Thermal and Heat Transfer Modeling of Lithium –Ion Battery Module during the Discharge Cycle

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Abstract

Climate change and concerns over the reliable supplies of hydrocarbons are aiding in the focus on Electric Vehicles (EVs) and Hybrid Electric Vehicles (HEVs). The Lithium-ion battery as a better solution for the energy storage in automobile applications is briefly introduced. Adverse effects of uneven temperature including thermal runaway, low temperature performance and performance degradation are described in detail. Furthermore, the progress on existing battery thermal management systems including both active and passive cooling methods are also described. Mainly, this paper investigates the temperature distribution and the heat generation characteristics of a cylindrical Li-ion battery cell and a battery module. Three sources of heat generation were considered in the modeling including Ohmic heat, the reaction heat and the polarization heat. The battery cell consists of spiral wounded cathode, anode, current collector and a separator. The material properties are those of a typical lithium-ion battery. Transient and thermo-electric Finite Element Analysis (FEA) of cylindrical lithium ion battery is presented. Adopting the cylindrical coordinates and lumped modeling theories simplified the model. The FEA was performed using COMSOL Multiphysics 5.5 software and the association of Battery and Fuel Cells module. Li-ion 1D model was also used from COMSOL application libraries to identify the exact amount of heat generation from the battery cell. The 1D model coupled with 3D model for the cell temperature distribution. The cell simulation model was then expanded for the battery module temperature profile simulation and the battery module consists of 59 cylindrical battery cells. Based on results, it can be confirmed that the temperature profile from analytical model had a similar tendency with the simulation model. In addition, the temperature distribution change based on different cell arrangements are also discussed and presented.

Keywords: Heat transfer, temperature distribution, Li-ion battery modeling

Introduction

The global concerns over reducing the dependence on fossil energy and ultimately producing less harmful emissions are aiding the focus on Electric Vehicles (EVs) and Hybrid Electric Vehicles (HEVs). The performance of EVs and HEVs are mainly dependent on the energy storage system such as batteries and the battery performance influences various parameters such as travelling distnace, acceleration and the charge acceptance during recovery from regenerative braking. Since the cost of the batteries, life –cycle and the durability affect the reliability of a battery powered vehicle, it is necessary to optimize the parameters which affect the efficiency of the batteries.

The Lithium-ion (Li-ion) battery is considered as the first –choice candidate for a power source of EVs and HEVs due to its many advantages such as low self-discharge rate, high efficiency, and high power to weight and energy to weight ratios [1]. In addition to EVs and HEVs, Li-ion batteries are commonly used in telephone communication and portable electronic devices as well. However, the thermal performance of Li-ion battery limits its long term stability and safety characteristics since the best operating temperature of the battery is typically between 30-40^{o}C [2]. Furthermore, it is necessary to operate the battery modules at a uniform temperature since the uneven temperature distribution will cause an electrically unbalanced module and shortened the battery life. In addition, thermal runaway may occur in a cell when heat is not properly controlled. Fire and explosion are the significant risks that can be happen due to uncontrolled heat distribution.

Many researchers have conducted investigations into the influence of the temperature and heat distribution on battery packs. Sherfey et al [3], Gross et al [4], Dibrov et al [5] and Chen et al [6] have adopted experimental approaches and used calorimeters to determine the heat output. In addition, two-dimensional Computational Fluid Dynamics (CFD) models were developed by Li [7]to conduct detailed simulations of the thermal management issues within a battery pack cooled by air. Previous studies focused on the investigation of commercial battery modules and contributed to the thermal management of Li-ion batteries. However, it can be found that there is less number of investigations have been conducted in terms of different cell arrangements and inter cell distance aspects. Therefore, this paper investigates the designs of cell arrangements together with different inter-cell for the battery module applied in high power lithium-ion battery pack. The FEA method and lumped model of a single cell have been

introduced in the simulations. Section 2 describes the analytical approach of heat transfer modelling of single cell Li-ion battery. In section 3, thermal modelling of a Li-ion battery module is discussed. The temperature distribution change in terms of different cell arrangements and inter-cell distances are discussed in Section 4. Finally, a discussion is provided on the simulation results.

