM by 9°C, 12°C, 20°C at the power densities of 399223W/m$^3$, 532297W/m$^3$, and 798446W/m$^3$, respectively.

- The effect of the heat transfer coefficient from the housing outer wall was examined. It was shown that the battery temperature increases at the same rate before melting. Nonetheless, longer melting time was observed with higher heat transfer coefficient. If the heat transfer coefficient was larger enough, 40W/m$^2$K in this case, PCM would not be fully melted even after 6000s.

- The effect of PCM onset melting temperature was examined. The lower the onset melting temperature was, the lower the plateau temperature was, whereas the difference of the plateau temperature and the onset melting temperature kept constant. On the other hand, it took longer time for the PCM to melt fully for higher onset melting temperature due to larger sensible heat before melting.

- The copper foam was inserted into the PCM to overcome the shortcoming of the low thermal conductivity. Numerical results showed that there was no obvious temperature plateau for the PCM composite with the copper foam case. In comparison with the pure PCM case, the battery temperature with PCM in copper foam was lower. The natural convection of the melted PCM in copper foam was also weaker than the pure PCM case, leading to a less inclined melting front.

Acknowledgments

Financial supports from the Eastern Scholar program by Shanghai Higher Education Institution and the project 14520501100 granted by Shanghai Scientific and Technological Commission are acknowledged.

A. 1

| Nomenclature | Greek symbols | Greek symbols |
|--------------|---------------|---------------|
| \(a_{sf}\) - interfacial surface area \((m^1)\) | \(\alpha\) - thermal expansion coefficient \((K^{-1})\) |  |
| C - inertial coefficient \((m^1)\) | \(\beta\) - liquid fraction |  |
| \(C_P\) - specific heat capacity \((J/kg K)\) | \(\omega\) - pore density \((PPI)\) |  |
| \(d_f\) - fiber diameter \((m)\) | \(\varepsilon\) - porosity |  |
| \(d_p\) - pore size \((m)\) | \(\mu\) - dynamic viscosity \((kg/ms)\) |  |
| \(d_k\) - characteristic length \((m)\) | \(\rho\) - density \((kg/m^3)\) |  |
| g - gravitational acceleration \((m/s^2)\) | \(\tau\) - time \((s)\) |  |
| H - latent heat of paraffin \((J/kg)\) | \(\chi\) - tortuosity coefficient |  |
| h - heat transfer coefficient \((W/m^2K)\) |  |  |
| \(h_{sf}\) - Interfacial heat transfer coefficient \((W/m^2K)\) |  |  |
| K - permeability \((m^2)\) |  |  |
| k - thermal conductivity \((W/m K)\) |  |  |
| \(k_e\) - effective thermal conductivity of paraffin \((W/m K)\) |  |  |
| \(k_{se}\) - effective thermal conductivity of copper foam \((W/m K)\) |  |  |
|  |  |  |
| \(P_r\) - prandtl Number |  |  |
| P - pressure \((pa)\) |  |  |
| q - heat density \((W/m^3)\) |  |  |
| \(R_e\) - Reynolds number |  |  |
| T - temperature \((^oC)\) |  |  |
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