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Computational Modeling of Positive Grid Structures in Lead-Acid Batteries and the Determination of Optimal Horizontal Bar Angles and Their Impact on Battery Service Life

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ABSTRACT : *The Lead-acid batteries are among the oldest and most widely used energy storage technologies, known for their reliability, low production costs, and ease of manufacturing compared to modern battery technologies. Despite significant advancements in energy storage solutions, these batteries continue to be widely used in various applications, including backup power systems, electric vehicles, industrial equipment, and renewable energy systems. Their stable performance, cost-effectiveness, and ability to operate in diverse environmental conditions make them a preferred choice for many industries. The performance and lifespan of lead-acid batteries are significantly influenced by several factors, with grid design playing a crucial role in determining the distribution and density of electric current. This distribution directly affects the rate of corrosion, as uneven current flow leads to localized degradation in different areas of the grid. Over time, this non-uniform corrosion reduces battery efficiency and contributes to its performance deterioration. Although previous studies have investigated the impact of tilting horizontal bars toward the lug, they primarily relied on arbitrary angle values without determining the optimal tilt angle. This study aims to bridge this knowledge gap by analyzing the effect of horizontal bar angles on battery performance and evaluating computational simulation results to derive the optimal values that enhance current distribution and minimize corrosion. Through this research, technical recommendations will be proposed to optimize grid design and improve battery efficiency, ultimately extending its service life and enhancing its reliability across various applications.*

KEYWORDS: Lead-acid batteries, Design and analysis of lead-acid battery grid, Horizontal bar angles, Operational and service life, Actual performance and deep discharge, Finite elements.

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I. INTRODUCTION

The basic composition of a lead-acid battery consists of two electrodes: a negative electrode made of pure lead (Pb) and a positive electrode composed of lead dioxide (PbO_2). These electrodes function together within an electrolyte solution of sulfuric acid. This configuration facilitates the electrochemical reactions that enable the battery to store electrical energy by converting it into chemical energy during charging and release it during discharge. Figure (1) illustrates the arrangement of these components within the battery. [1]

Research Problem Statement:

The grid is the fundamental component of the lead-acid battery and is often subjected to varying stresses due to repeated discharge and charge cycles. This can sometimes lead to corrosion, causing the active material to separate and resulting in the complete failure of the cell. Consequently, the battery's total voltage drops to 10 volts, and its effectiveness is lost.

The research problem is primarily summarized in the following points:

- Studying and analyzing the grid design to achieve the best distribution of voltage and current through the grid bars during discharge and charge cycles.
- In some cases, cell replacement may be necessary, which is very costly, and the issue could transfer to another cell, leading to the complete failure of the battery.
- Studying the variation of horizontal bar angles and their impact on current density, which may enhance grid efficiency in some cases but could also reduce it in others, making it essential to determine the optimal angle.

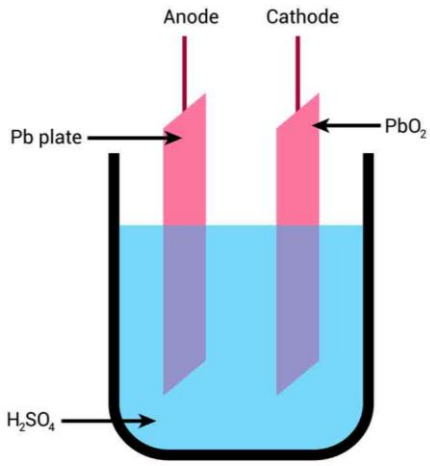

Figure (1): The electrolyte solution, with the lead-acid battery electrodes immersed in it.

Research Importance and Objectives:

This research aims to:

- Study the impact of grid design by analyzing the change in the angles of horizontal bars and the spacing between them on the distribution of voltage and current.
- Conduct initial simulations using Autodesk Inventor and COMSOL software to explore scenarios for current and voltage distribution.
- Find the optimal design that achieves the longest operational and service life for lead-acid batteries.

Research Methods and Materials:

- Study the working principle of lead-acid batteries.
- Design components using CAD software.
- Perform simulations for voltage and current distribution using COMSOL Multiphysics.
- Study and analyze designs to reach the optimal design that ensures the longest lifespan, best performance, and lowest cost.

Main Requirements for the Design Problem Under Study:

1. Design of the grid bar pathways.
2. Angles of the horizontal grid bars.
3. Lead mass used.
4. Distribution of voltage and current.
5. Battery lifespan.

