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Algorithm for the synthesis of equations of thermal conductivity of lithium-ion accumulator for finite volumes during division

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Abstract: The current level of technology development makes it possible to improve the volumes of on-board equipment significantly, the same applies to backup power supply systems, in which the use of lithium-ion batteries is promising, which, if there are significant advantages, have a number of disadvantages that must be taken into account when using them. First of all, this is thermal acceleration, which is caused by internal physico-chemical processes and improper operation. To prevent thermal overclocking, it is proposed to use a digital twin, the basis of which is a mathematical model of thermal processes of a lithium-ion battery, obtained by mathematical prototyping of energy processes. For the numerical implementation of the mathematical prototyping method, it is proposed to use a modified finite volume method with the implementation of the division procedure until the required accuracy of the model is obtained. The presented article discusses the procedure for the formation of thermal conductivity equations when modeling the dynamic distribution of the thermal field in a lithium-ion battery in a three-plane formulation of the problem. This procedure is necessary when implementing the modified finite element method using the method of mathematical prototyping of energy processes, which involves dividing finite volumes to achieve the required calculation accuracy. A special feature of the division procedure is the change in volumes, areas of contact of interacting elements, and the change in elements that are sources of heat. In the simulation cycle, it is necessary to re-form the system of differential equations, taking into account the changes that occurred after the division. For clarity, the article discusses the procedures for dividing volumes into two equal parts according to one of the coordinates, and the Cartesian coordinate system is also considered to obtain a model. The proposed procedure for forming a system of differential equations is implemented in Python, the simulation results have shown the adequacy of the model and the efficiency of the proposed method.

Key words: lithium-ion battery, modified finite volume method, diagnostic method, method of mathematical prototyping of energy processes.

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Алгоритм синтеза уравнений теплопроводности литийионного аккумулятора для конечных объемов при делении

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Аннотация: Современный уровень развития техники и технологий позволяет существенно улучшить возможности бортового оборудования, это же касается и систем резервного электропитания, в которых перспективным представляется применение литийионных аккумуляторных батарей, которые при наличии существенных преимуществ обладают рядом недостатков, которые необходимо учитывать при их использовании. В первую очередь это тепловой разгон, обусловленный внутренними физико-химическими процессами и неправильной эксплуатацией. Для предотвращения теплового разгона предлагается использовать цифровой двойник, основой которого является математическая модель тепловых процессов литийионного аккумулятора, полученная методом математического прототипирования энергетических процессов. Для численной реализации метода математического прототипирования предложено использовать модифицированный метод конечных объемов с реализацией процедуры деления до получения требуемой точности модели. В представленной статье рассматривается процедура формирования уравнений теплопроводности при

моделировании динамического распределения теплового поля в литийионном аккумуляторе в трехмерной постановке задачи. Эта процедура необходима при реализации модифицированного метода конечных элементов с помощью метода математического прототипирования энергетических процессов, который предполагает деление конечных объемов для достижения требуемой точности расчетов. Особенностью процедуры деления является изменение объемов, площадей соприкосновения взаимодействующих элементов, изменение элементов, которые являются источниками тепла. В цикле моделирования необходимо заново формировать систему дифференциальных уравнений с учетом тех изменений, которые произошли после деления. Для наглядности в статье рассматриваются процедуры деления объемов на две равные части по одной из координат, также для получения модели рассматривается декартова система координат. Предложенная процедура формирования системы дифференциальных уравнений реализована в среде Python, результаты моделирования показали адекватность модели и работоспособность предлагаемого метода.

Ключевые слова: литийионный аккумулятор, модифицированный метод конечных объемов, метод диагностики, метод математического прототипирования энергетических процессов.

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Introduction

The current stage of aircraft electrical engineering development is new chemical current sources – lithium-ion batteries and hydrogen fuel elements [1, 2], semiconductor, conductor and magnetic devices implementation. The given technologies make it possible to both significantly improve the volumes of on-board equipment and create new aircraft, in which the electromechanical engine is the basic element, empowered by chemical current sources [2, 3]. The same applies to backup power supply systems, in which the use of lithium-ion batteries is promising, which, if there are significant advantages among other battery types in terms of specific energy [4, 5], have a dramatic disadvantage – they are exposed to thermal acceleration in certain external conditions and while being recharged. Besides that, lithium-ion batteries (LIB) operation temperature increase significantly reduces its capacity, which affects its operation features.

There is a number of publications [6–9] on LIB thermal operation modes, in which diverse approaches of the given phenomenon prevention – by using new materials, technologies, operation rules, etc. [10–12] – are presented. It is important to reveal the reasons of emergency in advance, for instance, by forecasting the thermal limit values within the batteries [13–16] in terms of operation.

It is proposed to use a modified finite volume method, in which the thermal conductivity equation synthesis is the particular issue based on mathematical prototyping of energy processes [17–19] for forecasting the reaching of LIB thermal limit, as the regular capacity division procedure involves forming a new differential equations system for new finite capacities set.

It is assumed to use the presented thermal condition diagnosis and forecasting approach for lithium-ion current sources of on-board power systems as a thermal process digital twin [20–23], integrated into promising aircraft power system [24, 25] smart current distribution schemes.

