Performance of Lithium and Sodium Ion Batteries and their Efficiencies

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Kellog Honors College Capstone Project

CPP Student RSCA Conference 2024

I. Introduction

<u>Do you know any common household appliances that use lithium ion batteries?</u>

High reliance on lithium ion batteries, however sodium ion batteries could provide a better alternative.

<u>Applications</u> of this project seeks to enhance functionalities of existing Lithium ion batteries and explore Sodium-based batteries due to this greater abundance and economic viability. As society relies on portable electronic devices and renewable energy sources, optimizing battery performance becomes crucial.

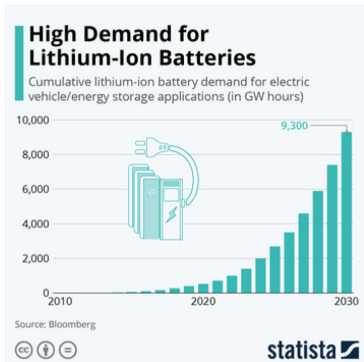

Figure 1: High Demand Usage for LIBs chart from statista.com

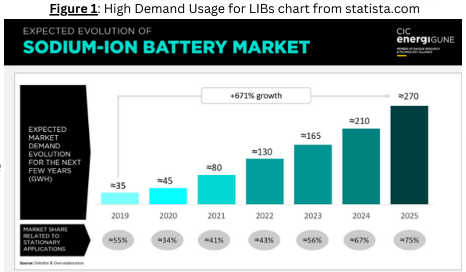

Figure 2: Projected SIB usage from cicenerygigune.com

<u>Industrial Innovation:</u> Exploration of SIB, positions itself as a potential next-generation industrial innovation, Typically have a lower environmental impact compared to LIBs.

<u>Electric Vehicles</u>: While LIBs dominate market, SIBs are being researched, abundance and lower cost of sodium make it an attractive alternative, sustainable and cost-effective

II. Objective

To conduct product design focusing on screening and optimizing various elements/ parameters to enhance performance of batteries.

Dielectric Constants, Valence Types, Molecular Weight

III. Background

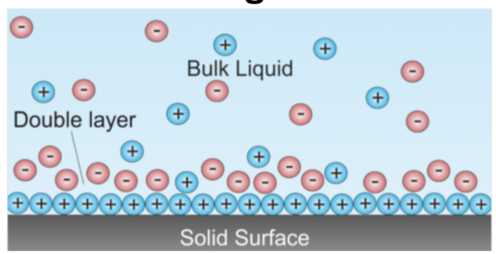

Figure 3: Electric Double Layer Charge Distribution

Guoy-Chapman Theory: describes electrical double layer; distribution of charges at interface between an electrolyte solution and a charged interface

$$\sinh\left(\frac{ze\phi(x)}{4kT}\right) = \sinh\left(\frac{ze\phi_s}{4kT}\right) \cdot \exp\left(-\frac{x}{\lambda}\right)$$

- $\phi(x)$ is the electrical potential at a distance x from the charged surface,
- ϕ_s is the potential at the surface,
- k is the Boltzmann constant,
- T is the temperature,
- e is the elementary charge,
- z is the ion valence,
- λ is the Debye length.

Debye Hückel Theory: measure of how far electric fields can penetrate into an electrolyte solution, predicts behavior of charged particles in a medium

$$\lambda_D = \left(\frac{\varepsilon \cdot k \cdot T}{n \cdot e^2}\right)^{1/2}$$

- λ_D is the Debye length,
- ε is the permittivity of the medium,
- n is the number density of ions in the medium.

Bjerrum Length: represents the distance at which the electrostatic interaction energy between two elementary charges equals the thermal energy; i.e. stability

$$\lambda_B = \frac{e^2}{4\pi\varepsilon\varepsilon_0 kT}$$

- λ_B is the Bjerrum length,
- ε_0 is the vacuum permittivity,

Linearized Guoy-Chapman Theory: provides approximation for the electrical potential as a function of distance from the charged surface, key assumption that the electric potential and ion concentrations near charged surface are small. Used Taylor series expansion

$$\phi(x) = \frac{2kT}{e}\ln\left(\cosh\left(\frac{ze\phi_s}{4kT}\right)\right) - \frac{ze\phi_s}{2}\tanh\left(\frac{ze\phi_s}{4kT}\right) \cdot \frac{x}{\lambda}$$

