Computational Optimisation of Battery Grid for Efficiency

and Performance Improvement

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Abstract

Battery is a critical system used in automobile, renewable energy, medical devices and mobile phones. Research efforts are directed to increase energy density, longevity and reduce the cost. This paper is related to computational optimisation of lead acid battery for efficiency and performance improvement. Battery grid is the precursor for the active material and current distribution in lead acid electrochemical cell. Battery grid are made by casting or expanded metal process. Configuration of the grid is critical for minimising ohmic drop, uniform current distribution and for more reaction sites. The governing transport mechanism for the electrochemistry of lead-acid battery is due to migration, diffusion and convection molar flux of charged species(j) and for this simulation COMSOL battery and fuel cell module is leveraged. The battery grid performance is governed by ionic transport mechanism and hence the Primary Current Distribution interface is used. The positive grid was used for the optimisation with the electrode, electrolyte and porous electrode. The volume fraction of the electrode, current density, electrode potential and total power dissipation density are monitored for performance comparison. The current density is correlated to corrosion resistance and long life cycle time. These investigations highlight the potential of Computational Electromagnetic (CEM) and electrochemistry simulations for innovative battery design.

1. Introduction

Batteries are classified based on the electrochemistry. Primary Disposable Batteries type includes, Zinc carbon, zinc chloride, Lithium, Silver, mercury oxide and Zinc air. The Secondary Rechargeable Batteries includes, Nickel cadmium, Nickel metal hydride, Alkaline, Lithium ion, Lithium ion polymer and Lead acid. Lead Acid battery, although a two hundred years old

technology, is the workhorse of the industry. Battery grid is the precursor for the active material and current distribution in lead acid electrochemical cell. Battery grid are made by casting or expanded metal process. Configuration of the grid is critical for minimising ohmic drop, uniform current distribution and for more reaction sites. The current density is related to corrosion resistance and long cycle time of battery performance [1]. Computational Electromagnetic (CEM) and electrochemistry simulations are increasing used for battery design and performance enhancement [2,3]. In this paper, a standard grid and new optimised grid system is modelled for performance comparison.

1.1 Working Principle of Lead Acid Battery

The storage battery or secondary battery is such battery where electrical energy can be stored as chemical energy and this chemical energy is then converted to electrical energy as when required. The conversion of electrical energy into chemical energy by applying external electrical source is known as charging of battery. Whereas conversion of chemical energy into electrical energy for supplying the external load is known as discharging of secondary battery. Lead-acid batteries are composed of a Lead-dioxide cathode, a sponge metallic Lead anode and a Sulphuric acid solution electrolyte. This heavy metal element makes them toxic and improper disposal can be hazardous to the environment.

1.2 Discharge

During discharge, the lead dioxide (positive plate) and lead (negative plate) react with the electrolyte of sulfuric acid to create lead sulfate, water and energy.

1.3 Charge

During charging, the cycle is reversed: the lead sulfate and water are electro-chemically converted to lead, lead oxide and sulfuric acid by an external electrical charging source.

The key components of lead acid battery are positive and negative electrode grid, active material, electrolyte and the enclosure.

2. CEM Formulation and Simulations:

For the battery performance evaluation, a symmetrical segment of the positive electrode grid, active material and electrolyte is used. Fig 1 and 2 shows the CAD model of the standard grid and the new optimised grid, respectively. The governing transport mechanism for the electrochemistry of lead-acid battery is due to migration, diffusion and convection molar flux of charged species(j) and for this simulation COMSOL battery and fuel cell module is leveraged. For the grid design, the Laplace equations can be used to model ionic transport performance. Appropriate Electrode equilibrium potential is used in the simulation. COMSOL Primary Current Distribution interface for the battery is used for the CEM simulations. The governing equation for the battery performance simulation is given below.

$$N_{j} = -z_{j}\mu_{j}FC_{j}\nabla \emptyset - D_{j}\nabla C_{j} + C_{j}\nu$$
$$\nabla_{i} = \sigma \nabla^{2} \emptyset$$
$$\nabla^{2} \emptyset = 0$$
$$\eta = E - E_{e} - \emptyset$$

Where N_j is iconic flow, Z_j is charge, D_j is the diffusion coefficient. μj is ionic electrochemical mobility, F is the Faraday's constant, c_j is the concentration, is electrostatic potential outside the electric double layer,



Fig 1. CAD Model of the standard grid



Fig 2. CAD Model of the new grid

2.1 Boundary conditions:

Fig 3 shows typical FEA mesh and boundary conditions on typical new optimised grid design. A discharge current of 100 A is applied to the end of the lug. The primary current condition, relating the electrolyte and electrode potentials is set to the equilibrium potential of 1.7 V.The potential in the electrolyte is set to zero at the external boundary that is parallel to the grid.