Research methods and methodology

Mathematical prototyping of energy processes method [18–20] is the basic one for LIB thermal condition diagnosis and forecasting, which a mathematical model, meeting the basic conservation and thermodynamic laws and analytic expressions for thermal scalar field distribution can be obtained with, allowing then to forecast thermal changes taking into consideration the known influencing factors.

The following general form of mathematical prototyping of energy processes equations presentation [19] should be used for thermodynamical problems:

$$
\begin{cases}
dW = dU - T^* dS, \\
dS = \sum\limits_{i=1}^{m_U} \dfrac{\delta Q_i}{T_i}, \\
U = \sum\limits_{i=1}^{m_U} U_i + \sum\limits_{i=m_U+1}^{\overline{m}_U} \Phi_i, \\
d\Phi_i = -\sum\limits_{k=1}^{m_x} X^o_{i,k} dx_k, \; i = \overline{m_U+1, \overline{m}_U}, \\
\dfrac{dx_k}{dt} = \sum\limits_{r=1}^{m_{\Delta x}} b_{k,r} \dfrac{\delta \Delta x_r}{dt} + \left(\dfrac{dx_k}{dt}\right)_{ext} + \left(\dfrac{dx_k}{dt}\right)^{(сл)}_{ext}, \; k = \overline{1, m_x}, \\
\dfrac{dU_i}{dt} = \dfrac{\delta Q_i}{dt} - \sum\limits_{k=1}^{m_x} X_{i.k} \dfrac{dx_k}{dt}, \; i = \overline{1, m_U}, \\
\dfrac{\delta Q_i}{dt} = \sum\limits_{j=1}^{i-1} \dfrac{\delta Q^{(пер)}_{i,j}}{dt} - \sum\limits_{j=i+1}^{m_U} \dfrac{\delta Q^{(пер)}_{j,i}}{dt} + \sum\limits_{r=1}^{m_{\Delta x}} \beta_{i,r} \dfrac{\delta Q^{(нек)}_r}{dt} + \left(\dfrac{\delta Q_i}{dt}\right)_{ext} + \left(\dfrac{\delta Q_i}{dt}\right)^{(сл)}_{ext}, \; i = \overline{1, m_U}, \\
\dfrac{\delta Q^{(нек)}_r}{dt} = \left(\sum\limits_{k=1}^{m_x} \left(\sum\limits_{l=1}^{m_U} X_{l,k} + \sum\limits_{l=m_U+1}^{\overline{m}_U} X^o_{l,k} \right) b_{k,r} \right) \dfrac{\delta \Delta x_r}{dt}, \; r = \overline{1, m_{\Delta x}}, \\
\Delta F_{\Delta x,r} = \left(\sum\limits_{i=1}^{m_U} \beta_{i,r} \dfrac{T^*}{T_i} \right) \left(\sum\limits_{k=1}^{m_x} \left(\sum\limits_{l=1}^{m_U} X_{l,k} + \sum\limits_{l=m_U+1}^{\overline{m}_U} X^o_{l,k} \right) b_{k,r} \right), \; r = \overline{1, m_{\Delta x}}, \\
\Delta F_{Q_{i,j}} = \dfrac{T^*}{T_i} - \dfrac{T^*}{T_j}, \; j = \overline{1, j-1}, \;\; i = \overline{2, m_U}, \\
\dfrac{\delta \Delta x_r}{dt} = \sum\limits_{l=2}^{m_U} \sum\limits_{g=1}^{l-1} a^{Q_{l,g}}_{\Delta x,r} \Delta F_{Q_{l,g}} + \sum\limits_{q=1}^{m_{\Delta x}} a^{\Delta x,q}_{\Delta x,r} \Delta F_{\Delta x,q}, \; r = \overline{1, m_{\Delta x}}, \\
\dfrac{\delta Q^{(пер)}_{i,j}}{dt} = \sum\limits_{l=2}^{m_U} \sum\limits_{g=1}^{l-1} a^{Q_{l,g}}_{Q_{i,j}} \Delta F_{Q_{l,g}} + \sum\limits_{q=1}^{m_{\Delta x}} a^{\Delta x,q}_{Q_{i,j}} \Delta F_{\Delta x,q}, \; j = \overline{1, i-1}, \;\; i = \overline{2, m_U},
\end{cases}
\tag{1}
$$

where U_i – energetic degrees of freedom (EDF) inner energies, which are the system condition coordinates;

x_k – other condition coordinates (condition coordinates vector plane);

Q_i – the *i*-th quantity of thermal component of the EDF system obtained;

$b_{k,r}$ – topology matrix components, commonly obtained from conservation laws;

$\left(\delta Q_i / dt\right)_{ext}$, $\left(\delta Q_i / dt\right)^{(сл)}_{ext} \left(dx_k / dt\right)_{ext}$ – external thermal streams in and out of EDF system and their occasional components;

$\left(dx_k / dt\right)^{(сл)}_{ext}$ – external streams in and out of other condition coordinates system(s) and their occasional components;

$Q^{(пер)}_{i,j}$ – thermal volumes between the EDF (destination from the smaller values to the bigger ones is considered to be the positive direction of every thermal between the EDFs);