III. Results

Sodium: NaClO4 in Ethylene Chlorate

Lithium: LiPF6 in Propylene Carbonate

Figure 4: MATLAB Code

```
clear
%==========================================================================
%  <<For Electric Double Layers at Battery Electrodes>>
%!  Linear Gouy-Chapman Calculations for Electric Double Layers:
%  (1) Calculate the Debye inverse length: kappa
%  (2) Calculate the surface potentials: beta.e.PSI(0)
%==========================================================================
%...(1)  Calculate Debye Inverse Length for NaCl Solutions
%==========================================================================
%      real*4 M,k,Ion,kappa,kappa2,Ionic,kappal,kappaxdA
%      character ntitl(10)
%      dimension M(6),d(6),c(6),rhop(6),rhom(6),Ion(6),kappa(6)
%      dimension sigmS(6)
%     data M/0.1,0.2,0.32,0.50,0.80,1.2/
%     data d/1.000115,1.00519,1.00998,1.0708,1.02865,1.04365/
%      data sigmaS/0.056/
%     open (15,file='Debye.txt',status='unknown')

%!...                 Input data
      e= 1.60206e-19                    %Coulomb of unit electron
   em= 78.358*111.2e-12 %permittivity of water at 25oC.  C^2/(N.m^2)
   k= 1.38054e-23                %Boltzmann constant. J/K
   T= 298.15                     %Kelvin
   zp= 1.0                             %Valence cation
   zm=-1.0                             %Valence anion
   WNaCl= 23.0+35.45        %Molecular weight of NaCl
   pi=3.14192653589793
%!...                 Calculation of Parameters
%...                        Bjerrum length (1 meter= 1.0e+10 Angstroms)
      B= e*e/(em*k*T)*1.0e+10  % B in units of Angstroms
%    print *, 'Bjerrum length, B=',B,' Angstrom'

%     Write(15,"('Bjerrum length:B=',g12.5,'  Angstrom')") B
%...                        Basis: 1000 g of pure water
%     write (15,"(//, ' beta.e.PSI    at   c(M)    sigma*')")

%6   format (i4,4f10.4)
```

```
%==========================================================================
%...    Calculate Electrostatic Potential, PSI , on EDL
%        By the Linear Gouy-Chapman Eq.
%         beta.e.PSI = 4pi  (B/d)*(sigma*)/(kappa*d)
%==========================================================================
%...                     Parameters for EDL
   dA= 3.0                                      %Diameter ion, Angstrom
   T= 298.15                               % Kelvin
      sigmaS= 0.0562                            % Reduced surface charge density:
sigma*dA^2/e
   cM= 0.1
%!...                    Bjerrum reduced B/dA
   BdA= B/dA       % B/diameter= dimensionless B
%     print *,' B/dA', BdA,', B(A)=',B
%...          Find kappa
      rhp= cM*6.022e-01/1000.                                   %Cation number
density, 1/A3
   rhm= cM*6.022e-01/1000.                                     %Anion number
density, 1/A3
   Ionic= 0.5*(rhp*zp^2 + rhm*zm^2)                  %Ionic strengths, 1/A3
   kappa2= 8.0*pi*B*Ionic                                     %Debye kappa^2=
8.pi.B.I, 1/A2
   kappal=sqrt(kappa2)



%                      Dimensionless kappa = kappa*dA
      kappaxdA=  kappa1*dA
%     print *,'kappa=',kappal,', kappa*dA=', kappaxdA,', dA=',dA
%    Calculate betaePSI
%         beta.e.PSI(0) = 4pi  (B/d)*(sigma*)/(kappa*d)

      betaePSI= 4.0*pi*BdA*sigmaS/kappaxdA
%     print *,'*** Beta.e.PSI=', betaePSI,', at      cM=',cM,'S*=',sigmaS
%     Write(15,"('beta.e.PSI=',3g12.4)") betaePSI,cM,sigmaS
%    stop
%    end
```

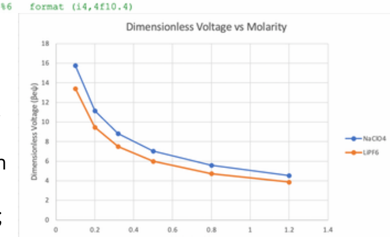

Figure 5: Dimensionless Voltage vs Molarity Graph

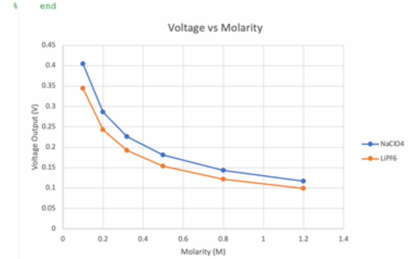

Figure 6: Corrected Unit Voltage vs Molarity Graph

Discussion: Sodium State Batteries showed higher electric potential by around ~18%. Sodium has larger atomic weight than Lithium, allows for greater separation of charge in anode and cathode, potentially leading to higher voltage. Redox potentials of sodium materials may be more favorable than those of lithium-based. Sodium-based batteries use different anode and cathode materials than lithium-based batteries.

Conclusion: Through this project, I was able to apply these 3 theories and formalize a code to compare Lithium and Sodium State Batteries. These theories are very limited as there is so much more research and testing needed to fully compare and ensure fair environments for both batteries. As we strive for advancements in battery technologies, particularly in comparing different elements like lithium and sodium, this project serves as a stepping stone. Understanding the complexities of battery performance is crucial for the development of more efficient and sustainable energy storage solutions. I thank Cal Poly Pomona and my advisors that I was able to have this opportunity to further my knowledge into my true passion which is sustainable development.

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