Thermal performance on the influence of filling ratio of an acetone thermosyphon through numerical modelling

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Abstract. A comprehensively numerical model is established to simulate the phase change in the evaporator section and condenser section in a two-phase closed thermosyphon (TPCT). Combination of Volume of Fluids (VOF) method and an user-defined function (UDF) sources is utilized to simulate the details of flow behaviors and heat transfer phenomena during heat and mass transfer inside the closed chamber. In order to investigate the effect of filling ratio of boiling pool, 50%, 75% and 100% filling ratio are obtained. The displayed contours are analyzed in the light of phase volume fraction, the vapor generation and falling droplets along the thermosyphon. Moreover, the thermal resistance and temperature distribution are conducted to investigate the thermal performance of liquid flow at the end of 10s. It is found that the thermal performance of TPCT reaches the best with 0.78K/W thermal resistance and smooth temperature distribution when the evaporator section is fully charged with acetone.

1. Introduction

With the development of economic society and the deepening of energy crisis, new energy vehicles will become the new focus of automobile industry development. Because of its high energy density, high specific power, light weight, low self-discharge rate and long cycle life, lithium-ion battery is widely considered as the most suitable energy storage device in electric vehicles [1]. However, lithium batteries are susceptible to the temperature fluctuation, especially the high temperature above 50°C will diminish the power capacity, damage reactive substances and shorten the cycle life, which can reduce the efficiency of the power battery [2]. The appropriate working temperature range of lithium battery is within 20°C to 45°C, in which the performance and cycle life of battery will keep a great balance. In addition, the temperature difference of a single cell should be no more than 5°C [3,4].

Nowadays, lithium battery should maintain rapid advancement of materials and performance due to the development of electric technology. In order to acquire higher energy density and extend mileage, and lower the cell temperature and diminish the uniformity of temperature difference during operating conditions, the battery thermal management system (BTMS) is paramount for lithium-ion battery in electric vehicles [5]. An excellent BTMS need to posse various characteristics: effective heat transfer performance, convenient operation and maintenance, and thermal runaway prevention [6].

The passive BTMS take advantage of heat pipe or phase change material to transfer the heat generated from the cell core. Heat pipe is considered to be an efficient heat sink, which is a sealed vessel formed by the two-phase conversion mechanism from evaporation to condensation [7,8]. It has the virtual of thermal homogeneity and low thermal resistance that can improve the heat transfer performance [9]. The TPCT, one of the heat pipe, transfers the vapor by pressure difference from evaporator section and flows the liquid back to the boiling pool by the gravitational forces, which consists of a circulation loop [10,11].
limited numerical investigation has been carried out to study the heat transfer performance and two-phase flow characteristics in the thermosyphon. Alizadehdakhel et al. [12] established a numerical thermosyphon, in which the temperature distribution was validated by the experimental apparatus through inserting a volume of fluid method, in which a vapor generation in the evaporator section and a liquid film in the condenser section could be observed. It was found that the numerical simulation was clearly described the phase transformation during the working state.

Fadhl et al. [13] made first attempt to inject two working fluids, R134a and R404a into thermosyphon at different constant heat flux. The results revealed that the average relative errors of the temperature distribution curves of the experimental and computational fluid dynamics (CFD) simulation were highly consistent, less than 2%. Xu et al. [14] developed a model considering the evaporator wettability and inclination contact, which showed that inclination angle of 90° had the lowest thermal resistance that decreased 44.1% with a hydrophilic surface than 20.6% with a hydrophobic surface for evaporator section. Fertahi et al. [15] built a comprehensive model to reproduce the phase change process from evaporation to condensation in a thermosyphon. In order to improve the thermal performance and heat transfer ability, tilted fins integration on the condenser section were implemented, which promoted the efficiency of thermosyphon to 16.05% and accelerated the energy transfer velocity.