Δx_r – other processes coordinates besides thermal shift between the EDFs;

$Q^{(нек)}_r$ – uncompensated thermals, arisen during physical and chemical processes (irreversible work shifting into thermal);

$\beta_{i,r} > 0$ – uncompensated thermal proportions by EDFs, meeting $\sum\limits_{i=1}^{m_U} \beta_{i,r} = 1$ condition;

$T_i > 0$ – the EDF temperatures;
$X_{i,k}$ – thermodynamic potentials of essential EDFs interaction by x_k condition coordinates;
$\Delta F_{Qi,j}$ – dynamic powers, thermal shift between EDFs driving processes;
$\Delta F_{\Delta x,r}$ – dynamic powers, driving the other processes;
T^* – the reference temperature, which the W system free energy is set through;
$\Delta a_{Qi,j}^{Ql,g}$, $\Delta a_{Qi,j}^{\Delta zq}$, $\Delta A_{\Delta x,r}^{Ql,g}$, $\Delta A_{\Delta x,r}^{\Delta x,q}$ – positive dissipative matrix components;
S – system enthropy;
U – total system inner energy;
Φ_i – EDFs interaction energies.

Setting the problem

The equilibrium thermodynamic system, in which all the components (finite capacities) are of constant thermal capacity and conductivity, thermolysis coefficients between the adjacent elements are also the constant ones, all the capacities are set by inequation systems and planes, parallel to the Cartesian coordinate system planes, is the subject of the given research.

The battery having a single electrode, both positive and a negative one (fig. 1), with an electrolyte in between, is then the object. Component densities and ohmic resistances are all constant ones. There are the extra areas (finite capacities) between the battery, imitating the area environment, which the inner boundary the temperature is constant on.

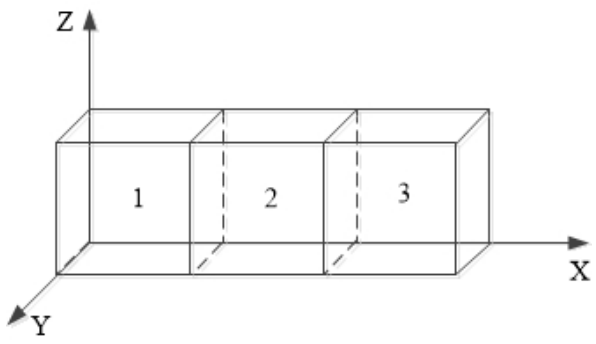


Fig. 1. Spatial model of the battery

The general matrix differential equation of a variable plane based on mathematical prototyping of energy processes method is made for temperature distribution calculation in the battery researched:

$$\boldsymbol{C\rho V}\frac{d\boldsymbol{T}}{dt}=\boldsymbol{\Lambda T}+\boldsymbol{T_{0I}T_0}+\boldsymbol{Q}, \qquad (2)$$

where $\boldsymbol{C}$ – thermal conductivity matrix of the researched objects;
$\boldsymbol{\rho}$ – matrix of capacity densities;
$\boldsymbol{T}=\left(T_1,...,T_n\right)^T$ – column vector of every capacity temperature;
n – capacity quantity, which all the researched space is divided into, this quantity increases after the division, which all the matrixes of equation (2) changing;
$\boldsymbol{\Lambda}$ – matrix for thermal conductivity, thermal transfer and thermolysis surface areas;
$\boldsymbol{T_{0I}}$ – matrix for conductivity thermal transfer with the environment;
$\boldsymbol{T_0}$ – environment temperature;
$\boldsymbol{Q}$ – inner thermal source due to currents in electrodes and an electrolyte.

