Development and comparisons of the thermal simulation models with various complexity of the electrolytic capacitor for functional verification purposes of super capacitor in different conditions of use

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ABSTRACT

Supercapacitor is perspective solution for electrical energy storage whereby its big advantage is that this energy is available to be utilized in a very short time. Disadvantage of such device is its low operating voltage (several Volts) and its high sensitivity against maximum temperature limit. Therefore for purposes of development of physical sample of supercapacitor it is suitable to develop also simulation model, which will be capable to exactly interpret physical behavior of considered supercapacitor in various conditions (electrical, thermal, environmental). For these purposes COMSOL Multiphysics 3.5a has been used. In this article we would like to describe development process of the thermal model of wound capacitor which is EDLC type (Electrochemical double layer capacitor), whereby main target is to reach very close proximity of simulation results comparing to measurements in various conditions. Targeting high degree of model’s accuracy, three alternatives of model complexity will be shown. Instead of accuracy the proper model for next steps of development has to fulfill also requirements on the computation time. In the final stage, we will describe how important is design of the computational mesh, whereby EDLC thermal model has to meet strict requirements on high degree of accordance with experimental measurements.

Keywords: supercapacitor, thermal model, simulation, electrolytic dual layer capacitor

1. THEORY

From macrostructure of EDLC it is possible to figure out, that for the heat conduction the volumetric properties of EDLC acts as anisotropic surroundings. This structure is in axial and radial direction of EDLC coil geometrically and physically different. Heat transfer through this structure is therefore different in axial direction against heat transfer in radial direction. At examined thermal model of EDLC, the waveform of axial and radial part of thermal constant (heat transfer by conduction) in the dependency on order of turn is designed. During operation of the EDLC its temperature rises above ambient environment. The core temperature inside the EDLC exceeds the temperature at the EDLC surface and in the steady state the applied electrical power \( P_C \) matches the heat power \( P_{Th} \) dissipated to the ambient:

\[
P_C = P_{Th}
\]

There are three types of cooling mechanism:

- convection type (free or forces)
- radiation type
- conduction type

Heat convection is governed by heat transfer from the can to the ambient environment. Convection is generally modeled as a surface effect. The parameter that describes the degree of thermal heat transfer coupling from a surface of area \( S \) to ambient fluid is known as the convection heat coefficient \( h \), which is a strong function of the fluid velocity \( v \) and mass transfer properties.
(density, viscosity). The power dissipated through convection is generally given by:

\[ P_{\text{conv}} = h.S(T_s - T_a) \]  

(2)

\( T_s \) – surface temperature EDLC,
\( T_a \) – ambient temperature,
\( S \) – area of surface sleeve of EDLC,
\( h \) – heat transfer coefficient convection.

The core temperature of EDLC can be estimated by:

\[ \frac{\Delta T_{c,s}}{R_{\text{th,core}}} = \frac{\Delta T_{s,a}}{R_{\text{th}}} \]  

(6)

\( T_{c,s} \) – temperature rise core surface,
\( T_{s,a} \) – temperature rise surface ambient,
\( R_{\text{th}} = 1/h_{\text{tot}}.S \)
\( R_{\text{th,core}} \) – combined thermal resistances of EDLC

From macrostructure of EDLC capacitor on fig.2 it is possible to conclude, that volume properties of EDLC acts as anisotropic surrounding for the heat conduction. This structure is in axial and radial direction geometrically and physically different.

In practical uses the total heat transfer coefficient (include convection and radiation) can by approximated by [1], [2]:

\[ h_{\text{tot}} \approx 5 + 17.(v + 0.1)^{0.66} \]  

(5)

Previous equations (2), (3) are expressing possible heat rise \( \Delta T \) of EDLC. Anyway they are not accepting many other important factors, such as gravimetric orientation, geometric ratio \( D/L \), type of air flow (laminar, turbulent). Therefore heat radiation is better to be expressed by Stefan-Boltzmann’s law:

\[ P_{\text{rad}} = \varepsilon.\sigma.S.(T_s^4 - T_a^4) = h_{\text{rad}}.S.\Delta T_{a,s} \]  

(4)

\( \varepsilon \) – emissivity,
\( \sigma \) – Stefan-Boltzmann’s constant,
\( h_{\text{rad}} \) – heat transfer coefficient radiation.