Fig 3. Typical FEA mesh and Boundary conditions

3. COMSOL multiphysics Simulation Results:

The Area fraction of the standard and optimized new battery grid is maintained at the same area/ volume fraction at 0.32f. The fig 4 and fig 5 shows the contour plot of electric potential. The fig 4. of standard battery grid that has electric potential of maximum and minimum values of 1.68 (V) and 1.52(V) respectively. The optimized design of the battery grid that possess maximum and minimum values of electric potential 1.66(V) and 1.56(V) respectively shown in fig 5. Table 1 shows the summary of electric potential results.

Fig 6 and fig 7 shows the contour plots of the electrolyte potential of standard and new optimized battery grid. The range of electrolyte potential of standard and new optimized battery grid, is 0.16 and 0.10 respectively. Table 2 shows the summary electrolyte potential results.





Fig 4. Electric Potential (V) of standard battery grid



Fig 5. Electric Potential (V) of new battery grid

Table 1

Electric Potential (V)	Max	Min	Range
CASE 1	1.68	1.52	0.16
CASE 2	1.66	1.56	0.10

Surface: Electrolyte potential (V)



Fig 6. Electrolyte Potential(V) of standard battery grid

Surface: Electrolyte potential (V)



Fig 7. Electrolyte Potential (V) of new battery grid

Table 2

Electrolyte Potential (V)	Range	
CASE 1	0.16	
CASE 2	0.10	

The contour plots of electrode current density of standard and new battery grid is shown in fig 8 and fig 9 with values of maximum 1.74E+07 (A/m²), $7.52E+06(A/m^2)$, minimum 1190 (A/m²), 2630 (A/m²) respectively. The range values for Standard and new grid are 1.74E+07 and 7.52E+06 respectively. Table 3 shows the summary of electrode current density for both the grid designs.



Fig 8. Electrode current density (A/m²) of standard battery grid



Volume: Electrode current density, norm (A/m²)



Fig 9. Electrode current density(A/m^2) of new battery grid

Table 3

ECD (A/m ²)	Max	Min	Range
CASE 1	1.74E+07	1190	1.74E+07
CASE 2	7.52E+06	2630	7.52E+06

The total power dissipation density of standard and new battery grid is compared for their efficiency and performance improvement. The maximum, minimum values of standard and new battery grid with 6E+07(W/m³), 1(W/m³) and 1.4E+07(W/m³), 0.2(W/m³) respectively shown in fig 10 and fig 11. Table 4, shows the total power dissipation density of standard and new battery grid results.



Fig 10. Total power dissipation density(W/m³) of standard battery grid



Fig 11. Total power dissipation density (W/m³) of new battery grid

Table 4

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TPDD (W/m ³)	Max	Min	Range
CASE 1	6E+07	1	59999999
CASE 2	1.4E+07	0.2	13999999.8

4. Results and Discussion

The electrode current density simulation results of the standard rectangular and the optimised grid configurations, are shown in fig 11 and 12, respectively. The optimised grid configuration shows 57% reduction in current density. Similarly, 76% reduction in Total Power Dissipation density is observed for optimised grid configuration.



Fig 12. The electrode current density (A/m^2) of standard battery

Volume: Electrode current density, norm (A/m²)



Fig 13. The electrode current density(A/m²) of new optimized battery grid

5. Conclusions

A brief introduction to the battery was given. The computational electromagnetics (CEM) formulation, battery performance modelling method, assumptions and input boundary conditions were detailed. The details of standard grid and new optimised grid configuration was provided. The CEM simulation results were reported. The electrode potential, electrolyte potential, electrode current density and the total power dissipation density are reported. The simulation results demonstrated that the new optimised grid shows significant reduction in electrode current density and the total power dissipation density. The electrode current density reduction can be correlated to reduction in corrosion resistance and increase in practical life cycle time of the battery. The computational electromagnetics (CEM) based battery performance modelling method showed insight into battery physics for performance optimization. These investigations highlight the potential of CEM and electrochemistry simulations for innovative battery design.

6. References

[1] Handbook for Stationary Lead-Acid Batteries, Part 1: Basics, Design, Operation Modes and Applications, Handbook (part 1) - 1 - Industrial Power, Application Engineering, Edition 6, February 2012.

[2] "The Effect of Grid Configuration of Potential and Current Density Distributions in Positive Plate of Lead-acid Battery Via Numeric Modelling", D Nakhaie, PH Benhangi, A Alfantazi, A Davoodi Electrochimica Acta 115, 189-196, January 2014.

[3] "Finite Element(FE) Modelling of Current Density on Valve Regulated Lead Acid Battery Positive Grid", RJ Ball, R Evans, R Stevens Journal of power sources 103 (2), 213-222, January 2002.

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