With $\boldsymbol{K}=\boldsymbol{C\rho V}$

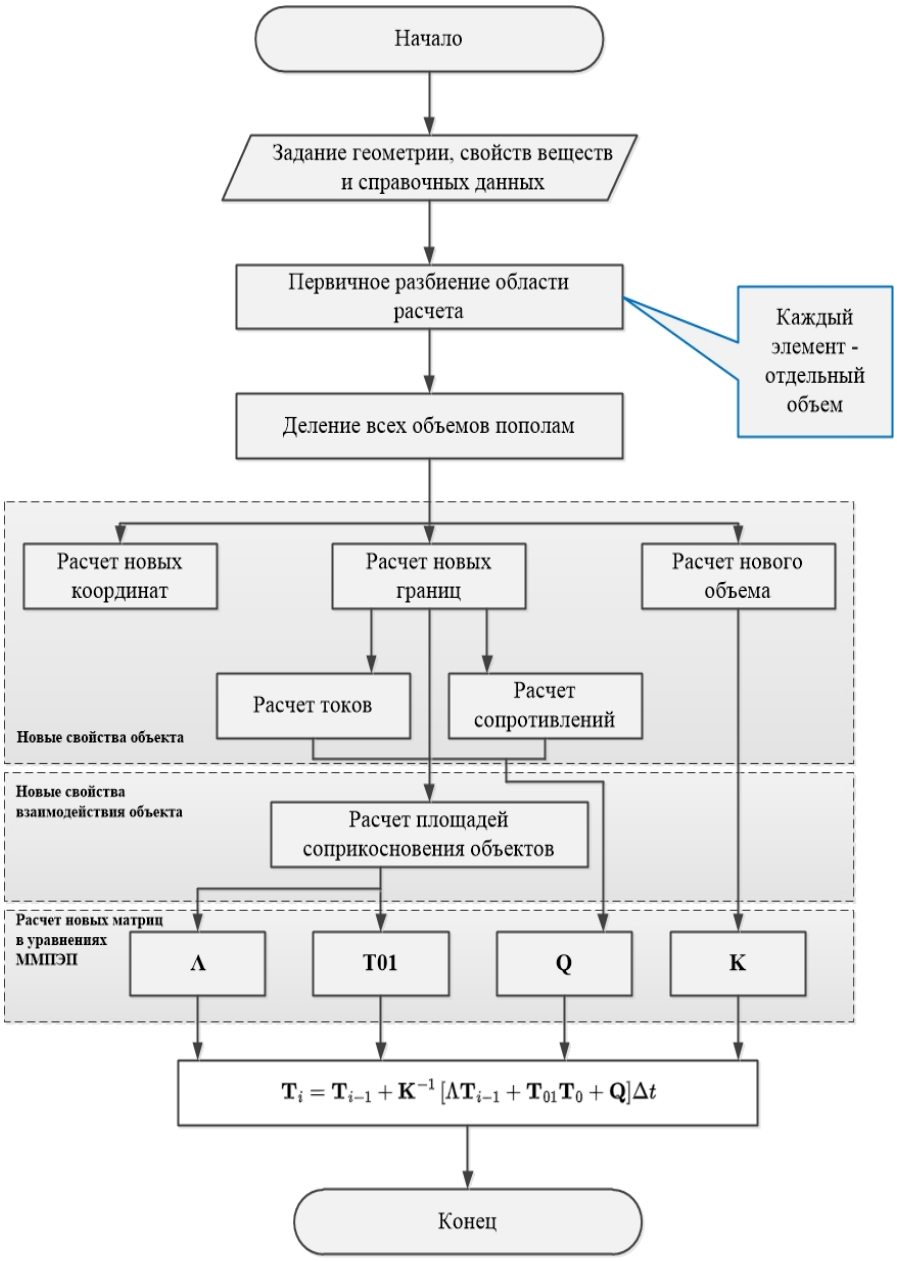
$$\boldsymbol{K}\frac{d\boldsymbol{T}}{dt}=\boldsymbol{\Lambda T}+\boldsymbol{T_{0I}T_0}+\boldsymbol{Q} \qquad (3)$$

is obtained.

It is necessary to divide subsequently the capacities, calculate all capacity temperature dynamics change and form thermal dynamic scalars analytic functions for the given geometry of the researched space in accordance with modified finite capacities method procedure.

Mathematical model equation synthesis algorithm

The quantity of equations in the model (all the matrix planes) and all the matrixes $\boldsymbol{K, \Lambda, T_{0I}, Q}$ themselves in equation (3) both change while implementing the given method, which is its fundamental problem. Changes in all



Начало – Start;
Задание геометрии, свойств веществ и справочных данных – Setting the geometry, substance features and reference data;
Первичное разбиение области расчета – Primary calculation area division;
Каждый элемент – отдельный объем – Every single element is a particular capability;
Деление всех объемов пополам – All the capabilities division in half;

Новые свойства объекта – New object features;
Расчет новых координат – New coordinates calculation;
Расчет новых границ – New boundaries calculation;
Расчет нового объема – New capability calculation;
Расчет токов – Currents calculation;
Расчет сопротивлений – Resistances calculation;

Новые свойства взаимодействия объекта – New object interaction features;
Расчет площадей соприкосновения объектов – Object contiguity squares calculation;

Расчет новых матриц в уравнениях ММПЭП – New matrixes in in the modified finite volume method calculation;

Конец – Finish

Fig. 2. The algorithm for the synthesis of thermal conductivity equations in the division of elements in the modified finite volume method

volume geometrical parameters are the first ground for it.

There is the algorithm of equation (3) forming and matrixes recalculation in Figure 2. Equation (3) is then presented as differential figure integration equation with Eyler's method.

$$\boldsymbol{T_i = T_{i-1} + K^{-1}\left(\Lambda T_{i-1} + T_{01}T_0 + Q\right)\Delta t.} \qquad (4)$$

Recalculation procedures are divided into two steps: forming the new object features after division and new system features, responsible for object interaction (thermal transfer in the given case), which is the algorithm peculiarity.

