Mathematical Model of Lithium-Ion Battery Cell and Battery (Lib) on its Basis

D I Smagin\textsuperscript{1}, A A Trofimov\textsuperscript{1}, K S Napreenko\textsuperscript{1} and A R Neveshkina\textsuperscript{1}

\textsuperscript{1}Moscow Aviation Institute (National Research University), Moscow, Russia

E-mail: 79637587781@yandex.ru

Received xxxxxx
Accepted for publication xxxxxx
Published xxxxxx

Abstract

The article considers a mathematical model of lithium-ion battery cell and battery (LIB) on its basis. The developed mathematical model allows predicting LIB temperature on different parts of its surface during charging and discharging by nominal and maximum currents. The results of the battery discharge process simulation and validation of the mathematical model based on the field experiment results are also presented.

Keywords: lithium-ion battery, mathematical model, power supply system, thermal analysis, electric transport

1. Introduction

The use of mineral fuel and energy resources and the depletion of its reserves are one of the most pressing problems in the modern world. The fuel use, which adversely affects the environment, provokes environmental issue. The environmental safety requirements, which are becoming more stringent every year, demand the development and creation of environmentally friendly energy sources that can replace traditional hydrocarbon reserves in the main industries, including transport [1-3].

Currently, one of the most relevant areas of the transport industry development is the creation of electric transport using lithium-ion batteries [4]. Such batteries have a few advantages, among which are high energy density, minimum self-discharge, weight and size indicators, etc. [5–7]. Today LIB applied in the areas of transport sector, public transport [8] (buses, trams and trolleybuses with increased autonomous course), sea and railway transport and aviation perspective aircraft with a high level of electrification [9].

Since power supply system is a fundamental system during development and operation of electric transport then for its full operation is necessary to have enough information about the performance of the components which constitute it.

One of the main factors affecting the work of LIB is heat. The operating temperature of the battery cells affects such important parameters of LIB operation as energy efficiency, reLIBility, service life and, as a result, the life cycle cost [10-12]. For a detailed thermal analysis of such energy sources it is advisable to use a mathematical model.

2. Mathematical model functions

The main functions of the mathematical model LIB are:

• Forecasting the temperature of battery cells under different operating modes;

• Analysis of LIB heat release under load with different currents.

3. Mathematical modelling of lithium-ion battery

The basis of the mathematical model is the heat transfer equations.

Conductive heat transfer is determined by the Fourier’s law of thermal conductivity:

\[ q = -K \frac{\partial T}{\partial n}, \]

where

\[ q \] — heat flow rate per unit area in direction \( n \);

\[ K \] — thermal conductivity in direction \( n \);

\[ T \] — temperature;

\[ \frac{\partial T}{\partial n} \] — temperature gradient in direction \( n \).
Convection heat transfer is determined by Newton’s law:
\[
q = h \cdot A \Delta T,
\]
where \(q\) — heat flow rate per unit area between surface and matter; \(h\) — convective film coefficient; \(A\) — area of surface; \(\Delta T\) — the difference in temperature between surface and matter.

Radiation is described by Stefan-Boltzmann law:
\[
q = \sigma \cdot \varepsilon \cdot A_i \cdot F_{ij} \cdot (T_i^4 - T_j^4),
\]
where \(q\) — heat flow rate from surface \(i\) to surface \(j\); \(\sigma\) — Stefan-Boltzmann constant; \(\varepsilon\) — emissivity; \(A_i\) — area of surface \(i\); \(F_{ij}\) — form factor from surface \(i\) to surface \(j\); \(T_i\) — absolute temperature of surface \(i\); \(T_j\) — absolute temperature of surface \(j\).

The heat conduction equation for a differential volume can be written in the form:
\[
\rho c \frac{\partial T}{\partial t} + \nabla \cdot q = Q - K \nabla^2 T = 0,
\]
where \(\rho\) — density of the substance; \(c\) — heat capacity; \(T\) — temperature; \(t\) — time; \(Q\) — the rate of internal heat generation per unit volume; \(K\) — specific thermal conductivity tensor; \(\nabla^2 T\) — temperature Laplacian.