After reviewing previous studies related to modifying the design of the lead-acid battery grid, it was found that cell modeling using the COMSOL platform allows for the analysis of current density [2]. Research also indicated that modifying the grid design directly affects the amount of metal used in the alloy [3], especially when changing the design of the grid bars, which in turn impacts the distribution of current and voltage density [4]. The operational purpose of the battery was considered, in terms of discharge and charge types and their speeds [5], in addition to linking these variables with the grid's corrosion rate [6]. Despite numerous studies addressing the impact of alloy components and their surface treatment [7], the design aspect has remained focused on the material costs of the manufacturing process [8]. However, the review showed that previous studies did not systematically address the effect of tilting the angles of the vertical bars or the spacing between them; instead, they limited their analysis to random value evaluations [9].

Boundary conditions for the study:

It is essential to define the boundary conditions and fix all parameters in the model before starting the study. Then, each parameter under analysis should be adjusted individually within the grid's structural design. This allows for a systematic analysis of the effects and a precise engineering correlation of the results, which contributes to reaching the optimal design.

Electrical Conductivity:

Electrical conductivity occurs due to the movement of positive and negative ions through the liquid. When two electrodes are immersed in the liquid, an electric current is generated, passing through it. In the case of direct current (DC), positive ions move in the direction of the electrical current, while negative ions move in the opposite direction.

The electrical conductivity of the liquid depends on the number of ions present and their mobility. The speed of the ions is influenced by the strength of the electric field, the mass of the ions, and other factors. Therefore, electrical conductivity can vary significantly between different liquids [10].

1. **Conductivity of Grid and Lug**

   Accepted Value: 4.8e6 [S/m]

Electrical conductivity represents the material's ability to conduct electric current, and it is the inverse of electrical resistivity. Pure lead has an electrical conductivity of approximately 4.8e6 [S/m]. Although this conductivity is lower than some metals like copper, it is considered sufficient in the environment of lead-acid batteries.

2. **Conductivity of Porous Electrode (Active Material)**

   Accepted Value: 9500 [S/m]

The porous electrodes in lead-acid batteries consist of lead dioxide (PbO_2) in the positive electrode and spongy lead (Pb) in the negative electrode. The electrical conductivity of these electrodes depends on their chemical composition and porous structure, which affects electron and ion transport.

3. **Conductivity of Electrolyte**

   Accepted Value: 90 [S/m]

The electrolyte in lead-acid batteries is a solution of sulfuric acid (H_2SO_4) in water. It plays a key role in ion transport between electrodes during charging and discharging processes. The conductivity of the electrolyte depends on the acid concentration and temperature. The electrical conductivity of the electrolyte ranges between 50 and 100 S/m under typical battery operating conditions, with the optimal sulfuric acid concentration around 4.2 - 5.0 mol/L. The chosen value of 90 S/m reflects a balance between electrical efficiency and minimizing undesirable side reactions.

4. **Electrolyte Volume Fraction**

   Accepted Value: 0.5

The electrolyte volume fraction represents the ratio of the electrolyte volume to the total volume of the porous medium within the grid. This parameter directly influences ionic transport and the rate of electrochemical reactions in a lead-acid battery.

In porous electrodes, the electrolyte volume fraction typically ranges between 0.3 and 0.6 to ensure a balance between ionic conductivity and energy storage capacity. The selected value of 0.5 reflects an intermediate state that provides a good distribution of the electrolyte while allowing sufficient space for the active material within the electrode.

5. **Density of Sites**

   Accepted Value: 1e-5 [mol/m^3]

This value represents the concentration of active sites that contribute to the electrochemical reaction at the electrode surface. The density of sites determines the reaction rate and the electrode's ability to exchange charges with the electrolyte.

This value depends on the nature of the active materials, such as lead dioxide (PbO_2) and spongy lead (Pb). Experimental studies typically use values ranging from 1e-6 [mol/m^3] to 1e-4 [mol/m^3], making the selected value suitable for representing electrode behavior under optimal operating conditions.