New object essential feature determination procedure is quite simplified due to use of object-focused programming technology: all substance features (thermal conductivity, thermal capacity, density, specific ohmic resistance, current densities at all the coordinates), along with integral features (mass, volume, ohmic resistance, mass centre coordinates) calculation

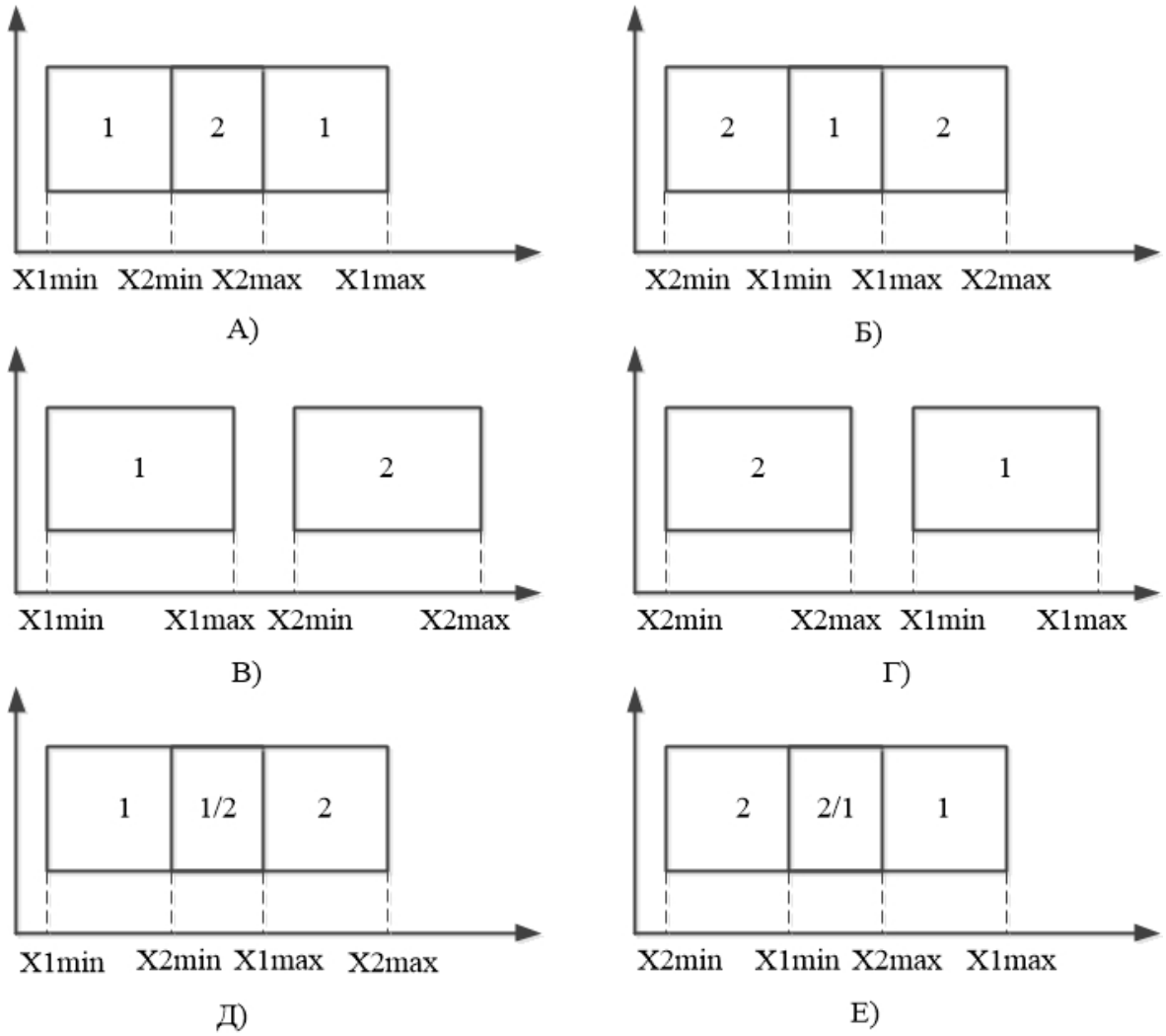


Fig. 3. Possible combinations of the intersection of the faces of two volumes along the X-axis that are in the same plane

methods are inherited from parental objects after division. Only boundary space coordinates are redetermined depending on division concept. Volume division in half at all the Cartesian coordinates is observed in the given paper – that is the new object boundary coordinate determination procedure is simplified due to without violating the general principle of mathematical model forming. These features are used for **K** and **Q** matrixes determination.

The procedure of new object interaction features determination, which is to be run again for all the system objects after the division, should be observed particularly. These features are necessary for thermal transfer parameter determination, primarily depending on their contiguity surface area.

Besides the new interacting couples multitude it is necessary to determine thermal transfer coefficients (during object interaction from different substances) or thermal conductivity coefficients (for the same substances in the object couple). These features are used for $\boldsymbol{\Lambda}$ and $\boldsymbol{T_{01}}$ matrixes forming.