In practical uses the core temperature of EDLC can be estimated by:

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From macrostructure of EDLC capacitor on fig.2 it is possible to conclude, that volume properties of EDLC acts as anisotropic surrounding for the heat conduction. This structure is in axial and radial direction geometrically and physically different.
Axial part of turn’s thermal resistance with „j-th“ order was computed using next formula:

\[ R_a(j) = \frac{L}{k_a(j) \cdot S(j)} \]  \hspace{1cm} (1)

\( L \) – is height of turn coil (m),
\( k_a \) – thermal conductivity in axial direction (W/m.K)

Equivalent axial thermal conductivity of one turn of EDLC shown on fig.2 is given by next equation:

\[
\frac{1}{R_a(j)} = \frac{1}{R_a^S(j)} + \frac{1}{R_a^{C-L}(j)} + \frac{1}{R_a^{AI}(j)} + \frac{1}{R_a^{C-R}(j)} \]  \hspace{1cm} (11)

\( R_a^{C-L} \) – axial thermal resistance of carbon layer on left side,
\( R_a^{C-R} \) – axial thermal resistance of carbon layer on right side,
\( R_a^{AI} \) – axial thermal resistance of extruded aluminum layer,
\( R_a^S \) – axial thermal resistance of separator layer

Dependency of thermal coefficient for heat transfer by conduction in one turn of EDLC with „j-th“ order should be expressed from (4,5,6) by next formula:

\[ k_a(j) = \frac{L}{R_a(j) \cdot S(j)} \]  \hspace{1cm} (12)

After adding several radial resistances we can obtain dependency of equivalent radial thermal conductivity in one turn with „j-th“ order as follows:

\[ k_r(j) = \frac{\ln r_j}{2 \pi L R_r(j)} \]  \hspace{1cm} (14)

2. DEVELOPMENT OF THERMAL MODELS OF EDLC

3D geometrical model of EDLC capacitor with minimal complexity is shown on fig.5. It is representing the scroll coil of mentioned sandwich structure (fig.1) with diameter of 28 mm and height of 125 mm. Compressed foils on top and bottom side are made from extruded aluminum and have prepared area for electrical contacts connection. The core of EDLC is separated from aluminum chat through electrolyte layer.

Each subdomain of EDLC has physical thermal coefficients defined using material libraries from COMSOL heat-transfer module [3]. Coefficient of core’s thermal conductivity creates tensor of 2 grade in which part of axial and radial thermal conductivity are being
included. For the higher accuracy of results from thermal simulations we decided to develop also other models whose geometrical properties will be in the closer proximity to real physical sample. Next figure is showing 1xEDLC improved complexity model.

![Fig.6. Improved complexity model of 1xEDLC](image)

### 3. RESULTS AND COMPARISONS OF SIMULATION AND MEASUREMENT EXPERIMENTS

Surroundings of EDLC model is air with temperature of $T_{\text{amb}} = 27,3 \, ^{\circ}\text{C}$. Heat power in the core EDLC was set to $P_{\text{loss}} = 0,56 \, \text{W}$. Next figure is showing result from simulation experiment of simple complexity model for steady state operation.

![Fig.7. Interpretation of temperature distribution in whole volume of EDLC - simple complexity model, $P_{\text{loss}} = 0,56 \, \text{W}, T_{\text{amb}} = 27,3 \, ^{\circ}\text{C}$](image)

These results have been compared to experimental measurement of physical sample. The parameters of experimental measurement where the same as during simulation experiment so $I_{\text{load}} = 30 \, \text{A}$, $\text{DCR}_{\text{EDLC}} = 0,63 \, \text{m}\Omega$, $P_{\text{loss}} = 0,56 \, \text{W}$, $T_{\text{amb}} = 27,3 \, ^{\circ}\text{C}$. Charging process of capacitor lasts 51 sec. with applied voltage of 2,5 V, discharge process starts after 0,5 sec. and lasts 51 sec. with applied voltage of 0 V. Next figure is showing result from thermal measurement of physical sample.

