Modeling lead-acid battery with organic materials

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Abstract

Lead acid battery is one of the most common types of batteries in the world. These batteries are used in various applications such as electric vehicles, energy storage systems and emergency power systems. Lead-acid battery modeling in Comsol software is an effective way to better understand battery performance and identify potential problems. In this modeling, the lead-acid battery is considered as a two- electrolyte system. The positive electrolyte is sulfuric acid and the negative electrolyte is water. Oxidation and reduction reactions take place in the two electrodes of the battery.

The results of this modeling can be used in the design and improvement of lead- acid batteries.

Keywords: *Battery Modeling, Lead-Acid Battery, Lead-Acid Battery Simulation*

Statement of the Problem

Batteries are of particular importance as one of the most important elements of energy supply systems for electrical and electronic devices. Among the different types of batteries, the lead-acid battery is known as the cheapest and oldest secondary battery and was the first battery used in commercial applications. Due to its advantages such as low material cost, high recyclability, high reliability, high discharge rate and safety, lead-acid battery has been used in a wide range of engineering applications such as hybrid-electric vehicle (HEV), uninterruptible power supply. Is Due to these advantages as well as new performance improvements, lead-acid batteries have become a key component in the automotive industry (for more than 100 years) and stand-alone renewable energy systems.

Despite the above advantages, temperature rise is an unavoidable problem that significantly affects the performance and life cycle of lead-acid batteries. Therefore, the thermal management of lead-acid batteries has been of interest for several decades as a challenging issue to increase reliability in small and large applications. Khan et al presented a comprehensive review of the literature on thermal management of battery systems with a focus on quality and safety standards. . In addition, suggestions were made from different points of view, including increasing lifespan, increasing performance, and maintaining reliability. Thermal management of stationary battery systems also plays a key role in renewable energy systems, directly affecting the cost of the cooling system and battery life. Henke and Haylo reviewed the thermal management of these systems, including the effect of temperature and heat generation on performance, thermal management methods, and future study areas.

It is worth noting that in order to minimize the negative effect of temperature on the performance and life cycle of the battery system in hybrid electric vehicles and

autonomous renewable energy systems, real-time monitoring can be used as a useful tool that can potentially provide high speed gives and detailed data of battery performance status such as battery voltage and current, state of charge (SoC), state of health (SoH) and temperature.

During the discharge and charge processes, heat is generated inside each cell, which increases the temperature inside the battery. However, the temperature rise may be limited due to heat loss to the surroundings. Joule heating is one of the main sources of heat generation inside the battery in both discharge and charge processes. On the other hand, the electrochemical reactions of a lead-acid battery are exothermic in the charging process while endothermic in the discharging process. Therefore, charging reactions are another source of heat generation that increases the temperature inside the battery. It is worth noting that at many practical discharge rates, Joule heating is the dominant heat source and thus the temperature also increases during the discharge process. However, in the process of charging and overcharging, when the internal heat production exceeds the heat loss, the temperature of the battery increases, which accelerates the exothermic reactions and causes the temperature to rise further? In this case, thermal runaway occurs, known as thermal breakdown, especially in sealed and valve-regulated lead-acid batteries that show, that the thermal analysis of lead-acid batteries and the use of numerical techniques are valuable and very necessary to prevent this state of failure. Also, since many of the chemical and physical properties of lead-acid batteries are dependent on temperature and are significantly affected by the increase in temperature, which consequently affects the performance, cost and lifetime of batteries, experimental and numerical research Much has been done to analyze the thermal behavior of these batteries.

Regarding experimental studies, McKinney et al. experimentally investigated the

thermal behavior of a lead-acid battery used in electric vehicles (EVs) during different discharge cycles. The results showed that the circulation of the electrolyte using a pump significantly affects the thermal behavior, so that less heat is produced in the charging process, the peak temperature of the cell decreases and the temperature distribution becomes more uniform. In addition, the effect of external air cooling on battery thermal management at different ambient temperatures was investigated. In addition, the results showed that the temperature of the battery increases in both discharge and charge rates. Chang et al. experimentally studied the effect of rapid charging on thermal behavior. Although experimental evaluation of lead-acid batteries provides valuable data, it is expensive and time-consuming. Thanks to the development of computational resources, mathematical modeling and numerical simulation have been used as a suitable alternative to cheap, fast and accessible experimental tests. During the past decades, various numerical models and techniques have been developed to simulate the thermal, electrochemical and dynamic behavior of lead-acid batteries.