However, the CFD studies on the heat transfer analysis of TPCT are insufficient to investigate the phase change and thermal performance. Coupled with the power batteries, the working fluid in the thermosyphon should be operated within the optimal temperature, therefore, an acetone medium can be utilized to investigate the thermal characteristics. In addition, the influences of filling ratio are explored and performance indicators are defined to access the heat transfer effect.

In this paper, a numerical TPCT model charged with acetone by considering filling ratio is established. Combination of VOF method and UDF sources is inserted to simulate the two-phase change during heat and mass transfer from boiling pool to condensed chamber. This work contains observation about the thermal performance of an acetone thermosyphon at constant heat flux generated by the discharging batteries.

2. Model description
The numerical simulation of TPCT is based on the VOF method by momentum solver to monitor the phase volume fraction through the computational domain in the ANSYS FLUENT 18.0. The Euler-Euler approach is utilized to calculate the multiphase flow and the Navier-Stokes equations are solved to track the flow behaviors of each phase. Moreover, an UDF is implemented as source terms, namely energy, liquid and vapor sources, to predominant the mass and heat transfer mechanism during the evaporation and condensation.

2.1. Navier-Stokes equations
The two-phase interface is monitored and solved by the continuity equation (volume fraction equation), as listed as follow:

\[
\frac{\partial (\alpha_l \rho_l)}{\partial t} + \nabla \cdot (\alpha_l \rho_l \vec{u}) = S_m
\]  

In above the subscript \(l\) and \(v\) represent the liquid and vapor phase, respectively. Where \(\alpha\) is the volume fraction, \(t\) is the time, \(\rho\) is the density, \(u\) is the velocity and \(S_m\) is the mass source.

The velocity of mixture phase is solved by the momentum equation, which is obtained as follow:

\[
\frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \left[ \mu \left( \nabla \vec{u} + \nabla \vec{u}^T \right) \right] + \rho \vec{g} + \vec{F}_{CSF}
\]  

Where \(\mu\) is the dynamic viscosity, \(p\) is the pressure, and \(g\) is the gravitational acceleration.

A continuum surface force (CSF) model has been proposed by Brackbill et al. [16] as follow:

\[
F_{CSF} = 2\sigma_{ls} \frac{\alpha_l \rho_l C_i \nabla \alpha_l + \alpha_v \rho_v C_l \nabla \alpha_v}{\rho_l + \rho_v}
\]  

Where \(\sigma_{ls}\) is the surface tension, and \(C\) is the curvature.
The energy equation is shown below:
\[
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot [\bar{u}(\rho E + P)] = \nabla \cdot (k \nabla T) + S_E
\]
(4)

Where \( k \) is the thermal conductivity and \( T \) is a mass-averaged variable of temperature. \( E \) is the energy and \( S_E \) is the extra source term to transfer the energy.

2.2. Mass and heat transfer
An UDF is compiled in the numerical setup to simulate the transformation between the vapor and liquid regarding the saturation temperature as the variable indication along the computational zone, which compares the mixture temperature of two phases with saturated temperature. The mass and heat transfer occurs inside the transformation chamber through latent heat. The construction of source terms is listed in table 1.

| Temperature condition | Phase change process | Phase | Source term |
|-----------------------|----------------------|-------|-------------|
| \( T_{mix} > T_{sat} \) | evaporation          | Liquid| \( S_{ml} = -0.1 \alpha_f \rho \frac{T_{mix} - T_{sat}}{T_{sat}} \) |
|                       |                      |       | \( S_{ml}' = -S_{ml} \) |
|                       |                      |       | \( S_{El} = S_{ml} \cdot LH \) |

| \( T_{mix} < T_{sat} \) | condensation         | Vapor | \( S_{ml} = 0.1 \alpha_f \rho \frac{T_{sat} - T_{mix}}{T_{sat}} \) |
|                       |                      |       | \( S_{ml}' = -S_{ml} \) |
|                       |                      |       | \( S_{El} = S_{ml} \cdot LH \) |

Where \( S_{ml} \) is the mass source term, \( S_E \) is the heat source term, \( T_{mix} \) is the mixture temperature of two phases, \( T_{sat} \) is the saturation temperature, and \( LH \) stands for the latent heat.