6. Equilibrium Potential

Accepted Value: 1.75 [V]

The equilibrium potential is the potential difference at chemical equilibrium between the two electrodes when no electric current is flowing. It is determined according to the basic electrochemical reactions in the battery. The equilibrium potential depends on the Nernst equation and the concentrations of the reacting chemical species. For lead-acid batteries, the typical equilibrium potential falls within the range of 1.7 - 2.1 volts. The chosen value of 1.75 volts reflects a realistic operating state during charging and discharging processes. The Nernst equation is an essential tool in electrochemistry used to calculate the electric potential of an electrochemical cell under non-standard conditions, i.e., when the ion concentrations in the solutions are unequal. This equation considers the effect of ion concentrations and temperature on the cell's electrical potential [11].

Nernst Equation Formula:

$$\ln Q \frac{RT}{nF} - E^0 = E$$

Where:

- **E** is the electrical potential of the cell at the specified concentration and temperature.
- **E°** is the standard electrical potential of the cell (at 25°C and standard ion concentrations).
- **R** is the universal gas constant (8.314 J/ (mol. K)).
- **T** is the absolute temperature in Kelvin (K).
- **n** is the number of electrons transferred in the chemical reaction.
- **F** is the Faraday constant (96485 C/mol).
- **Q** is the product of the concentrations of the products divided by the product of the concentrations of the reactants, taking into account the reaction coefficients (called the reaction quotient).

This equation helps in calculating the electrical potential of the cell under non-standard conditions, depending on the ion concentrations and the temperature, which affect the chemical reactions inside the cell.

Application of the Nernst Equation to the Lead-Acid Battery:

The lead-acid battery consists of two main reactions that occur at the electrodes:

- **At** the positive electrode (cathode):

$$2H_2O + 4PbSO \rightarrow -2e + 4H_2SO + 2PbO$$

- At the negative electrode (anode):

$$-2e + 4PbSO \rightarrow 4H_2SO + 2PbO$$

During the charging process, the reactions occur in the opposite direction. The Nernst equation is utilized to calculate the cell's electrical potential under specific operational conditions. If the concentration of sulfuric acid (H_2SO_4) and the temperature deviate from standard values, the resulting potential will be altered. For instance, if the sulfuric acid density, as measured by the hydrometer, is 1225, this indicates a higher acid concentration than the standard concentration. This variation in concentration will influence the value of Q in the Nernst equation, subsequently affecting the calculated electrical potential. [11]

7. Boundary Electrolyte Potential

Adopted value: 0 [V]

This potential represents the reference zero potential within the electrolyte at the battery boundaries. It is used as a reference for calculating potential differences within the system. The boundary electrolyte potential is typically set to 0 volts to facilitate a direct comparison of the electrical potentials of different components within the battery. This selection aligns with standard computational methods in numerical simulations.

8. Inward Electrode Current

Adopted value: - 100 [A]

The inward current represents the amount of charge flowing into the internal electrode of the battery, influencing the rate of electrochemical reactions and the battery's ability to deliver energy. The negative value indicates that the current flows from the electrode into the electrolyte (i.e., battery discharge). High currents, such as 100 amperes, are used in applications requiring high power, such as UPS systems or electric vehicles. This value represents the simulation of performance under high-load conditions.

9. Boundary Electric Potential Initial Value

Adopted value: 1 [V]

The initial boundary electric potential represents the starting value for numerical calculations to simulate voltage distribution in the battery. Typically, an initial value close to the open-circuit voltage (OCV) of the battery is chosen, which ranges between 1.8 to 2.1 volts under fully charged conditions. Selecting 1 volt allows for monitoring the gradual voltage change during the simulation, facilitating the analysis of the battery's electrical stability.

II. RESULTS AND DISCUSSION

Effect of Changing the Angles of Bars on Current Density Value:
Traditional Design:

The traditional design relies on perpendicular bars at 90-degree angles, which represent the initial configuration of lead-acid battery cells. To verify the obtained values, this design was modeled using Autodesk Inventor and then transferred to the COMSOL Multiphysics platform to analyze the maximum current density values and their distribution, as shown in Figure (2).