But it has limited physical meaning and performs poorly when extrapolated from its parameterization. It includes detailed descriptions of the physical, chemical, and electrical processes that occur inside the battery, thereby increasing predictability. However, these mechanical models require much more computing power. Battery management could be improved if there were easy-to-solve models with more mechanical details, and aspect ratio of the cell. Most of the work is done in the context of a single discharge, but the extension of a model for recharge has also been investigated. Models that account for degradation are not considered, but the framework developed allows such effects to be included.

Due to their sensitivity to high and low temperatures, lead-acid batteries may experience problems if they are placed in high or low temperature environments.

The aim of this thesis is the simulation and modeling of lead-acid battery with software and its analysis.

When Gaston Plante invented the lead-acid battery more than 160 years ago, he could not have predicted that it would spawn a multi-billion dollar industry. Despite their seemingly low energy density – 30–40% of the theoretical limit versus 90% for lithium-ion batteries (LIBs) – lead-acid batteries are made from abundant, inexpensive materials and a non-flammable water-based electrolyte, while manufacturing methods that at a recycling rate of 99%, it significantly minimizes the environmental impact [35]. However, predictions of the demise of lead-acid batteries have focused on the health effects of lead and the rise of LIBs. The large gap in technological developments should be considered as an opportunity for scientific collaboration to extend the scope of lead-acid batteries to power grid applications, which currently lack a single energy storage technology with optimal technical and economic performance.

In principle, lead-acid rechargeable batteries are relatively simple energy storage devices based on lead electrodes operating in aqueous electrolytes with sulfuric acid, while the details of the charging and discharging processes are complex and efforts to improve their efficiency have It faces challenges. Lead-acid batteries are currently used in uninterruptible power modules, power grid and automotive applications, including all hybrid and LIB vehicles, as a stand-alone 12V source to support starting, lighting and ignition modules, As well as critical systems, in cold conditions and in case of high voltage battery failure.

Although the principle of operation has not changed, manufacturers have improved the technology by optimizing the performance of electrodes and active components, mainly for use in vehicles. Future performance goals include increasing material utilization through more efficient access to active materials, achieving faster recharge rates to further increase cycle life and calendar life, and reducing their overall life cycle cost with a direct impact on the performance of grid storage systems.

Despite the fact that lead-acid batteries have been on the market for over 165 years, many aspects of their performance are still partially or poorly understood. This is because the governing physical laws are a matter of high complexity involving numerous interrelationships, which can usually be ignored for a given range of conditions. Finding reasonable simplifications and useful assumptions to develop solutions that may significantly reduce the environmental footprint of our civilization is one of the main motivations behind this work.

The continuous dissolution and re-deposition of the cell's active materials during each charge-discharge cycle creates a situation where the morphology and microstructure of the positive and negative electrodes are constantly changing. These structural changes cause corrosion of the electrode grids, which are usually made of pure lead or lead alloys. -Calcium or lead-antimony are made and affect battery cycle life and material efficiency. Since such morphological evolution is an integral part of lead-acid battery performance, the discovery of its governing principles at the atomic scale may open new exciting directions in the fields of material design, surface electrochemistry, high-precision synthesis, and dynamic management of energy materials. to open Electrochemical interfaces This understanding can have a direct impact on battery life, as maintaining the overall electrode surface ensures efficient charge-discharge processes.

The complex relationship between the acid concentration gradient in the electrode pores and the dissolution rate of lead sulfate underscores the challenge of improving the battery's ability to recharge at rapid rates.