3. Numerical modelling

3.1. Simulation setup and solution
A new two-dimensional model is established in figure 1. The liquid is heated in the boiling pool of evaporator section and the vapor is condensed in the upward chamber, then the liquid film flows back to the downward zone by the gravity. The whole length of the thermosyphon is 150mm in on the basis of CATL battery: 95mm length of evaporator section, 15mm length of adiabatic section and 45mm length of condenser section. The thickness of the thermosyphon shell is 0.5mm and the outer diameter of it is 6.5mm. The TPCT is made of aluminum with 50%, 75%, 100% filling ratio. The heat flux, imposed on the evaporator section, is 4984W/m², and that of adiabatic zone is 0W/m². The condenser section is maintained at 25°C as the temperature of constant cooling water. Additionally, the interface between the fluid zone and solid place is set as coupled wall, which can only transfer heat but not the phase. The working fluid is acetone and its physical properties are listed in the table 2.

A transient time step is 0.0005s that is carried out to distinctly simulate the phase change process, and the simulation process achieves a steady state at the end of 30s. The pressure-based Navier-Stokes solution algorithm, based on the SIMPLE algorithm, is adopted to adjust the pressure relaxation factor. The Geo-Reconstruct and PRESTO scheme are adopted for the volume fraction and pressure, respectively, a first order upwind scheme is used for momentum and energy equations to accelerate convergence.
Table 2. Physical properties of acetone.

| Thermal property              | Units            | Acetone (l)    | Acetone (v)    |
|-------------------------------|------------------|----------------|----------------|
| Density                       | kg/m³            | y = -0.0011x² - 0.4841x + 1023.1 | 1.3031         |
| Specific heat                 | kJ/kg·K          | 2181.8         | 1472.4         |
| Thermal conductivity          | W/m·K            | 0.14913        | 0.015365       |
| Viscosity                     | Kg/m·s           | 0.0002674      | 8.4146e-06     |
| Latent heat of evaporation    | kJ/kg            | 518.89         |                |
| Molecular weight              | kg/kmol          | 58.08          |                |
| surface tension               | N/m              | \(\sigma LV = 0.5e^{-0.8x²} - 1.5541e{-0.04x} + 6.4578e{-0.02}\) |
| Saturated vapor pressure      | kPa              | 53.32 (39.5°C) |                |

Figure 1. Geometry and boundary condition of thermosyphon.

Figure 2. Two types of mesh structure for independence test.

3.2. Mesh independence
Due to the heavy workload of computational task for simulation while acquiring the accurate precision, a mesh independence test is conducted. Two types of mesh structure with grid numbers of 51968, 71958, are simulated, which are presented in the figure 2. With the filling ratio of 100%, the deviation of temperature distribution of TPCT in both grids is within 2% that can be ignored in the results. Therefore, the grid numbers of 51968 are adopted for the next two-phase flow simulation.

4. Results and discussion

4.1. Thermal performance at different filling ratio
The simulated thermal resistances vary from 1.53-2.03 K/W, 0.80-1.51 K/W and 0.78-1.40 K/W at various filling ratio of 50%, 75% and 100%, respectively. As presented in the figure 3, the thermal resistance rapidly decreases at the beginning and gradually stabilizes due to the constant temperature at the condenser section rather than the heat transfer coefficient when the evaporator section of thermosyphon is charged with 75% and 100% acetone. The thermal resistance of 75% filling ratio is 2.6% higher than that of 100% filling ratio at the end of 10s, of which the boiling pool is filled with liquid, so it takes a long time for bubbles to generate and the temperature in the condenser is fluctuated leading to the unsteady thermal resistance from 3s to 8s. Additionally, When the filling ratio is 50%, the upper zone of the evaporator section and adiabatic walls have heat accumulation, where the falling
droplets are heated and prevent the heat from going up by the steam pressure. Then, a huge thermal resistance comes into being inside the liquid chamber.