It is necessary to observe all the couples of the system object multitude, which is the procedure peculiriality, then there are 6 interaction variants for all the coordiantes (x, y, z) of all the volumes couples in case the object faces are in the same plane:

variants 1 and 2 – the second object boundary surface area is within the first object surface area (fig. 3, *А*, *Б*) or the first object boundary

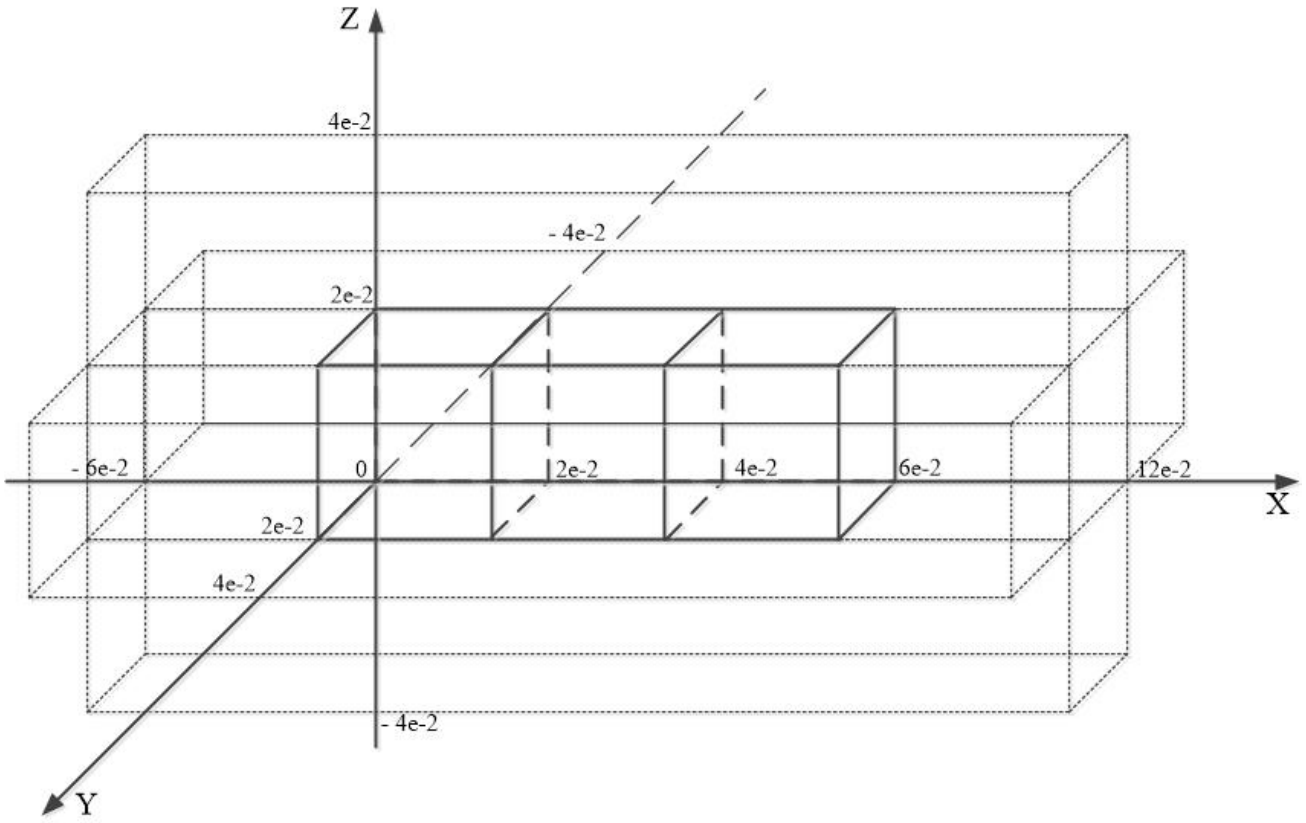


Fig. 4. The initial scheme for calculating the temperature field of a lithium-ion battery

surface area is within the second object surface area;

variants 3 and 4 – surface areas do not overlap (fig. 3, *В*, *Г*);

variants 5 and 6 – surface area overlapping, during which every couple object surface areas overlap only partly (fig. 3, *Д*, *Е*).

Research results

The presented synthesis algorithm is implemented in Python environment with object-focused technology use. The following procedures are implemented in program complex:

- the initial material features reference data setting;
- forming a fundamental "volume" unit, which is a predecessor of all the new units;
- forming a unit collection, inherited from the fundamental one and their interaction parameter determination;
- object division (in half with a plane) at all the Cartesian coordinates;
- geometrical parameters and $\boldsymbol{K, \Lambda, T_{01}}$ and $\boldsymbol{Q}$ matrixes calculation;
- support procedures.

Numerical experiments demonstrated that the given method allows to determine temperature field and obtain thermal scalar field analytical functions quite accurately even having done a small amount of divisions and, consequently, having obtained a small amount of object which the researched space is divided into.

There is the initial battery geometry in Figure 4:

- X(0; 0,02); Y(0; 0,02); Z(0; 0,02) – volume for modelling the electrode 1;
- X(0,02; 0,04); Y(0; 0,02); Z(0; 0,02) – volume for modelling an electrolyte;
- X(0,04; 0,06); Y(0; 0,02); Z(0; 0,02) – volume for modelling the electrode 2;

and extra air volumes:

- X(–0,06; 0); Y(0; 0,02); Z(0; 0,02) – volume for modelling air boundary with electrode 1 (by X axis);