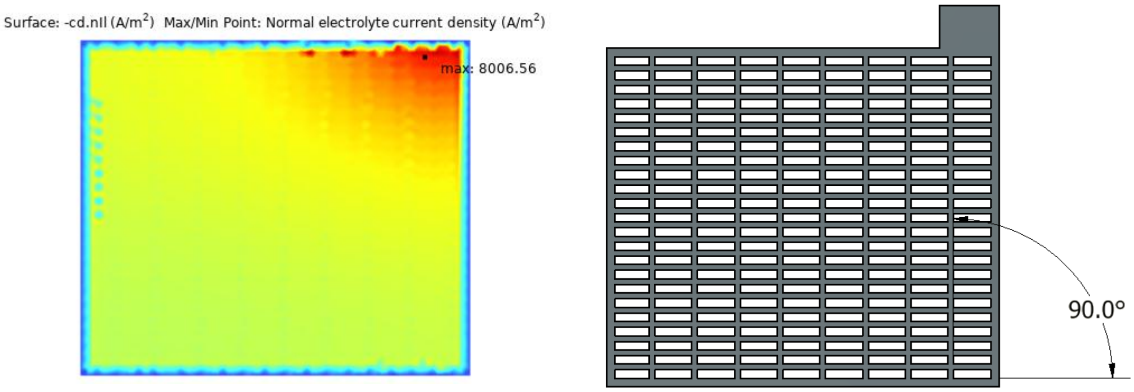

Figure (2): The conventional design and the current density analysis results in COMSOL Multiphysics.

The highest current density concentration is found to be **8006.56 A/m²**, which is located near the lug. This result indicates that the simulation closely replicates previous experimental behavior.

The Studied Design with Vertically Adjusted Bars at 76°:

It maintains the same constraints as the traditional design but differs in the inclination of the vertical bars, which are tilted at an angle of **76°** relative to the horizontal bars. In other words, the bars were inclined by 14° to investigate the effect of this tilt on current density. The model was developed using Autodesk Inventor and then transferred to the COMSOL Multiphysics platform to analyze the maximum current density values and their distribution.

A previous study analyzing various vertical angles showed that the maximum current density decreased to 6715.07 A/m², identifying 76° as the optimal vertical angle. In another study we conducted, we found that the optimal spacing between the bars is 13 mm. Based on these findings, further research will be conducted to examine the impact of varying horizontal bar angles on the modified design [12].

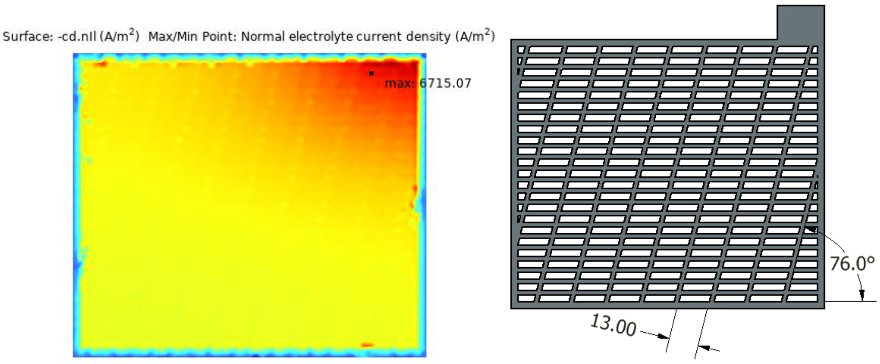

Figure (3): The modified design with vertical bars at a 76° angle and the current density analysis results on the COMSOL Multiphysics platform.

The conventional design relies on horizontal bars that are parallel to the horizon and perpendicular to the vertical axis at a 90° angle.

Based on this, a modified design with vertically inclined bars at angles of (90, 85, 80, 75, 70, and 50) degrees, respectively, and a vertical bar spacing of 13 mm was selected. The models were designed using Autodesk Inventor and then transferred to the COMSOL Multiphysics platform to analyze the maximum current density concentration and its location.

