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Mathematical Modeling for Cooling of Cylindrical Li-ion Batteries

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Abstract –*As the conventional crude oil reserves are getting scarce by the very day, the demand for alternative fuels is thriving. Alongside which the engine modification has reached a limiting value thus giving a meager scope for further research. These issues have paved a way for new technologies like fuel cell, battery electric vehicle, and supercapacitor. Battery technology is at its peak research since it is a quintessential and a flexible power source for almost all electrical and electronic technology. Future of Battery Technology is at the heart of the battery electric vehicle's research and development. But despite its merits, it faces a lot of setbacks such as thermal management and cooling, energy density (energy to size or mass), fast charging and proper storage. This paper performs an analysis of heat generation in single cell Lithium-ion batteries and its cooling using forced air convection through a special arrangement. Mathematical modeling for temperature distribution, forced air convection and free convection is studied.*

***Key Words*:** Lithium-ion cell, Theoretical modeling,Dynamic model, Simulation

1. INTRODUCTION

Lithium-ion batteries (LIB) are being used in almost all fields of electric and electronic systems because of their superior properties. Electric vehicles, consumer electronics, aerospace industries are the fields where they are used heavily. High capacity, high efficiency, long life, low self-discharge, high energy density [1,2] makes them distinct from others. But despite this advantage, they pose some serious problems like thermal management and cooling, size and compatibility, high charging time.

The safe and efficient range of working temperature for lithium-ion batteries is around 0°C to 40°C; but it can go as high as 60°C thus, compromising performance. Above this range, there will be a phenomenon of thermal runaway where an increase in cell temperature leads to further increase in temperature thus ending in failure of the cell. Thus, a keenly designed module structure and cooling method should maintain the temperature within the operating range

1.1 Literature Survey

Due to the significance of thermal management, a lot of works are widely studied. Different thermal models, cooling techniques of cell or cell pack have been under research. Sefidan[3] studiedNano fluid based cooling of cylindrical lithium-ion batteries and analyzed it for the different battery pack and flow configurations analytically and using computational fluid dynamics models. Wang [4] studied cell arrangement with forced air cooling for different heat generation models. Mondal [5] studied cooling with Nano fluids like $Al_2O_3 + water$ and their thermal management. Ziebert[6] simulated Li-18650 cylindrical lithium ion batteries in COMSOL Multiphysics considering various parameters and for different heat generation models. Jingzhi Xun[7] conducted experiments on air cooled module of cylinder lithium ion batteries usingcomputational fluid dynamics analysis and numerical methods; with different combinations of Reynolds number, pack stacking.

1.2 Brief Methodology

In this discussion initially model of Li-18650 is simulated using COMSOL Multiphysics by considering electrochemical properties [6]. Later heat generation model for an isoperibolic condition is added to the single cell. The cell is cooled using ambient air which is analyzed through a laminar flow model. This result is used for theoretical modeling of unit cell pack. The mathematical modeling is carried by finding an overall heat transfer coefficient using suitable correlations. Grashoff's number is used in static model whereas Nusselt's number is used in the dynamic model The purpose of this study is to understand the working of the cell along with heat generation models thus to find the considerations in its thermal management.

2. THEORETICAL DISCUSSION

It is necessary to look at what happens inside a cell mathematically by considering theories and formulas of heat transfer.

2.1 Electrochemical Model

A lithium ion cell works under the principle of a redox reaction. It has Li and oxides of some metal as electrodes. During the charging cycle, Li-ions will move from the positive electrode and are deposited into the negative electrode. Reverse process will occur during the discharge cycle. The cell reaction is given as in Eq. (1) [7] for Li-ion cell with CoO

Anode: $Li \rightarrow Li^{+} + e^{-}$
Cathode: $CoO_2 + Li^{+} + e^{-} \rightarrow LiCoO_2$
Overall: $CoO_2 + LiC_6 \rightarrow LiCoO_2 + C_6$.... (1)

Positive Electrode: $LiCoO_2$ on 10-25mm thick Al Foil

Negative Electrode: Graphite on 10-12mm thick Cu Foil

Separator: 16-25mm thick POLYOLEFINE MEMBRANE (PE, PP, PE/PP)

