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Thermal profiling of ultracapacitor modules : A layered analysis

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Abstract

This study explores heat dissipation in supercapacitor modules tailored for energy-intensive applications. The research investigates the influence of different electrode material combinations on key performance parameters. Employing MATLAB and COMSOL simulations, the thermal conductivity of various layers within the supercapacitor module is analyzed. Findings reveal that polythene separators, responsible for encapsulating and segregating the module's electrodes, represent critical points for controlled heat transfer. Significantly, the use of metal oxide in electrode construction contributes positively to regulated heat dissipation. Substituting polythene separators with synthesized materials is proposed to optimize heat dissipation. This research pioneers a data-driven analysis and software simulations to augment the study's outcomes.

Subject Classification: *65-XX.*

Keywords: *Supercapacitor, Electrodes, Electrolyte, MATLAB, Thermal.*

1. Introduction

In recent advancements, supercapacitors have evolved as a compelling alternative to batteries, demonstrating notable improvements in their characteristics. Despite batteries boasting significantly higher energy storage capacity (10-100 times more), supercapacitors excel in practical applications, particularly as power boosters [1]. Although they may exhibit limitations in potential window [2], the integration of supercapacitors with batteries has yielded substantial enhancements in the automotive industry [3]. Their rapid charge and discharge characteristics make them ideal for applications requiring swift impulse current generation [4-6].

Several research papers discuss supercapacitor behavior and emphasize the necessity for further extensive studies on supercapacitors [7-9]. Alternative electrode materials such as carbide-derived carbons and zeolite-templated carbons are being explored [10]. The growing focus on sustainable development goals has led to an increased utilization of biomass-based materials in supercapacitor electrode preparation [11-12]. The formation of the electrode-electrolyte double layer in supercapacitors is instrumental in enhancing storage capacity [13-15].

Various statistical modelling techniques have been employed to study the performance contributing parameters of asymmetrical supercapacitors [16-18]. There has also been considerable research done on the structural integrity and electrode structure correlating it with the performance of supercapacitors [19-21]. Various charge storage volumes with different electrolytes are the result of electrochemical reactions [22-25]. The

imperative to predict the temperature rise in each layer of a supercapacitor, addressing the heat dissipation challenge, is highlighted. A notable drawback of supercapacitors is their tendency to heat up during operation, often overlooked due to their pulse current nature. This paper aims to investigate the thermal effects across different supercapacitor materials using MATLAB and COMSOL simulations.

The simulations provide insights into the heating patterns of each supercapacitor layer, assessing the ease or difficulty of heat dissipation. Such analyses contribute to preventing thermal runaway, addressing a significant research gap. The research paper is organized into subsequent sections, starting with Part 2 detailing electrode materials, separators, and packaging. Part 3 outlines the considered supercapacitor parameters, followed by their analysis using MATLAB and COMSOL in Part 4. The paper concludes with final remarks.

2. Materials used in the construction of supercapacitors

The production of supercapacitors predominantly utilizes activated carbon due to its cost-effectiveness, high surface area, electrode manufacturing methods, and widespread availability. The storage capacity of supercapacitors is significantly influenced by the interface resulting from double layer formations between the electrode and electrolyte. Capacitance relies heavily on the Specific Surface Area (SSA) available for electrolyte ions, termed as available SSA. Examples of carbon materials used in electrode fabrication include carbide-derived carbon, zeolite-templated carbon, onion-like and graphene.

Activated carbon is a common choice for electrode preparation in almost all supercapacitors due to its substantial surface area, cost-effectiveness, larger pores, and favorable electrical properties. The production of activated carbon involves both physical and chemical procedures from carbonaceous materials. This research assesses VULCAN XC-72R, NORIT, PICA, and YP50 for parametric mismatches. The SEM image of Vulcan XC-72R suggests a clustered and curvilinear particle structure. With continuous technological advancements, single-walled and multi-walled carbon nanotubes shall play a crucial role, known for their unique pore composition, thermal and mechanical stability, and excellent electrical characteristics. Graphene, also known as carbon-fiber-reinforced polymer, has gained acceptance. Metal oxides, particularly manganese dioxide, are blended with activated carbon to reduce internal resistance. Manganese dioxide, often used interchangeably with “metal

oxide," displays large specific capacitance, low resistance, cost-effectiveness, and environmental friendliness.

Efforts have been made to replace polythene separators in supercapacitors due to environmental concerns. Researchers have explored materials like paper, PBI, PVC, AGM, with limited success. Polythene's porous and non-decaying characteristics make it practical for use in supercapacitors. The current collector, a crucial component of the supercapacitor electrode, is ideally permeable. Aluminum and stainless steel, in the form of foil or wire mesh, are the most commonly used current collector materials to date.