![Fig.8. Result from experimental measurement of EDLC, $P_{\text{loss}} = 0,56 \, \text{W}, T_{\text{amb}} = 27,3 \, ^{\circ}\text{C}$](image)

Relative error between simulation and measurement for subdomains - core of EDLC and case of EDLC, were computed based on next equation:

$$T_{\text{rel.err}} = \frac{\nabla T}{T_{\text{amb}}} = \frac{T_{\text{core,meas}} - T_{\text{core,sim}}}{T_{\text{amb}}} = \frac{318 - 319.87}{27,3} = -0,68\% $$

| | | | |
|---|---|---|
| $I_{\text{RMS}} \, [\text{A}]$ | $P_{\text{loss}} \, [\text{W}]$ | $T_{\text{rel.error}}$ |
| CORE | 30A | 0,561 | -0,68 % |
| CASE | 30A | 0,561 | -5,32 % |
| CORE | 50A | 1,33 | -0,34 % |
| CASE | 50A | 1,33 | -9,5 % |

As was previously mentioned, facing requirements on higher accuracy of simulation model, we decided to develop improved complexity model. This model has against simple complexity model two added subdomains: aluminum coat, and air between aluminum coat and minimal complexity model (fig.6.). The problems which became into account after adding this subdomains was increased number of total elements of computation mesh (from $10^4$ to $10^5$). This fact has reflected into longer computation time. Therefore the optimization of mesh size manually have been done to improve computational time whereby, better accuracy of model had to be maintained.

Comparisons of results from simulation of minimal complexity and improved complexity model are shown on fig.8. The figure represents dependency of temperature distribution in the core of ELDC in x-cut direction in the middle of EDLC height. From fig.9. it can be seen that due to improvement of 1xEDLC model the temperature
difference between core, and between can of EDLC is much higher. This is caused due to air layer, which is located between aluminum coat and minimal complexity model (see fig.6.). From this simulation experiment it is clear to say that aluminum coat (width = 0.5mm) and air gap (width = 0.5mm) are causing that temperature inside of EDLC is higher compared to minimal complexity model by 3.74 ºC at $P_{loss} = 1.62$ W.

Next we have compared simulation results of improved complexity model at conditions which were similar to the conditions for simple complexity model. One important change came into account, DCR - series resistivity of EDLC of physical sample was changed due to several non-specified reasons. We would like to note, that reference measuring points have been changed against first experiments (fig.10). The results from this comparisons are listed in table 2.

4. IMPACT OF COMPUTATION NET DENSITY ON ACCURACY OF RESULTS

Previous experiments has confirmed that improvements of simulation model of EDLC has led to higher accuracy/lower relative error when compared to measurements of physical sample. On the other hand optimization of computational mesh was necessary due to requirements on duration of simulation time. Therefore we have also analyzed the accuracy of thermal field computation in dependency on density of computation net. For determination of relative error next equation have been used:

$$\Delta T(x) = T(x, \text{extra fine}) - T(x, \text{mesh size})$$  (15)

$T(x,\text{extra fine})$ - temperature calculated in EDLC at highest density of computation net

$T(x,\text{mesh size})$ - temperature calculated in EDLC at given density of computation net

In the COMSOL environment pre-defined mesh sizes menu offers you selection of pre-defined mesh sizes that automatically determine the parameters in the custom mesh size menu.