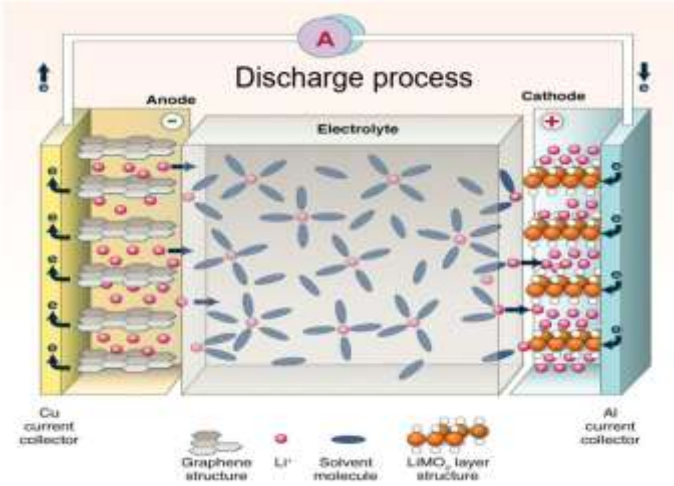

Fig-1: Schematic diagram of Lithium-ion cell

2.2Various Heat Generation Model

i. **Adiabatic Measurement**: No heat exchange between cell and surrounding. Cell temperature increases rapidly until the cell breaks down due to thermal runaway. [6]$\dot{Q}_{gen} = mc_p\frac{dT}{dt}$ ....(2)

ii. **Isoperibolic Measurements**: Approximately isothermal conditions; the outer environment is maintained at a constant temperature.
[6]$\dot{Q}_{gen} = mc_p\frac{dT}{dt} + Ah(T_s - T_c)$ ....(3)

iii. **Measurement of Reversible&Irreversible heat:** This includes heat generated due to Joule heating effect which is irreversible and second term due to entropy changes which are reversible.

$\dot{Q}_{gen} = -I(E_0 - E) - IT\frac{dE_0}{dT}$This can be also re-written as $\dot{Q}_{gen} = i^2R - T\Delta S\frac{i}{nF}$ .... (4)

$$Q_{gen} = Q_{Electrochemical} + Q_{Exothermic}$$

2.3Mathematical Model of Temperature Gradient

Fig -2: Plane View of cylindrical battery

For the purpose of analysis let us consider the cylindrical lithium-ion cell as a cylinder with heat generation at its center. Certain assumptions are made to simplify the analysis:

- Only radial conduction is assumed.
- Heat conduction due to radiation is neglected. Complete heat gets transferred to coolant fluid in contact.
- Material is isotropic.
- Heat is generated at the center and distributed radially which is a function of time and position (radius).
- Variations of parameters like density, viscosity, etc. are neglected and their average values over working range are taken.

The general heat transfer equation is given as follows:
$\nabla^2 T + \dot{Q}_{gen} = \frac{1}{\alpha}\frac{\partial T}{\partial t}$ .... (5)

Considering only radial heat transfer to obtain temperature distribution across the cell

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \dot{Q}_{gen} = \frac{1}{\alpha}\frac{\partial T}{\partial t} \qquad \text{.... (6)}$$

This is in the form of $\boldsymbol{T(r,t) = G(r).S(t)}$; which is a partial differential equation and homogenous and non-homogenous are solved separately.

a). Solving the non-homogenous part:

$$\frac{1}{r^2}\frac{d}{dr}\left(r\frac{dT}{dr}\right) = -\frac{\dot{Q}_{gen}}{k} \qquad \text{.... (7)}$$

$$T = -\frac{\dot{Q}_{gen}}{4k}r^2 + C_1 lnr + C_2 \qquad \text{.... (8)}$$

At r=0 → $C_1 = 0$ and $r = R$ → $C_2 = T_0$

$$T = T_0 + \frac{\dot{Q}_{gen}}{4k}(R^2 - r^2) \qquad \text{.... (9)}$$

b). **Solving homogenous part by the method of separation of variable**

$$T(r,t) = G(r).S(t) \qquad \text{.... (10)}$$

$$\frac{1}{G}\frac{\partial}{\partial r}\left(r\frac{\partial G}{\partial r}\right) = \frac{\rho C_p}{kS}\frac{\partial S}{\partial t} = -\lambda^2 \qquad \text{.... (11)}$$