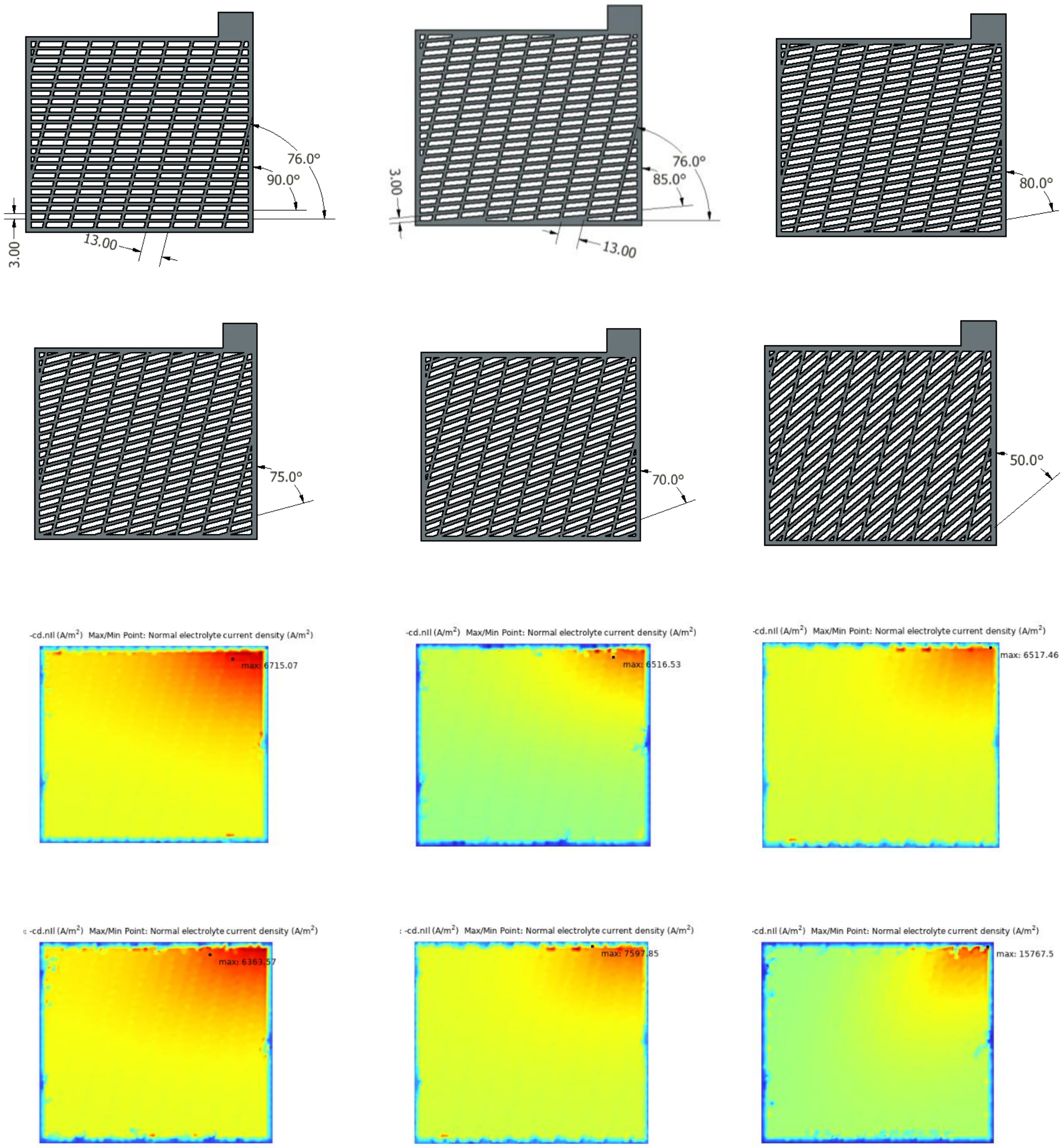

Figure (4) Analysis results of current density values for the designs within the COMSOL Multiphysics platform.