The Biot Number and The Fourier Number are used to determine the optimal integration step in the mathematical model.

The Biot Number characterizes the relationship between the temperature difference in the two points of the body at a certain distance and the temperature pressure – the difference between the body surface temperature and the ambient temperature. The Biot Number is determined by the dimensionless ratio:
\[
Bi = \frac{h \Delta x}{K},
\]
where \(Bi\) — The Biot Number; \(h\) — average heat transfer coefficient; \(\Delta x\) — average width of the element; \(K\) — average thermal conductivity.

The Fourier Number characterizes the ratio between the thermal conditions rate change in the environment and the rate of temperature field change within the system (body):
\[
Fo = \frac{4K \Delta t}{\rho C (\Delta x)^2},
\]
where \(Fo\) — The Fourier Number; \(K\) — average thermal conductivity; \(\Delta t\) — time frame; \(\rho\) — density of the substance; \(C\) — heat capacity; \(\Delta x\) — average width of the element.

In case the Biot Number is less than one for the calculation of the integration is used Fourier number. Otherwise, for the calculation of the integration is used determination of this numbers.

As the research objects it were selected battery cells with a nominal capacity of 170 Ah of each one. The main technical characteristics of the cell are presented in table 1.

| Dimension | Value  |
|-----------|--------|
| Length    | 150 mm |
| Width     | 85 mm  |
| Height    | 346 mm |

Table 1. Battery cell specifications

| Parameter                | Value         |
|--------------------------|---------------|
| Nominal Capacity         | 170 Ah        |
| Nominal Voltage          | 3.2 V         |
| Weight                   | 6.9 kg        |
| Internal Impedance at 1 kHz | 0.5 mOhm    |

Figure 1. Battery cell 3D model.

The battery cell core material is considered as homogeneous [13]. Core characteristics (density, thermal conductivity and heat capacity) correspond to those described in articles [13–15].

The internal heat release of the battery cell depends on the amount of current flowing.

4. Simulation result

In this example, heat exchange with the external environment is due to natural convection, the coefficient of convective heat transfer is 5 W/(m²·°C). Radiation in this task can be neglected, because the temperature on the surface of the battery cell is slightly higher than the ambient temperature and, therefore, the effect of radiation on the heat release process will be insignificant.

The calculated temperature distribution for the case of the battery cell is shown in figure 2, for the case of the battery consisting of 4 cells — in figure 3.
Figure 3. Calculation results for the battery.

5. Testing LIB

The aim of the exercise tests was determination of lithium-ion battery temperature on different parts of its surface during the discharge of nominal and maximum currents.

The test bench is a processing board of information coming from the temperature sensors, which are placed on LIB.

The experiments were conducted at an ambient temperature of 19.5 °C and natural convection. The battery consisting of 4 such cells was assembled for achieving the required discharge current. Sensor readings are recorded every 3 seconds. Sensors were located on the most exposed to heat LIB elements — terminals, cell connectors and on the surface of the body. The schematic arrangement of the sensors is shown in figure 4. It allows obtaining a wide picture of the main LIB sections temperature distribution. Temperatures in the controlled points at the discharge current 1C are shown in figure 5.

DS18B20 digital sensors with ±0.5°C measurement error was used as temperature sensors [16]. Information is exchanged with the master (microcontroller or Arduino board) via the 1-wire bus. LIB temperature was also controlled by thermal imager (figure 6).

Figure 4. The location of the temperature sensors.

Figure 5. Temperature of LIB elements at discharge current 1C.

Figure 6. LIB temperature distributions by thermal imager.

It should be noted that the thermal analysis of the LIB results is comparable with the heat release of batteries studied in articles [14, 17].

Validation of thermal mathematical model was carried out based on experiments on the discharge of a lithium-ion battery consisting of 4 cells.