There are different ways to determine the parameter values for different

components in the battery circuit. One way is for example to measure in graphs that contain recorded data from battery tests and simulations, resulting in a set of parameters for each temperature and state of charge. Another way is to find equations for each parameter and then determine the constants in those equations by looking at the graphs from the battery test. The reason it is possible to search for parameters in the graphs is that some behaviors in the data are related to different parameters and are only visible in the simulation.

Energy storage systems based on rechargeable batteries exist directly or indirectly in the daily life of the majority of the population worldwide. They are used as a power source by consumer electronics, power tools, and wireless devices. Many of us cannot imagine life without them. In addition, they are also installed in fixed applications such as data centers, hospitals, telecommunications stations, wind farms and conventional as a backup power supply. Another large segment of the battery business is occupied by the motor segment, including conventional, hybrid and electric vehicles, wheelchairs, e-bikes, lift trucks and golf carts. Their role in moving towards more environmentally friendly energy production and consumption is huge and should not be underestimated.

In this research, the simulated battery is assumed to be healthy and the losses can be ignored after full charging. Discharge and charge of electrodes can be considered as dissolution in dilute solutions of lead ions and plating outside of it. Battery active materials can be recycled into forms suitable for reuse with minimal processing.

The questions of this research include whether other materials can be used in the structure of batteries? And also, can it be simulated and its effects evaluated? And compared it with existing batteries? Did you examine the effects of heat?

Research objectives

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Significance of research

It is a study and simulation of lead-acid battery modeling with organic materials, which is considered variable according to previous studies and materials and solvents. So that it's thermal behavior can be evaluated.

Conclusion:

In this thesis, by using simulation, the behavior of lead-acid battery was studied in different conditions. Modeling and simulation system was used to simulate lead- acid battery. In this method, the mathematical model including mass and energy equations, electrical circuits, and side parameters such as battery temperature and environmental conditions were used to simulate the lead-acid battery.

Lead-acid battery modeling in Comsol software can be used to better understand battery performance and identify potential problems. The results of this modeling can be used in the design and improvement of lead-acid batteries.

In this modeling, the lead-acid battery is considered as a two-electrolyte system. The positive electrolyte is sulfuric acid and the negative electrolyte is water. Oxidation and reduction reactions take place in the two electrodes of the battery.

The modeling results show that the electric potential at the boundary between the electrolyte and the electrode decreases with time. This reduction is due to the oxidation of lead at the anode and the reduction of lead sulfate at the cathode. Also, the concentration of lead sulfate in the electrolyte increases with time. This increase is due to the production of lead sulfate in the cathode. The results of lead- acid battery modeling in Comsol software can be used for the following:

Better understanding of lead acid battery performance Identification of possible problems with lead-acid batteries Design and improvement of lead acid batteries

In the following, some specific applications of lead-acid battery modeling results in COMSOL software are given:

Battery life prediction: Using the modeling results, battery life can be predicted.

This is especially important for batteries used in time-sensitive applications, such as electric vehicles.

Optimizing the battery design: Using the modeling results, the battery design can be optimized. This can lead to improved battery performance, reduced cost and increased battery life.

Diagnosis of battery problems: Using the modeling results, battery problems can be diagnosed. This can help prevent battery failure and reduce maintenance costs.

With the advancement of technology, lead-acid battery modeling in COMSOL software has become a powerful tool to better understand, design and improve this type of battery.

By simulating the lead-acid battery, the behavior of the battery was studied in different conditions. Finally, by analyzing the obtained results, we reached the following conclusions, the most important of which are:

- As the temperature increases, the efficiency of the battery decreases.
- Increasing the internal resistance of the battery reduces the power that can be extracted from the battery.
- As the intensity of the output current increases, the battery voltage decreases.
- As the usage time increases, the battery capacity decreases.

In general, the results obtained from the simulation of the lead-acid battery showed that the internal resistance, temperature, intensity of the output current and time of use are important parameters that should be considered in the design and use of the lead-acid battery. Also, these obtained results can provide great help to the designers and manufacturers of lead-acid batteries in optimizing and improving the efficiency of their lead-acid batteries.

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