3. Factors influencing heat dissipation in supercapacitors

This paper employs a simulation approach to identify issues related to the characteristics of materials utilized in supercapacitors. The focus is on thermal conductivity and particle size, deemed critical parameters for heat dissipation in supercapacitors. This section provides a theoretical analysis of these two parameters.

a) *Thermal Conductivity*

The efficacy of a supercapacitor is significantly influenced by the efficiency of heat transfer volume, playing a crucial role in determining the device's lifespan. Given the substantial current drawn by supercapacitors, effective heat dissipation to adjacent components is essential for optimal utilization throughout its intended operational lifespan. Table 1 outlines the thermal conductivity of materials employed in supercapacitors.

Table 1 delineates that the thermal conductivity of the current collector surpasses that of both electrode materials and separators. It is evident that the thermal conductivities of these materials must align within a specified range to facilitate rapid heat conduction; otherwise, it could lead to the deterioration of the supercapacitor. Research in material

Table 1

Thermal Conductivities(W/m*K) of materials employed in supercapacitor construction.

Packaging Materials	Separator materials	Electrode materials	Current Collector materials
0.09-0.63	0.2-0.5	0.5-0.7	200-210

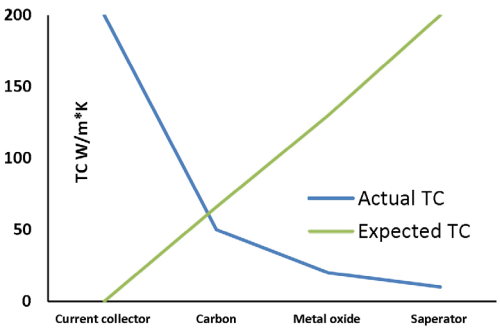


Figure 1

Mismatch of thermal conductivity

engineering is imperative to explore this aspect further. Enhancing the thermal conductivity of separators could be a groundbreaking solution to address these concerns.

Figure 1 is the graphical representation of mismatch of thermal conductivity for generally used materials in supercapacitor and expected thermal conductivity (TC) variation. The thermal conductivities of supercapacitor materials do not fall under identical range. For high performance of supercapacitor, the heat transfer rate shall be as gradual as possible however the graph cannot be parallel to the reference horizontal axis because the rate of heat transfer reduces when heat transfer advances from one material to another.

b) *Particle Size*

Ensuring that the pore size and particle size are well-matched is crucial. The more closely the size of electrolyte molecules or ions aligns with the pore size of the electrodes, the more efficient charge accumulation occurs, resulting in increased capacitance. Greater linkage between electrode particles and electrolyte particles is anticipated to enhance heat dissipation within the supercapacitor. Table 2 provides details about the particle and pore sizes of materials used in supercapacitors. Figure 2 depicts the relative positioning of these materials in relation to the supercapacitor, with each material having its specific particle size that impacts the thermal stability of the overall supercapacitor structure.

Table 2

Particle Size (um) of commonly used materials in supercapacitor.

Electrolyte materials	Electrode materials		Separator Materials
	Vulcan XC-72R	Metal Oxide	
0.03-0.2	0.02-0.05	0.057	50-60

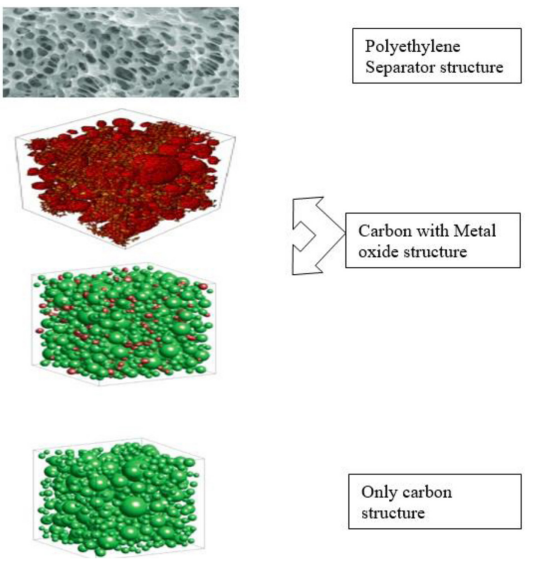


Figure 2

Possible particle interface among electrode material and separator in Supercapacitor

4. Evaluation of Heat Dissipation through MATLAB

Input parameters such as electrode dimensions, porosity, material type, material density, thermal conductivity, heat capacity, electrical conductivity, etc., were utilized in MATLAB to analyze the temperature rise at each layer of supercapacitors. The graphical user interface in Figures 3, 4, and 5 illustrates the temperature distribution in various layers using different combinations of electrode materials, separator materials, and electrolytes. The simulation revealed noteworthy insights, indicating that heat flow is influenced by factors like particle size mismatch and thermal conductivity. This simulation methodology can be extended for the analysis of diverse electrical energy storage devices such as batteries,

capacitors, and fuel cells. Given the increasing integration of supercapacitors in battery-operated and fuel cell-based vehicles, this simulation provides valuable insights for researchers to determine optimal material characteristics, preventing thermal runaway and thereby enhancing the device's lifecycle. This pioneering simulation represents a significant contribution to the research presented in this paper.