Solving for $G(r)$:

In general Bessel Function is of the form

$$\mathrm{r}^2.\frac{\mathrm{d}^2\mathrm{f}}{\mathrm{dr}^2} + \mathrm{r}.\frac{\mathrm{df}}{\mathrm{dr}} + (\lambda^2 - \mathrm{n}^2)\mathrm{r} = 0$$

$$\mathrm{r}^2\frac{\mathrm{d}^2\mathrm{G}}{\mathrm{dr}^2} + \mathrm{r}\frac{\mathrm{dG}}{\mathrm{dr}} + \lambda^2\mathrm{r}^2\mathrm{G} = 0 \text{Here n=0} \qquad \text{.... (12)}$$

$$G(r) = C_1 J_0(\lambda r) + C_2 Y_0(\lambda r) \qquad \text{.... (13)}$$

$$G(R) = T_0 \; i.e. \; J_0(\lambda_k) = T_0 \qquad \text{.... (14)}$$

Where $\lambda_k = \frac{\alpha_0 k}{R^2} = \lambda^2$;

Solving for S(r):

$$\frac{dS}{dt} = -\frac{\lambda_k k}{\rho c_p}S \qquad \text{.... (15)}$$

$$S_k(t) = e^{-\frac{\lambda_k k}{\rho c_p}}$$

Combining these two equations;

$$T(r,t) = T_0 + \frac{\dot{Q}_{gen}R^2}{4k}\left[1 - \frac{r^2}{R^2} + \sum_{k=1}^{\infty} a_k J_0\left(\frac{\lambda_k r}{R}\right)e^{-\frac{\lambda_k k}{\rho c_p}t}\right] \qquad \text{.... (16)}$$

Normalizing the solution:

$$\boldsymbol{T(r,t) = T_0 + \frac{\dot{Q}_{gen}R^2}{4k}\left[\sum_{k=1}^{\infty}\frac{8k}{\lambda_k^3 J_1(\lambda_k)}J_0\left(\frac{\lambda_k r}{R}\right)\left(1 - e^{-\frac{\lambda_k k}{\rho c_p}t}\right)\right]} \qquad \text{....(17)}$$

By using computational software, we can find temperature along the radial profile.

2.4 Heat Transfer from Surface to Coolant Fluid

Heat transferred from surface to the coolant fluid, in a given time are found thus finding values of surface temperature and coolant fluid. In calculation, the resistance offered by metallic separator is neglected. It is assumed that heat transferred from four quarters of the cylinder is equivalent to heat transferred by one cell.The coolant inside the duct receives this heat energy and its temperature changes in subsequent time.

$$Area\ of\ Duct = d^2 - \frac{\pi}{4}d^2 \qquad \text{.... (18)}$$

Effective Diameter=Hydraulic Diameter $D_H = D = \frac{4A_c}{P}$ (19)

The Fig-3 shows the plane view of the duct that is formed by four adjacent Lithium-ion cells. Thus,the area of duct formed is equal to the area of the fluid entry region. The fluid enters through a duct from one side and exits from other carrying away heat along its path. Fluid friction, turbulence effects, boundary layer formation is neglected in the study. The region is within the hydro dynamically developing region.