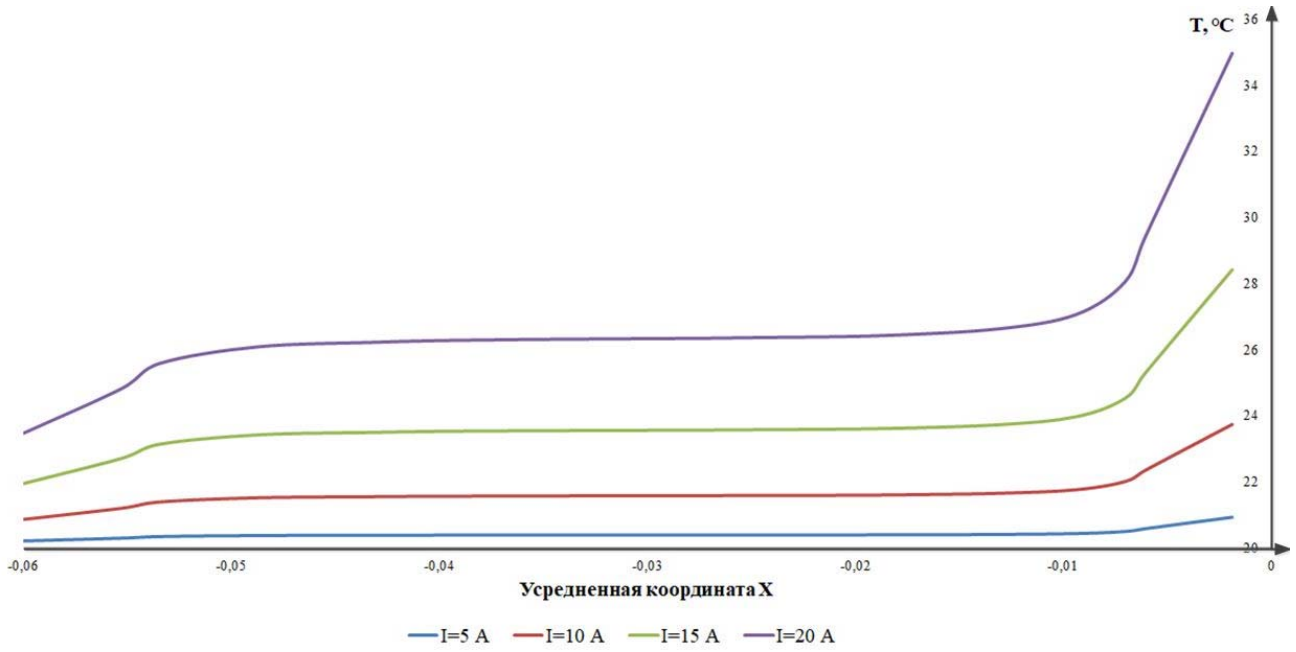


Fig. 5. Temperature distribution inside the volume X = (–0,06; 0); Y = (0; 0,02); Z = (0; 0,02) when dividing by coordinate X (Усредненная координата X – Mean X coordinate)

- X(0,06; 0,12); Y(0; 0,02); Z(0; 0,02) – volume for modelling air boundary with electrode 2 (by X axis);
- X(–0,06; 0,12); Y(0; 0,02); Z(0,02; 0,04) – volume for modelling the above air boundary with the battery (by Z axis);
- X(–0,06; 0,12); Y(0; 0,02); Z(–0,04; 0) – volume for modelling the below air boundary with the battery (by Z axis);
- X(–0,06; 0,12); Y(0,04; 0,02); Z(0; 0,02) – volume for modelling the front air boundary with the battery (by Y axis);
- X(–0,06; 0,12); Y(–0,04; 0); Z(0; 0,02) – volume for modelling the back air boundary with the battery (by Y axis).

Temperature field was calculated with the modified finite volumes method for the initial scheme (fig. 4). Temperature field was calculated for air volumes. The results are presented in Figures 5–7.

Judging by graphs in Figures 5–7 obtained, area above the electrolyte is the most heated one, which matches the experiment results. The data obtained may be used for forming the analytical expression, which lithium-ion battery pre-failure stages diagnosis method will be based on.

Conclusion

1. Automatical thermal conduction equation synthesis algorithm is obtained through modified finite volume method, involving space division during calculation, with, consequently, equation synthesis at every iteration required.

2. The algorithm is implemented in the Python object-focused program environment for lithium-ion battery fundamental prismatic geometry, graphs of temperature dependence on space coordinates, analysis of which has demonstrated the appropriate resemblance with genuine physical processes, are obtained.

3. The equation synthesis algorithm presented is developed considering the assumption about all the volumes presented as rectangular parallelepipeds, which faces are parallel to the basic Cartesian coordinates planes. It is necessary to revise some of the algorithm procedures for any other division shape.

4. The direct forming of electrotechnical aircraft equipment temperature scalar field analytical dynamic models is the development of the algorithm presented.