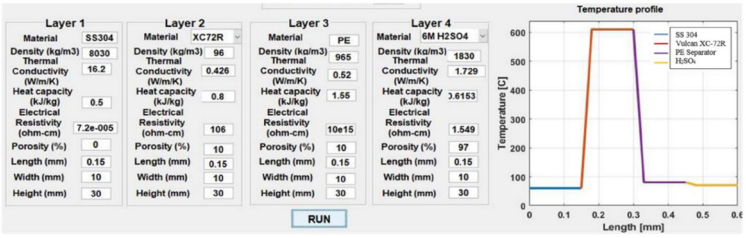


Figure 3

Temperature variation in the supercapacitor with Vulcan XC-72R as electrode material

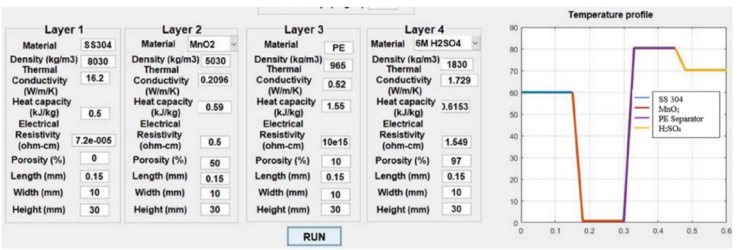


Figure 4

Temperature variation in the supercapacitor with manganese oxide as electrode material.

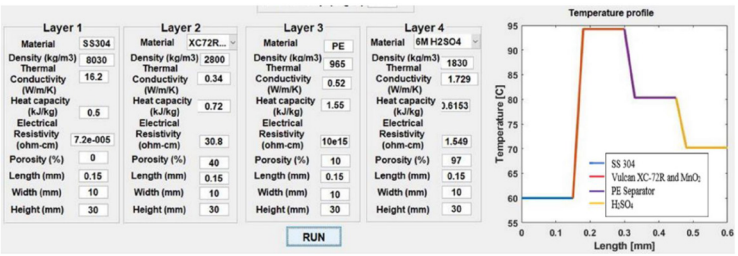


Figure 5

Temperature variation in the supercapacitor with Vulcan XC-72R and manganese oxide as electrode material.

Figure 3 illustrates the temperature changes within the supercapacitor using Activated Carbon as the electrode material. The simulation displays the temperatures of the current collector, electrode material, electrolyte, and separator, with a maximum temperature reaching 600 degrees Celsius. In Figure 4, the temperature variations in the supercapacitor with a metal oxide as the electrode material are presented, showing temperatures of the current collector, electrode material, electrolyte, and separator, with a maximum temperature of 80 degrees Celsius. Notably, metal oxide contributes to efficient heat dissipation. Figure 5 depicts the temperature fluctuations in the supercapacitor using both metal oxide and activated carbon as electrode materials. The simulation reveals temperatures of the current collector, electrode material, electrolyte, and separator, with a maximum temperature of 95 degrees Celsius. A key outcome of this simulation is the efficacy of metal oxide in facilitating rapid heat dissipation.

5. Evaluation of Heat Dissipation through COMSOL

In the field of supercapacitor research, an exhaustive examination of crucial parameters, such as electrode dimensions, porosity, material properties, and their impact on temperature elevation within the device, has been conducted. This section employs COMSOL Multiphysics as the simulation platform, expanding the capabilities for thorough exploration. The simulation process involves the systematic variation of these input parameters, generating temperature rise profiles across different layers within the supercapacitor. Figures 6, 7, and 8 depict the user interface in COMSOL after input parameterization, displaying temperature distributions for a diverse range of electrode materials, separator materials, and electrolytes. Significant insights have emerged from this extended simulation effort. The analysis clarifies that heat flow within the supercapacitor system is intricately influenced by factors such as thermal conductivity, among others, revealing the complex interplay of these variables. Furthermore, the significance of this research extends beyond supercapacitors alone. While the focus has been on this pulse current device, the methodology presented here holds the potential for broader applications encompassing the analysis of various electrical energy storage devices, including batteries, capacitors, and fuel cells. Given the imminent integration of supercapacitors into the realm of electric vehicles, our simulation findings bear profound implications.