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**Table 2.** Relative errors between simulation (improved model) and measurement for reference measuring points of EDLC

<table>
<thead>
<tr>
<th>Face:</th>
<th>Temperature of Simulated model [Ts]</th>
<th>Temperature of Measured cell [Tm]</th>
<th>Difference (Ts-Tm)</th>
<th>Relative error (Ts-Tm)/Ta</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 L B</td>
<td>32.99</td>
<td>31.00</td>
<td>1.99</td>
<td>0.08</td>
</tr>
<tr>
<td>1 R B</td>
<td>33.05</td>
<td>31.00</td>
<td>2.05</td>
<td>0.08</td>
</tr>
<tr>
<td>1 L F</td>
<td>33.04</td>
<td>31.50</td>
<td>1.54</td>
<td>0.06</td>
</tr>
<tr>
<td>1 R F</td>
<td>33.04</td>
<td>31.30</td>
<td>1.74</td>
<td>0.07</td>
</tr>
<tr>
<td>1 up</td>
<td>33.15</td>
<td>31.70</td>
<td>1.45</td>
<td>0.06</td>
</tr>
<tr>
<td>1 down</td>
<td>32.92</td>
<td>32.70</td>
<td>0.22</td>
<td>0.01</td>
</tr>
</tbody>
</table>

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**Fig.9.** Plot of temperature of minimal and improved complexity model. Radial direction x-line for height ($z$) = 0.04 m

**Fig.10.** Reference measuring points for verifications of improved complexity model

**Fig.11.** Temperature in cross section area of EDLC in dependency on density of computation net
Pre-defined mesh size can generate from extremely fine to extremely coarse (extra fine, finer, fine, normal, coarse, coarser, extra coarse). Fig.11 is showing line plot of temperature in cross section area of EDLC (x-cut, through diameter of EDLC). Figure represents temperature in dependency on density of computation net. Fig.12 is showing line plot of relative error of temperature which was computed based on equation (15).

Therefore we have analyzed also machine time calculation in dependency on density of computation net. Table 3 is showing mentioned results. It can be seen that targeting relative error around 0.05% it is sufficient to utilize finer or fine mesh size. In comparisons with extremely fine settings the error is higher by around 0.04% but computation time is lowered by 98%. This is very important result almost for applications and/or research where high number of simulation experiments have to be made in less time but have to have high accuracy level.

5. CONCLUSION

This paper describes methodology of design of thermal model of supercapacitor which is electrolytic dual layer type. After development of mathematical model we have design thermal model in COMSOL 3.5a environment. Next we have performed simulation experiments which were compared to exact measurements of physical sample. Targeting higher accuracy of thermal model for future purposes we have designed second model with improved complexity. In this way we were able to aim higher accuracy when compared to experimental measurements, but on the other hand complexity of model became critical in the meanings of density of computation net. Therefore we have analyzed relationship between relative error, density of computation net and computational time. From results it is clear that for requested accuracy the fine settings of net density is very sufficient. Almost this setting secures very good accordance to experimental measurements with low value of relative error. In next steps we are going to develop thermal models with higher number of EDLC cells. For these purposes the analysis of net density is very necessary.

Table 2. Machine time for computation of simulation results for thermal distribution of EDLC (improved model)

<table>
<thead>
<tr>
<th>Mesh size</th>
<th>Number of elements</th>
<th>Machine time of simulation [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>EXTREMELY FINE</td>
<td>378 302</td>
<td>1 703, 280</td>
</tr>
<tr>
<td>EXTRA FINE</td>
<td>123 289</td>
<td>271,205</td>
</tr>
<tr>
<td>FINER</td>
<td>58 023</td>
<td>69,453</td>
</tr>
<tr>
<td>FINE</td>
<td>29 814</td>
<td>27,656</td>
</tr>
<tr>
<td>NORMAL</td>
<td>19 491</td>
<td>14,100</td>
</tr>
<tr>
<td>COARSE</td>
<td>6 421</td>
<td>3,437</td>
</tr>
<tr>
<td>COARSER</td>
<td>3 452</td>
<td>1,578</td>
</tr>
<tr>
<td>EXTRA COARSE</td>
<td>1 765</td>
<td>Unsuccessful computation</td>
</tr>
<tr>
<td>EXTREMELY COARSE</td>
<td>620</td>
<td>0,437</td>
</tr>
</tbody>
</table>

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6. REFERENCES