Analytical model for Li-ion battery single cell heat transfer

Batteries mainly generate heat during charge and discharge due to enthalpy changes, resistive heating inside the cell and the electrochemical polarization. The heat originates from the enthalpy change associated with electrochemical reactions. The ohmic heat is the energy loss caused by the transport resistance in solid and electrolyte phases. The polarization can be identified as the deviation between the cell open-circuit potential and the operating potential. However, there is resistance to hinder the charge transfer process at the solid – electrolyte interface. The energy which is required to overcome the resistance is referred to as the active polarization heat [2].

The energy balance equation for a cylindrical Li-ion battery cell is developed by considering the energy conservation law and the equation can be expressed as follows:

$$\rho C_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(k_r r \frac{\partial T}{\partial r}\right) + \frac{1}{r^2}\frac{\partial}{\partial \varphi}\left(k_a \frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right) + \dot{Q} \quad (1)$$

Where, ρ is the density of active battery material (kg/m^3) and C_p is for specific heat capacity (J/kgK). T denotes the absolute temperature (K) and r represents the radius of the battery cell (m). k_r , k_a and k_z denote the thermal conductivity for radial axial and z directions respectively (W/mK). Furthermore, $\dot{Q}$ denotes the volumetric heat generation rate for the battery cell (W).

The term on the left hand side represents the energy accumulated inside the battery and the right side terms demonstrate the three dimensional heat conduction and the volumetric heat generation rate expression respectively.

Generally, the cell consists of layers of cathode, separator, current collector and anode wound spirally into a cylinder. Although those layers have different thermo-physical properties theoretically, each cell of the battery module is considered as a homogenous body with effective thermo-physical properties [8]. By considering the above facts, the effective value of density and heat capacity of a single cell can be presented as follows.

$$\rho C_p = \frac{\sum_i \rho_i C_{p,i} V_i}{\sum_i V_i} \quad (2)$$

Where, $V_i$denotes the volume of each component. In addition, the thermal conductivity of the cell is anisotropic and therefore, the thermal conductivity in radial and axial direction is defined as follows.

$$k_r = \frac{\sum_i L_i}{\sum_i L_i / k_{T,i}} \quad (3)$$

$$k_a = \frac{\sum_i L_i k_{T,i}}{\sum_i L_i} \quad (4)$$

Where, $L_i$is the thickness of each component (m) and $k_{T,i}$ represents the total thermal conductivity of each component (W/mK).

The lumped capacitance model was assumed in the analytical solution method for the heat transfer in battery cell. Generally, lumped capacitance thermal modelling is a transient conduction approach. In lumped thermal modelling, it is assumed that the temperature of a solid is spatially uniform and is a function of time (t) only. This implies that the temperature gradient in a solid is negligible and the thermal conductivity is infinite. Although in reality this is not true, it can be approximated only if the thermal resistance to conduction within the solid is significantly less than the thermal resistance to convection between the solid and the surrounding [9].

$$\frac{L_c}{k} \ll \frac{1}{h} \quad (5)$$

Where $h$the convection heat is transfer coefficient (W/m^{2}K) and L_c is the characteristic length (m). Characteristic length is the ratio of volume to surface area of the solid. In addition, the equation (6) formulates the dimensionless Biot (Bi) number.

$$Bi = \frac{hL_c}{k} \ll 1 \quad (6)$$

The ratio of the heat transfer resistance inside and at the surface of the battery cell is represented as the *Bi* number and the Bi number has to be significantly less than 1 to be applied in a lumped capacitance model. It is because, when Bi <0.1, the error of transient heat model is less than 5%. When considering the parametric values of current scenario, the Bi number is also less than 0.1. Therefore, it is possible to apply the lumped capacitance model for the Li-ion battery cell heat transfer and the equation can be simplified as follows:

$$\rho C_p \frac{\partial T}{\partial t} = hA(T - T_{amb}) + \dot{Q} \quad (7)$$

Where, T_{amb} is the absolute temperature at the ambient condition (K).