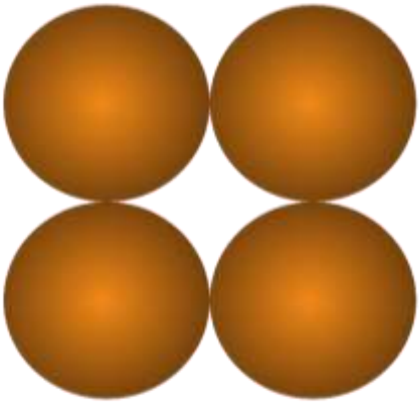

Fig -3-Plane View of the cell pack

There are two possible ways in which fluid flow. In one method fluid is made to flow continuously i.e. dynamic model and another one in which fluid is made to flow only in intervals when the fluid reaches a certain temperature in duct thus saving pumping power.

a. Dynamic Model:

Here Reynolds number plays a significant role and isused to find the overall heat transfer coefficient. The model should obey the momentum equation, the continuity equation, and the energy equation.

$$Nu = C.Re^{m}.Pr^{\frac{1}{3}} \qquad .... (20)$$

For Reynolds number between 40.0 to 4000, we have C=0.683 and m=0.466

$$Nu = 0.683.Re^{0.466}.Pr^{\frac{1}{3}} \qquad ....$$
(21)

$\frac{\partial}{\partial t}(\rho_f \vec{v}) + \nabla.(\rho_f \langle \vec{v}|\vec{v}\rangle) = -\nabla\vec{p}$; Momentum Equation [7]

$\frac{\partial}{\partial t}(\rho_f C_{pf} T_f) + \nabla.(\rho_f C_{pf} T_f) = -\nabla.(\mathrm{k_g}\nabla T_g)$; Energy Equation [7]

$\frac{\partial}{\partial t}(\rho_f \vec{v}) + \nabla.(\rho_f \vec{v}) = 0$; Continuity equation [7]

$$h = \frac{k}{D} 0.683.Re^{0.466}.Pr^{\frac{1}{3}} \qquad .... (22)$$

$$Q = h.A_s.(T_s - T_{f0}) = -\dot{m}.t.C_{pf}.\frac{dT}{dt} \qquad .... (23)$$

Here T_s is constant for the first iteration and it gets updated for subsequent iterations. Thus, the final equation

$$\ln(t) = \frac{mC_{pf}}{hA} \ln\left[\frac{T_s - T_{f0}}{T_s - T_{f1}}\right] \qquad .... (24)$$

Table-1 gives values of calculated parameters. [10]

Table -1: Parameters and their values

b. Static Model:

Here natural convection is considered fluid is replaced only after certain time interval i.e. when it reaches threshold temperature.

Determining overall heat transfer coefficient, Grashoff's number $Gr = \frac{D^3 g\beta\Delta t}{\nu^2}$ .... (25)

Mc-Adams Correlation:

$$Nu = \left\{\begin{matrix} 0.59(Gr.Pr)^{0.25}, & for\ laminar\ flow\ Gr.Pr < 10^9 \\ 0.10(Gr.Pr)^{\frac{1}{3}}, & for\ turbulent\ flow\ 10^9 < Gr.Pr < 10^{12} \end{matrix}\right\}$$

$$\beta = \frac{1}{\rho}\left(\frac{\partial p}{\partial T}\right)_p \qquad .... (26)$$

$$h = \frac{k}{D} 0.59(Gr.Pr)^{0.25} \qquad .... (27)$$

$$Q = h.A_s.(T_s - T_{f0}) = -mC_{pf}\frac{dT}{dt} \qquad .... (28)$$

Here T_s is constant for the first iteration and it gets updated for subsequent iterations; $T_f\ varies\ as\ T_{fo}\ T_{f1}\ T_{f2}$ for further iterations.

Thus, the final equation is

$$t = \frac{mC_{pf}}{hA_s} \ln\left[\frac{T_s - T_{f0}}{T_s - T_{f1}}\right] \qquad ....$$
(29)

3. RESULTS AND DISCUSSION

Cell temperature is the major parameter that is considered for analysis anddiscussion.Fig-4 shows the temperature of the surface with respect to time. Cell temperature increases with time because of heat generated gets gradually accumulated in the domain. But the temperature has been within safe limits during the half cycle. In the rest half of the discharge cycle, the heat generation will be less thus the temperature will be in the acceptable limit. The peak temperature after the 1500s is 321K.