The ability to determine precise material specifications for supercapacitor construction, mitigating the risk of thermal runaway, and enhancing the overall lifecycle of these power devices, is a pivotal contribution of this research. One significant revelation from the investigations is the identification of the polyethylene separator as the primary factor limiting heat dissipation within supercapacitors. This discovery underscores the critical role played by the separator material in thermal management. As depicted in Figure 9, a three-dimensional representation of the supercapacitor subjected to the same parameters as those studied in the previous MATLAB analysis is presented. Notably, despite variations in electrode materials, the volume of the supercapacitor module remains relatively constant at approximately 0.18 cm3. Consequently, the observed temperature drops across different scenarios are of minor significance, hovering at around 1% across all cases.

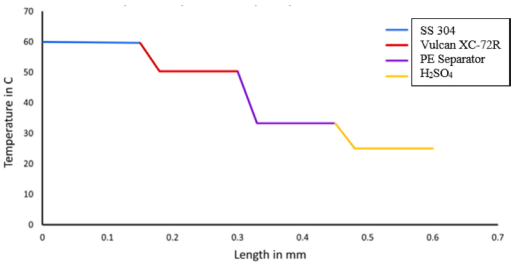


Figure 6

Temperature variations in the supercapacitor with Activated Carbon as electrode material in COMSOL.

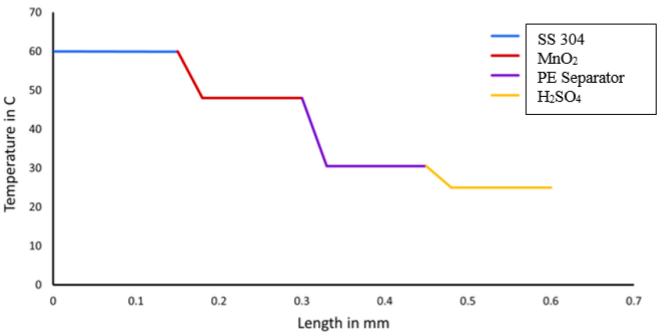


Figure 7

Temperature variations in the supercapacitor with metal oxide as electrode material in COMSOL.

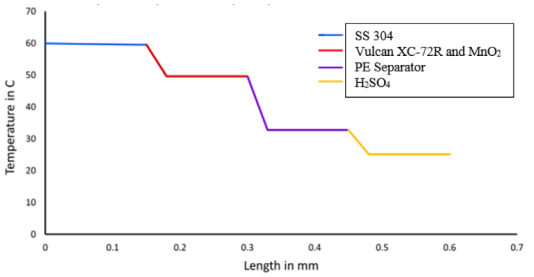


Figure 8

Temperature variations in the supercapacitor with activated carbon and metal oxide as electrode material in COMSOL

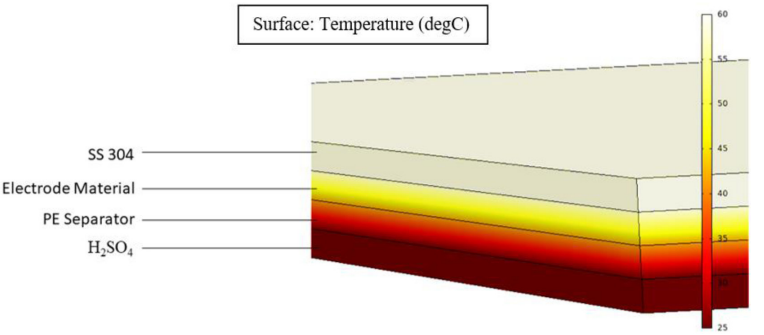


Figure 9

Thermal analysis of supercapacitor module with PE separator

Figure 9 offers a visual representation of the thermal analysis within the supercapacitor, illustrating the temperature variations which are not possible in MATLAB simulation. This simulation does not give temperature variation at each layer in gradient form as it considers average temp variation within the module. It underscores the stability of thermal performance within the compact volume of the supercapacitor. It also shows a significant temperature drop at the PE separator layer which is not clearly coming out in MATLAB simulation.

6. Conclusions

As evident, the thermal conductivity of materials utilized in supercapacitors is still insufficient to ensure unimpeded heat transfer. MATLAB simulation underscores the significance of metal oxide in heat transfer, revealing its dual role not only in additional charge storage for

improved capacitance and reduced internal resistance but also in facilitating heat transfer within the electrode material. According to COMSOL simulation, a separator with high thermal conductivity is crucial to minimize thermal runaway in the device, with the separator identified as the weakest link in heat transfer. Investigating separator materials with optimal thermal conductivity holds substantial promise for enhancing the supercapacitor's performance in terms of heat transfer. The utilization of synthesized materials as separators could pave the way for a supercapacitor with optimized functionality. While MATLAB simulation provides internal temperature rise in graphical form, COMSOL offers a three-dimensional visualization of the device, capturing nuances that thermal imaging cameras may overlook. It's noteworthy that COMSOL can't capture internal temperature spikes, a capability clearly demonstrated by MATLAB simulation.

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