In 1995, John Newman and Caroline [10] published the first equation related to the heat transfer in single Li-ion battery cell and the equation (7) confirms the Newman's equation of heat transferring for Li-ion battery cell.

Thermal modelling of Li-ion battery module

The 3D simulation model for the Li-ion battery cell was developed as a CFD model by using COMSOL Multiphysics 5.5 software [11]. Apart from the basic package, the add-on modules "Heat transfer in Solids and Fluids" and "Batteries and Fuel Cells" are used in the modelling.

The simulation model for a single cell contains a 1D model and a 3D model and the two models were coupled with each other in the simulation. In order to identify the exact heat generation inside the cell, the 1D model is used. The 1D model also facilitates the required battery cell chemistry for the simulation. The 3D model is used to model the temperature profile of the battery cell and it was developed based on the Newman's [10] heat transfer model which was already confirmed analytically.

The Li-ion 1D model from COMSOL application libraries [11] contains three domains; negative porous electrode, separator and positive porous electrode. Furthermore, as indicated in application library, 0V is set on the negative electrode's current collector for the electronic current balance and the current density is specified at the positive electrode current collector in the model. Moreover, the model has a discharge cycle which is followed by interval of zero current and a final charging stage [12].

As mentioned above, the 3D model is mainly identified as the thermal model and developed using COMSOL Heat Transfer in Solids and Fluids interface [11]. As indicated in Figure 1, the geometry consists of four domains including active battery material domain, cylindrical battery connector, and mandrel and flow compartment. The heat source is associated with the active battery material and, as above, the active battery material domain is considered to represent all layers of the Li-ion battery cell. In addition, the active battery material domain adopts effective material properties as in analytical model. The battery connector material is steel and the nylon isolator around which the battery cell sheets are wound is identified as the mandrel. Since the research focused on the18650 standard air-cooled Li-ion battery cell, the cell has the radius of 9 mm and the height of 65 mm. For simulation purpose, the flow compartment is filled with air.

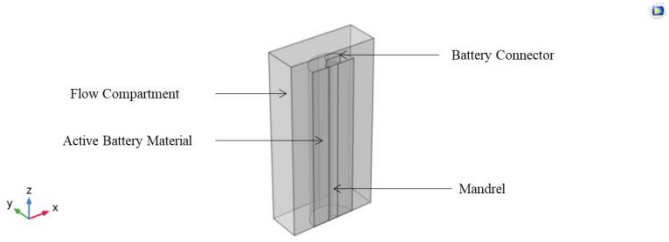

Figure 1.3D Battery model

As boundary conditions, both inlet and initial temperatures are set to 298.15 K in the 3D model. The airflow velocity is taken as 0.1 m/s at the inlet for x direction and a pressure of 1 atm is considered. Symmetry boundary conditions are applied to the battery walls. As indicated in COMSOL application library [11], a square wave function is used to demonstrate the alternating charge and discharge current at 7.5 C rate and the cycle time of 600s including a relaxing period after 1500s is applied. Furthermore, the initial State of Charge (SoC) is taken as 10% for the model [12].

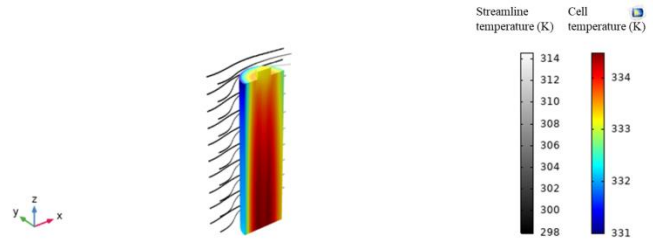

Figure 2. Temperature distribution results of a single cell

The result indicates that the maximum temperature is more than 334 K and the temperature of the flow varies between 298 K and 314 K. Maximum temperature is marked at the mandrel and active battery material. The outer boundary of the cell has the minimum temperature since the outer boundary touches the airflow.