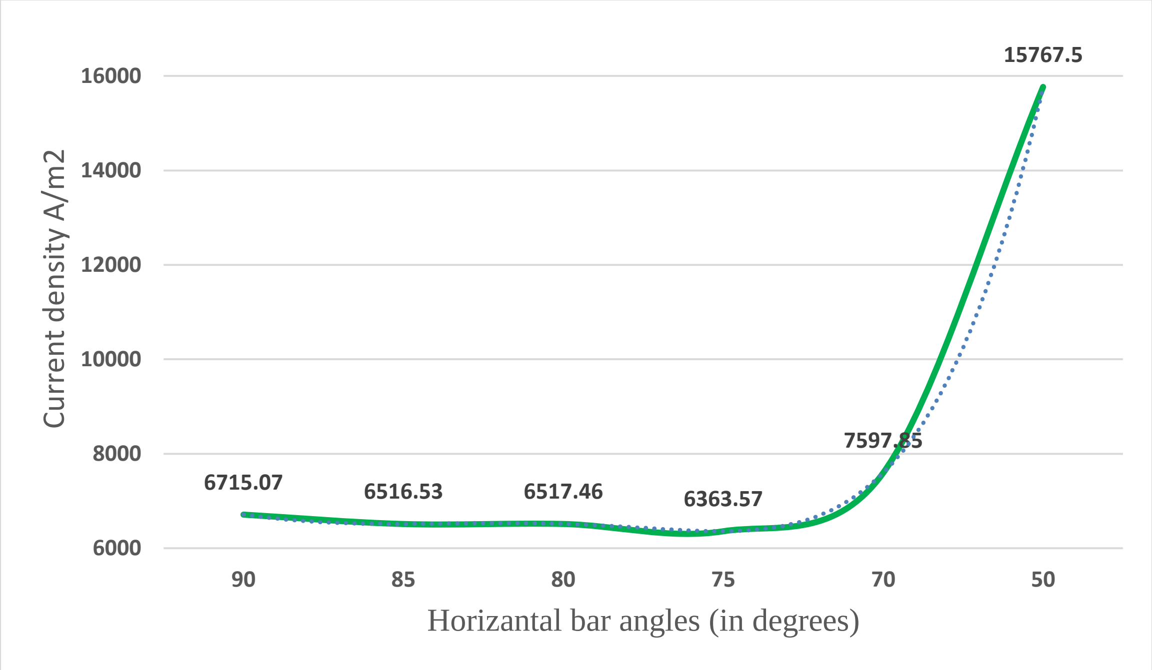

Figure (5) Graph of the relationship between the horizontal bar angles of the lead-acid battery grid and the current density values.

By representing the previous results in a graphical chart shown in Figure (5), the following points are recorded:

- At an angle of 75 degrees, a decrease in current density concentration is observed, reaching a value of **6363.57 A/m²**, indicating increased stability and reduced current density concentration towards the lug.
- As the angle decreases beyond 70 degrees, the maximum current density increases and becomes more concentrated towards the lug.
- From the plot, it can be inferred that the 75-degree angle, according to the trend line, may not be the optimal value. Therefore, a more precise study with smaller increments will be conducted, considering the following angles: 74°, 75°, 76°, and 77°.
- The models were designed using Autodesk Inventor and then transferred to COMSOL Multiphysics to analyze the maximum current density values and their distribution.

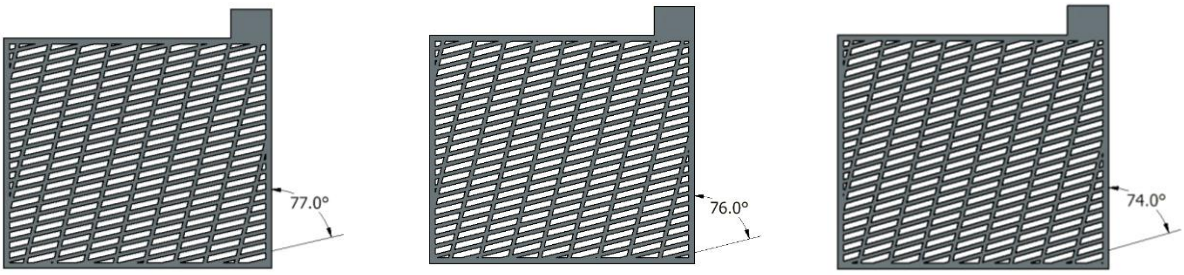

Figure (6): Designs of the models with variations in the horizontal bar angles within a smaller range.

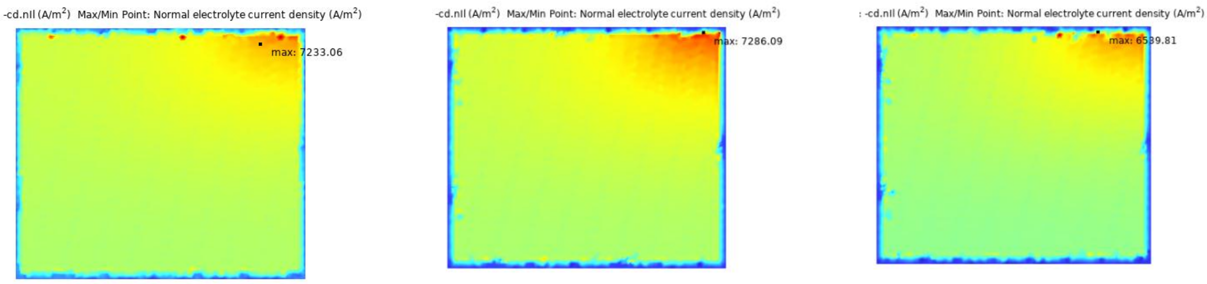

Figure (7): Analysis results of current density values for the designs using COMSOL Multiphysics.