![Figure 3](image3.png)

**Figure 3.** The influence of filling ratio on thermal resistance of thermosyphon.

4.2. *Temperature distribution of thermosyphon*

The temperature distribution along thermosyphon has been monitored at diverse filling ratio in the simulation. Figure 4 reveals the temperature values in the fluid zone are recorded along the Y axial position from 0 to 150mm. That liquid absence at the evaporator section will raise the temperature because the droplets are evaporated before it reaches the boiling pool when the filling ratio is 50% and 75%. The temperature along the central axis at 100% filling ratio is lower than that of other two cases all the time. The average temperatures of evaporator section, adiabatic section and condenser section are 317.66°C, 314.83°C and 310.13°C, respectively. It is obvious that the temperature fluctuations of phase chamber smooth with increasing filling ratio. Therefore, the optimal heat performance is acquired at the filling ratio of 100%.

![Figure 4](image4.png)

**Figure 4.** The effect of filling ratio on temperature distribution of thermosyphons.

4.3. *Flow vision of evaporator section*

As shown in figure 5, the two-phase flow behaviors taking place in the evaporation section has been observed during the operating condition. The volume fraction of vapor phase stands for the red colour, and the blue color means the liquid state. The primary boiling pool is filled with acetone as working fluid, while adiabatic and condenser sections are charged with gaseous acetone. With simulated duration increased, the bubbles generated by the heat flux occupies the evaporator and continues to ascend up from 1s to 10s. The vesicular flow initially happens between 1s and 2s, where the liquid temperature has just reached a saturation temperature and the microbubbles are emerged from the
adjacent walls, which absorb the amount of heat and grow up. Then, the newly slug flow, formed by the collision and coalescence of small bubbles, occurs in the upper zone of boiling pool between 3s and 5s. The slug flow bears large fluctuation of flow rate and pressure, and instability, so the bubbles turn into bulk state that absorb the energy along the high temperature walls when the evaporator section is in a steady state of 10s.

**Figure 5.** Two-phase flow behaviors in the evaporator section of thermosyphon.

**Figure 6.** Droplets and liquid film in the condensation process of thermosyphon.

### 4.4. Condensation process

The condensation process is described in the figure 6, in which the droplets and liquid film absorb the heat flux. For adiabatic section, the hot vapor also obtains amount of heat in the upper zone of evaporator, and the particle path of droplets further improves the heat transfer. The liquid film flows back to the boiling pool to accomplish a two-phase change circulation in the thermosyphon, which can offset the loss of liquid phase.

### 5. Conclusion

The heat transfer characteristics of thermosyphon charged with acetone at shallow temperature are numerically investigated in this paper. From the flow figure, the numerical simulation can reproduce the dynamic motion of the thermosyphon by utilizing A VOF method and an UDF to simulate the two-phase flow behaviors. In the established model, the vapor ascends to the adiabatic and condenser section by the pressure and the droplets goes down to the evaporator section by the gravitational force. The bubble flow becomes slug flow from 1s to 5s, and finally the block flow comes into being at the steady state. Meanwhile, the droplets and liquid film can be observed during the simulation. A set of physical indicators are monitored to calculate the thermal performance of the thermosyphon between the boiling pool and condensed chamber. It is found that the 50% filling ratio will accumulate the heat at the adiabatic zone, and 100% filling ratio of evaporator can reach the best performance with 0.78K/W thermal resistance at the end of 10s, 2.6% lower than that of 75% filling ratio. Additionally, it has stable temperature fluctuation with 7.53°C of average temperature difference between evaporator and condenser sections.

**Acknowledgments**

The authors acknowledge the financial support received from National Nature Science Foundation of China (Grant No.51965008), Major Science and Technology projects of China of Guizhou ZNWLQC [2019]3012.
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