The steel battery canister is not considered in the thermal modelling simulation, as the battery canister does not contribute to the heat generation of the battery cell. Battery canister facilitates a cover to the active battery material of the cell and has a thickness of 0.25 mm. Since the thickness is low, the heat transfer effect from the battery canister is also considered as negligible. However, in order to confirm that there is no impact from the battery canister for the heat transfer, simulations were conducted by considering a 2D model. On the battery canister surface, a heat flux boundary condition is specified using a heat transfer coefficient of 20 W/m^2K and simulation results confirmed that the effect is negligible as well.

In order to investigate the temperature distribution and the heat transfer of a battery matrix, a matrix which contains 9 (3×3) cylindrical battery cells is used.

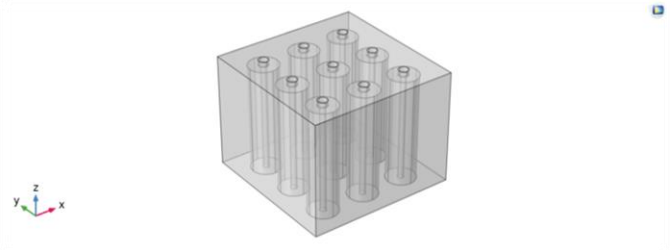

Figure 3. 3D Model of the battery cell matrix

Four main domains, such as active battery material, battery connector, mandrel and the flow compartment are associated with the matrix model. As mentioned above, both 1D and 3D models are coupled with each other. Furthermore, the same boundary conditions as in the previous modelling are applied to the battery matrix too. In addition, the properties of the flow are not assumed to vary with the temperature. However, the fluid flow is allowed to influence the heat transfer rate.

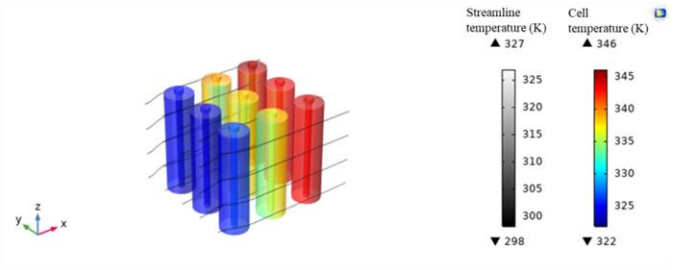

Figure 4. Temperature distribution results at 1500 s

As shown in Figure 4, in a matrix of nine battery cells, the temperature distribution varies between 322 K and 346K. The flow temperature is also varied between 298 K and 327 K. It indicates that the exhaust flow has the maximum temperature and the battery cell situated nearest to the outer boundary indicates the maximum temperature of the matrix.

The matrix was then extended for a battery module. Generally, a Li-ion battery consists of repeated modules and the virtual analysis is only focused on the elementary cells array. A linear layout, where cells are ordered in parallel rows is widely used. In the layout, the cells are arranged in a zigzag form as shown in Figure 5. According to industry and the related literature, it is mentioned that the offset structure is commonly used for cylindrical elements while the parallel shape is mostly used for the soft pouch type cells.

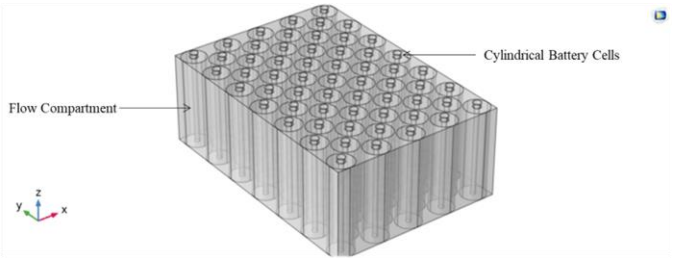

Figure 5. Battery module with 59 battery cells

The CFD simulation was conducted using a module containing 59 cells and the space dimension of the battery cell unit is fixed. Moreover, the inlet and outlet sections have already been defined too. Simulation reproduces the thermal behavior of a battery module under the same operating conditions as mentioned above.