Table-1: Properties

Parameter	Value
Prandtl Number; Pr	0.701
Density of air; ρ_{air}	1.165 kg/m^3
Thermal conductivity of air; k_{air}	0.02675 W/mK
Specific heat capacity of the air; c_p	1005 J/kg
Dynamic Viscosity of air; μ	18.63×10^{-6}
Area of Conduit;D_h	69.53×10^{-6}
Air Velocity; v_{air}	0.25m/s

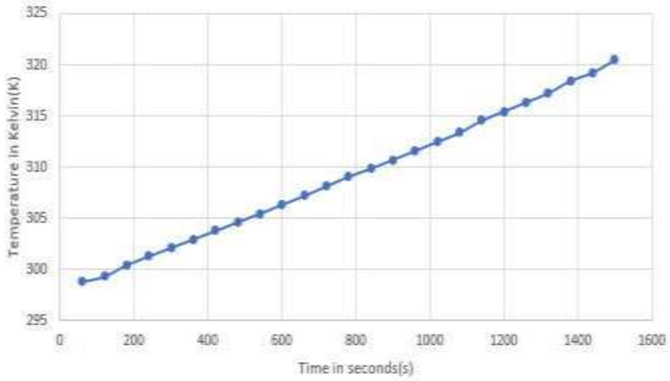

Fig -4: Time v/s Cell surface temperature

The Fig-5 shows the average fluid temperature reached in each iteration. The initial temperature rise is less compared to that in further stages. As time increases the temperature increases; this is partly due to the increase in the temperature gradient between incoming fresh air and cell temperature and other contribution due to there is a continuous thermal layer attained. The peak temperature reaches up to 315K. There is a slight deviation in the curve

4. CONCLUSION

From this discussion, it is seen that cell temperature can be regulated efficiently by using suitable coolant. The method considers certain assumptions,in reality, there will be deviations from these expected theoretical results; thus, certain regulation can be taken regarding thesame. For more accurate results friction factor, turbulence region, thermal and fluid boundary layer should be analyzed thus having the future scopein this analysis.

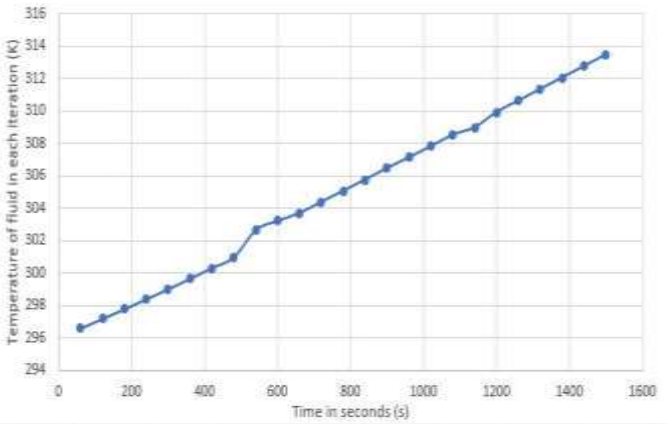

Fig -5: Time v/s Fluid temperature

Nomenclature

T-Temperature; Kelvin –K

$\dot{Q}$-Heat generated per second; Watts-W

t-Time; Seconds s

h-Heat transfer coefficient;W/m^2K

α-Thermal Diffusivity; m^2/s

k-Coefficient of Thermal Conductivity;W/mK

r-Radius from symmetry axis; m

β-Coefficient of Thermal Expansion;K^{-1}

g-Acceleration due to gravity; 9.81m/s^2

D_h-Hydraulic Diameter; m

ν-Kinematic Viscosity;m^2/s

μ-Dynamic Viscosity; Pa.s

Re-Reynolds Number

Gr-Grashoff's Number

Pr-Prandtl Number

Nu-Nusselt Number

p-Pressure; Pa

P-Perimeter;m

A-Area;m^2

$\vec{v}$-Velocity;m/s

R-Cell Resistance;Ω

i-Current Density; A/m^3

E-Cell Voltage;V

E_{oc}-Cell open circuit voltage; V

ΔS-Entropy change of cell;J/K

ρ-Density;kg/m^3

c_p-Specific heat capacity;J/kg

Subscripts

s-Inner Surface

c-Cross Section

S-Cell surface

f-fluid

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