Figure 7 shows a graph of the battery current 1C discharge, which shows the results of the experiment (temperature of the sensor located on the terminal) and mathematical modeling at the same point. Dashed line indicates a range of ±1.5°C from the experimental data.

Figure 7. Temperature versus time graph for stationary operation.
Figure 8. A graph of the discharge current.

For estimating the unsteady process, the discharge current ranged from 1C to 2.8 C, as it is shown in figure 8.

Figure 9 shows a graph illustrating the results of the experiment and mathematical modeling at the same point for the unsteady process. The dashed line indicates the range of ±1°C from the experimental data.

Figure 9. Temperature versus time graph for non-stationary mode.

As can be seen from the graphs shown in figure 7 and 9, the greatest discrepancy between the results of the experiment and mathematical modeling is about 1 °C for a stationary process and does not exceed 0.6 °C for a non-stationary one. This discrepancy results may be caused by the inaccuracy of the temperature sensors and possible minor computational errors associated with the construction of a computational grid. The results of the battery validation allow us to conclude that all the parameters of the battery cell are considered correctly, and the developed mathematical model can be used to analyze the heat release of LIB, consisting of battery cells given number.

6. Conclusion

The developed lithium-ion battery mathematical model showed good convergence of the results with full-scale tests, which will not only predict the heat release of the battery in different operation modes with a high degree of accuracy, but also to use this mathematical model in the future, for example, in the development of a thermostatic system.

References

[1] Boureima F S 2011 Environmental Assessment of Conventional and Alternative Vehicles and Fuels in a Belgian Context PhD Thesis (Brussels, Belgium: Vrije Universiteit Brussel)
[2] Van Mierlo J and Maggetto G 2003 J. Automobile Engineering 7 583–93
[3] Chemical sources of current: The manual ed by Korovin N In and Skandin A M 2003 (Moscow: MPEI Publishing house)
[4] Chen S C, Wan C C and Wang Y Y 2005 Journal of Power Sources 140 111–24
[5] Pollet B, Staffell I and Shang J 2012 Electrochem. Acta 84 235–49
[6] Wu B, Yufit V, Marinescu M, Offer G J M, Ricardo F and Brandon N P 2013 J. Power Sources 243 544–54
[7] Bystrov Y A, Kudryavtsev N A, Krasnobryzhy V A, Loginova M M and Zhdanov V V 2007 Underwater research and robotics 2 34–7
[8] Klimchuk A K and Temirgaliyev E R 2017 Possibilities of introduction of public electric transport instead of traditional (on the example of St. Petersburg) Proceedings of the scientific conference with international participation (St. Petersburg: Federal state Autonomous educational institution of higher education “Peter the great St. Petersburg Polytechnic University”)
[9] https://www.aeroflap.com.br/airbus-conclui-que-bateria-de-litio-ion-do-a350-e-confiavel/
[10] Pesaran A A 2002 J. Power Sci. 110 377–82
[11] Rothgang S, Rogge M, Becker J and Sauer D U 2015 Energies 8 6715–37
[12] Shabani B and Andrews J 2015 Int. J. Hydrogen Energy 40 5509–17
[13] Liu X, Zhang Y and Li X 2017 Battery Pack’s Structure Design Based on the Heat Flow Field Simulation 2nd International Conference on Industrial Aerodynamics (ICIA 2017) pp 614–23
[14] Samba A, Omar N, Gualous H, Van den Bossche P, Van Mierlo J and Boubekeur T I 2013 Development of 2D Thermal Battery Model for Lithium-ion Pouch Cells EVS 27 Barcelona, Spain
[15] Arunkumar R, Anbumalar S, AvilaPriya F and Poongothai K 2015 Int. J. of Sci. & Eng. Res. 6 4 74–8
[16] http://pdf.datasheetcatalog.com/datasheet/maxim/DS18B20.pdf
[17] Yi J, Koo B and Shin C B 2014 Energies 11 7586–60