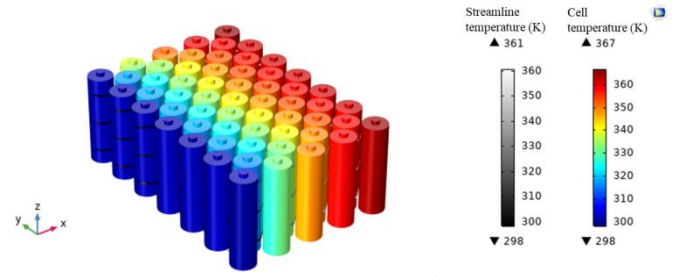

Figure 6. Temperature distribution results of a battery module at 7.5 C discharge rate after 1500s

Figure 6 shows the temperature profile related to the simulation with discharge rate of 7.5 C. The maximum cell temperature simulated after 1500s is 367 K while the maximum value of stream line temperature is 361 K.

Temperature distribution of Li-ion battery module with different cell structures

It is found that the temperature distribution of batteries is quantitatively dependent on cell arrangements and the inter-cell distance of a module [13]. In order to investigate this, simulations were conducted considering 24 battery cells in different arrangements. Four different cell structures were considered including 1×24, 3×8, 4×6 rectangular arrays and 19 cells of hexagonal arrangement. Although, it is not a 24 cells arrangement, 19 cells hexagonal arrangement was selected by mainly considering the space utilisation effect.

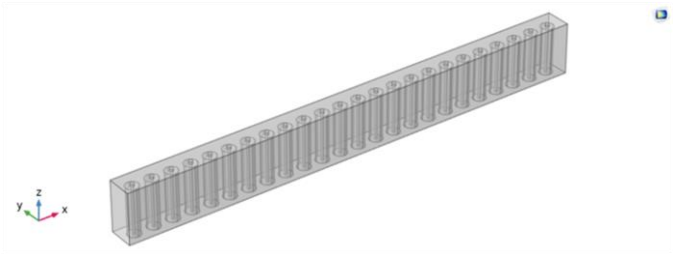

Figure 7. 1x24 Cells arrangement

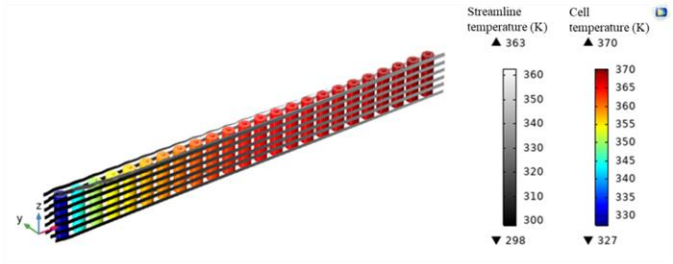

Figure 8. Temperature distribution results at 7.5C discharge rate

Figure 7 and 8 show the cell arrangement and the temperature distribution of the battery module at 7.5 C discharge rate respectively. An airflow of 0.1 m/s in the x-direction is applied for the module since the air-cooled battery module is considered. As indicated in results, it can be seen that the temperature of the cells are high and relatively uniform. During discharge heat generated of each cell is considered as constant. The self and mutual heating contribute to the rise of battery temperature. Furthermore, it is observed that the highest temperature of cells under this orientation falls outside the optimal range of 30-40°C.