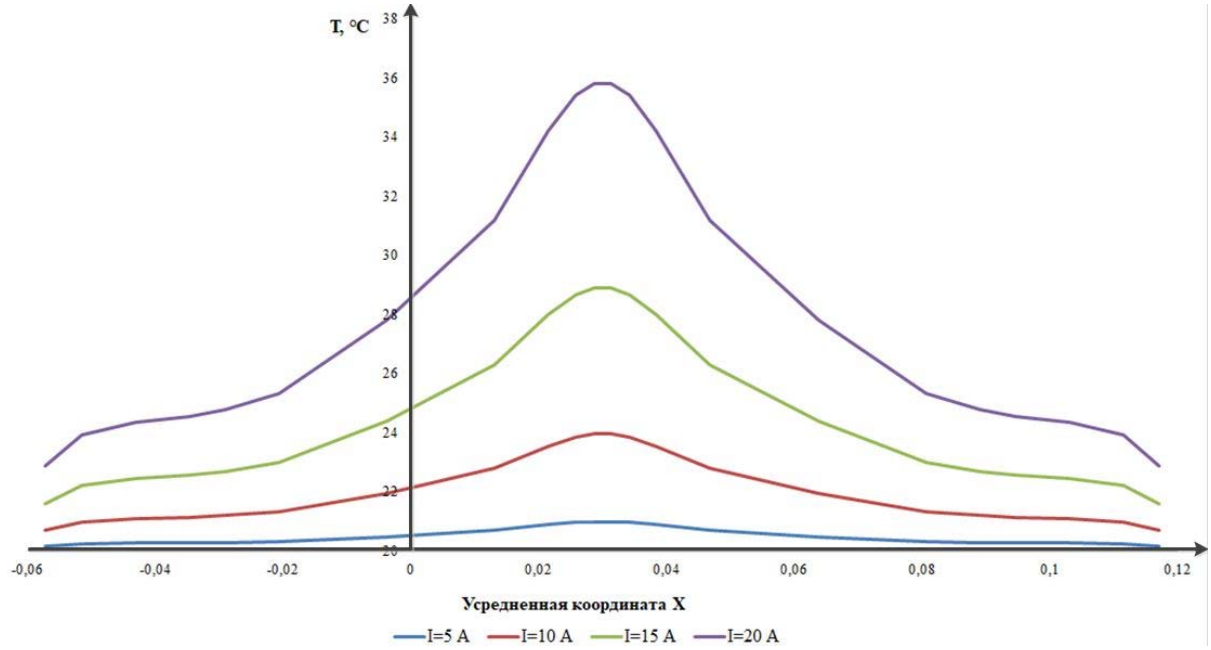


Fig. 6. Temperature distribution inside the volume X = (–0,06; 0,12); Y = (0,00; 0,02); Z = (0,02; 0,04) when dividing by coordinate X (Усредненная координата X – Mean X coordinate)

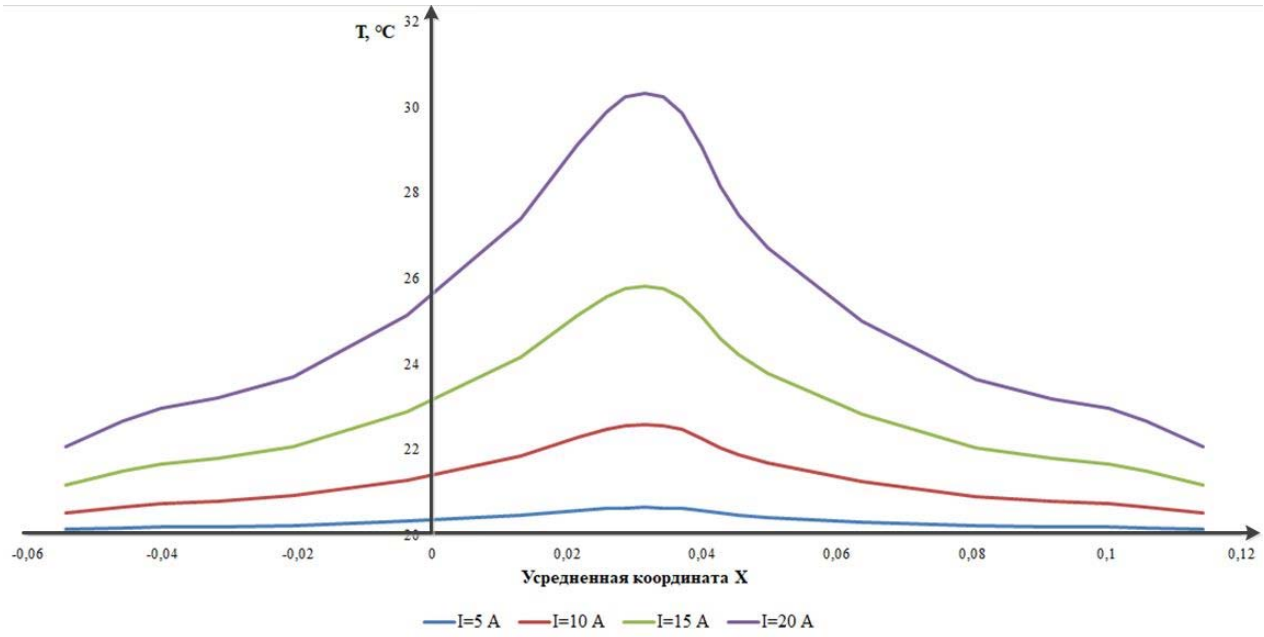


Fig. 7. Temperature distribution inside the volume X = (–0,06; 0,12); Y = (0,02; 0,04); Z = (–0,02; 0,04) when dividing by coordinate X (Усредненная координата X – Mean X coordinate)

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