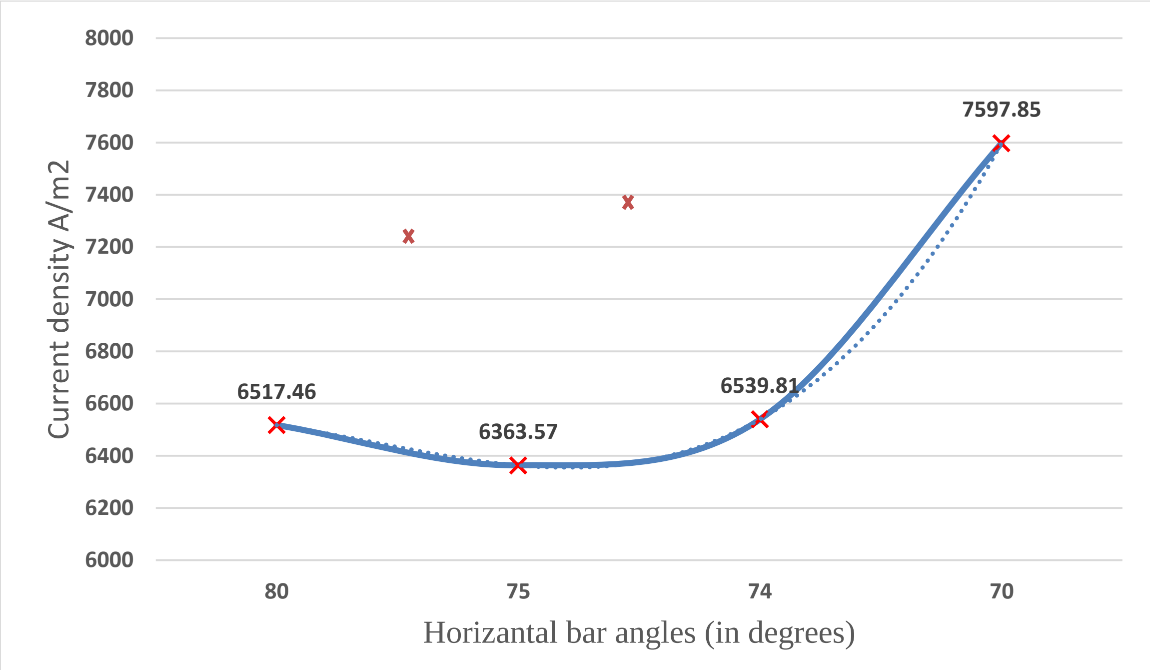

Figure (8): Graph depicting the relationship between the horizontal bar angles of the lead-acid battery grid and the corresponding current density values.

By representing the previous results in the graphical plot shown in Figure (8), the following points are recorded:

- At an angle of 75 degrees, a decrease in current density is observed, reaching 6363.57 A/m², indicating increased stability and reduced current density concentration towards the lug.
- Thus, the optimal angle for the inclination of the horizontal bars relative to the vertical frame of the lead-acid battery grid is 75 degrees, as it results in the lowest current density concentration.
- The current density values increase significantly at angles 76° and 77°, and these values can be considered as outliers.

III. CONCLUSION AND RECOMEDATIONS

Conclusions:

1. A computational model was developed that simulates the real model of lead-acid batteries available in Syrian markets using reverse engineering.
2. Understanding the physical and chemical model and the function of the design before starting reverse engineering significantly improves the accuracy of the obtained results.

3. The optimal parameters for the grid (based on experimental inputs) were determined as follows:

Table (1) shows the optimal values for the model.

Grid Parameter	Optimal Value	Grid Parameter
Vertical bar angle	76°	6715.07 A/m²
Horizontal bar angle	**75°**	**6363.57 A/m²**

4. The traditional design does not meet the requirements for deep discharge and household use.

Recommendations:

1. Study alternative designs to achieve an optimal model that meets deep discharge requirements.
2. Investigate a manufacturing method that ensures the proper positioning of the lug in the center without assembly issues.
3. Analyze the effect of antimony content in the lead alloy to determine the optimal percentage for maximizing operational lifespan while minimizing costs.

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