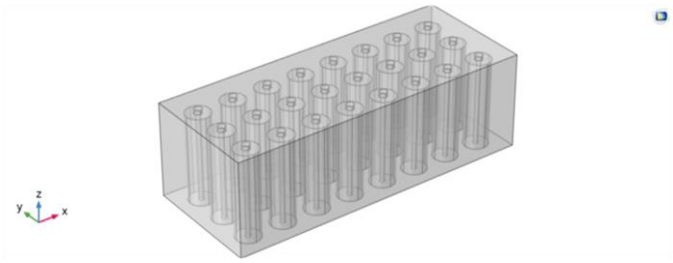

Figure 9. 3x8 Cells arrangement

When the cells in the model are arranged in 3×8 structure as shown in Figure 9, the results is almost equal as in the structure of 1×24. The results (see Figure 10) indicate that the furthest batteries acquire the highest temperature resulting from the combination of heat flux which is flowing with the airflow and the heat generated by neighboring batteries.

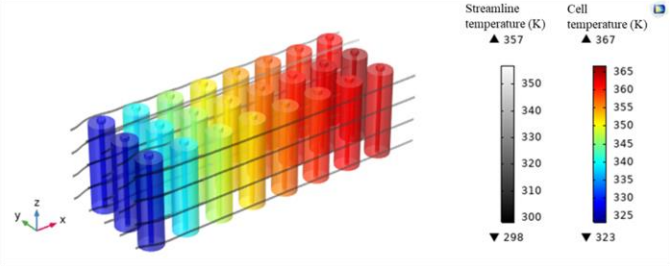

Figure 10. Temperature distribution results

Although the cooling air is heated up as well, the stream flow temperature is less than when compared to 1×24 cell arrangement and which implies that the longer the airflow path, the poorer the airflow cooling ability.

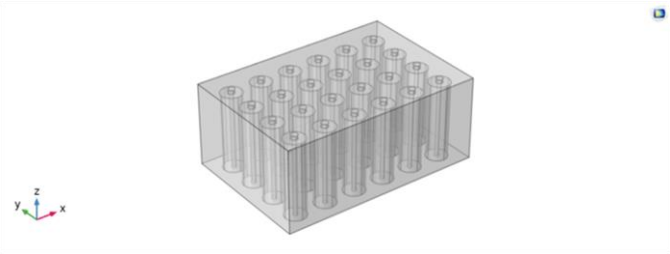

Figure 11. 4x6 Cells arrangement

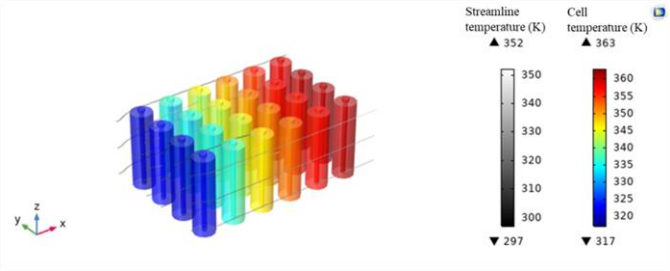

Figure 12. Temperature distribution results

To improve airflow cooling ability, the airflow path should be shortened and for this purpose, a 4×6 cubic structure was designed (See Figure 11). Thermal behavior of this battery module with air cooling is shown in Figure 12. The temperature distribution pattern follows the same rule as both 3×8 and 1×24 cell arrangement structures.

Generally, the temperature distributions of batteries are quantitatively depend on both cell arrangement type and the inter–cell distance. When considering the cooling efficiency with x-directional flow and cost, 4×6 cubic arrangement is a good choice.

However, when designing a battery module, it is required to consider about the space utilisation as well since the space occupation rate is another important scenario for a battery module. In order to investigate the temperature distribution results with the space utilisation factor, 19 cells hexagonal arrangement is used.

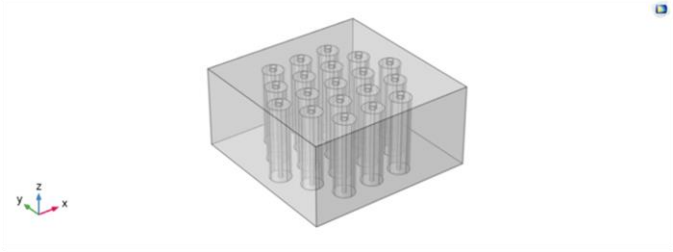

Figure 13. 19 Cells hexagonal arrangement

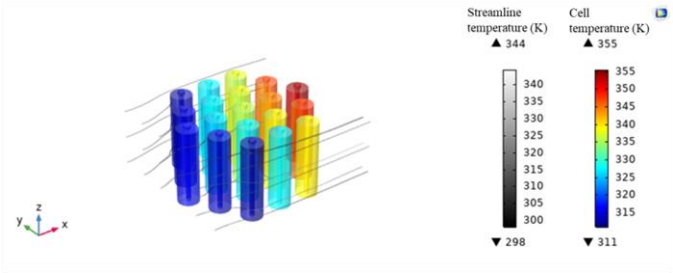

Figure 14. Temperature distribution results

19-cells hexagonal arrangement and thermal behavior of this arrangement are shown in Figure 13 and Figure 14 respectively. The indices demonstrate that the temperature distribution of 19 cells hexagonal module is much lower to that of 4×6 cubic module. It is because, that the number of battery cells occupied in the structure is less than 4x6 cubic structure. However, it is possible to predict that even if it has 24 cells, the maximum temperature is not more than 365 K.

Furthermore, in order to investigate the effect of inter-cell distance, a 19-cell hexagonal arrangement was used too. The inter-cell distance of the cell arrangement was changed from 0.027 m to no-gap situation by keeping all other boundary conditions as constant and simulations were conducted. The 19-cell hexagonal arrangement with no gap is presented in Figure 15. As indicate in results (See Figure 16), when there is no gap between cells, the temperature distribution is higher when comparing to the structure which has the gap between battery cells. It is because when there is the gap, more air occupies the space and it will reduce the mutual heating between battery cells.

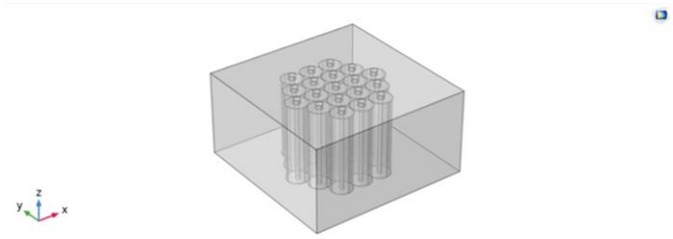

Figure 15. 19 Cells hexagonal arrangement with no gap between cells

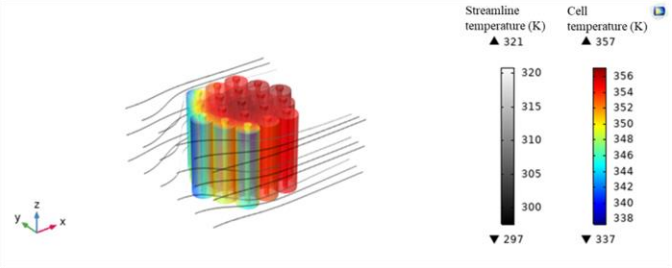

Figure 16. Temperature distribution results

Conclusions

In this study, the thermal performance of Li-ion battery module is discussed by considering both analytical and simulation methods. Assumptions of the lumped model are applied in the analytical method of a single cell. Simulations are conducted by coupling both 1D and 3D models. In addition, thermal performance analyses are performed for different cell structures and the arrangement structures include 1×24, 3×8, 4×6 arrays rectangular arrangements and 19 cell hexagonal arrangement. Among all structures discussed in the study, 4×6 cubic structure is identified as the best choice in terms of the cooling capability and simulations are conducted for hexagonal structure with 19 cells by considering the space utilisation factor and inter-cell distance. Results confirmed that the having a gap between battery cells reduces the mutual heating effect and increases the cooling effectiveness.

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