International Journal on Recent and Innovation Trends in Computing and Communication
ISSN: 2321-8169 Volume: 11 Issue: 11
***Article Received:** 10 September 2023 **Revised:** 20 October 2023 **Accepted:** 30 October 2023*

Comparative Performance Analysis of Different Cathode materials of Solid State Lithium ion Battery

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Abstract: In this paper , a single dimensional solid state lithium(Li)-ion batteries are simulated at different C-rates to analyze the characteristics like discharge curves, electrolyte potential along the thickness of electrolyte and variation of concentration along the electrolyte and positive electrode by using multi-physics simulation software tool, COMSOL. Li-ion batteries can be designed with different cathode materials but every material has its own advantages and disadvantages along with their applications. So, the main focus of this paper is to compare the characteristics of different cathode materials of Li-ion battery at different C-rates with similar design operating parameters.

Introduction:

Due to lowest weight of Lithium (Li) and its high energy density, Li –ion battery with liquid electrolyte was successfully implemented in consumer electronics, hybrid vehicles applications, etc. The performance of battery depends on its operating conditions like load current, internal temperature raise, etc. So battery performance has to analyze at every instant of its operation which can easily done by modeling tools. Dubarry M, Liaw [1] proposed the universal modeling tool to analyze the Li-ion batteries. Li-ion batteries can easily implement to consumer electronics and for low power applications without any hurdles. But , in high power applications like EVs [2],[3]and power grid storage systems, many Li-ion batteries are connected in combination of series and parallel. The different internal resistance of the batteries and minute internal chemical changes of the batteries could not operate satisfactorily. So a special circuitry is needed for monitoring the batteries at high power applications. Lul, Han X et al [4] presented a detail review on the key issues of Li-ion batteries working for high power applications. The key reason for looking to alternative energy resources is not only for global warming but also for preserving of fossil fuels and unable to recycle them. So recycling of used materials is also an attractive branch of science in the research world. To preserve the Li-ion deposits for future, Sonoc A et al [5] gave a review on recycling of Li-ion batteries to recover Li and other materials like cobalt (Co), Titanium (Ti),etc. Li-ion batteries are manufactured at prescribed conditions like temperature and pressure to avoid its reaction with the environmental gases. It will easily react with environment and extinguishes as fast as possible. So sufficient safety measures has to take at manufacture and packaging levels and recycling as well. Arora A et al [6] and Lisbona D et al [7] and Pistoia G [8] proposed different safety measures that has to be taken for Li-ion batteries especially at manufacturing and for EV application level. Liquid electrolyte Li-ion batteries has a limitation of risk of extinguishing at the over load conditions like high C-rates. Gray M et al [9] introduced the usage of polymer in place of liquid electrolyte to overcome mentioned limitation. The polymer Li-ion batteries have higher energy density than liquid electrolyte Li-ion batteries. If the battery management system is failed to monitor the batteries behaviour in battery back there is a chance of some batteries get overcharged during charging.

The study of effect of overcharging battery in pack is also needed at the time of designing the battery pack for the applications like EVs and power grid storage systems. Leising RA et al [10] proposed the method of analysis the overcharge reaction of Li-ion batteries for various applications. Polymer electrolytes are not complete solid electrolytes although they overcome the limitations of liquid electrolytes but their performance also affect at high temperatures and high C-rates. Solid electrolyte successfully overcomes the limitations of polymer electrolyte, called solid state batteries. Kotobuki M et al [11] explained the need of all solid state batteries for future energy store systems which mainly attracts its high energy density. Tadaka L et al [12], Weppner W[13] and Baggetto L

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et al [14] explained recent progress in the solid state batteries to extend their applications for high power applications. They majorly focus on improvement of ionic conductivity through solid electrolytes. Oudenhoven JFM et al [15] suggested some techniques for improving ionic conductivity by micro structures called micro batteries. The nonlinear systems are analyzed by using equivalent electric circuit parameters which are linear in nature. Many researchers suggested renewable energy generation such as wind, solar, tidal, etc for controlling the global warming which are generated at off peak load conditions. These can successfully connected to the grid by storing the generated energy. Swierczynski M et al [16] proposed an analysis of synchronizing the wind power generation to the grid by energy storage with Li-ion batteries. The working of the designed energy storage systems can be analyzed by proper modeling. Yann Liaw et al [17] proposed a simple equivalent circuit model for Li-ion battery for analysing the open circuit voltage (OCV) of battery which is used for EV application. The simple equivalent circuit model could not reflected complete internal operation of batteries which have majorly effects with chemical imbalances. Developing of mathematical equations to address the operation of batteries at different load conditions would project the way to analyze their working. Doyle M and Newman J [18] and Gomadam PM et al [19] proposed the use of mathematical modeling of Li-ion polymer batteries and nickel cadmium batteries at designed level which can use to analyze them further. By successfully implemented the designed battery to the required application, monitoring of its characteristics such as state of charge (SOC), terminal voltage of the battery is also a major challenge. Rong P et al [20] and Jagannathan M et al [21] proposed the modeling of Li-ion battery to predict the remaining capacity of the battery during its operation called analytical modeling of Li-ion battery. The models which are proposed until took some assumptions which majorly ignore small chemical imbalances at time of heavy load conditions of the battery. So a model which covers all the physics of the system such electrical, chemical, thermal, etc has to use to analyze the battery. Allu S et al [22] introduced a new computational frame work for solving high complex systems called multiphysics simulation. Nesro MS et al [23] proposed the method of implementing the all solid state batteries in COMSOL, which is simplified multiphysics simulation tool. Alex Bates et al [24] are used COMSOL multiphysics to simulate the two dimensional lithium ion battery with different operating parameters. The literature which is described in the foremost portion has covered all basics of primary and secondary batteries, methods of analysis tools like analytical, mathematical and electrochemical etc and the safety concerns on lithium batteries. Major applicable areas of secondary batteries and their analysis tools like equivalent electric circuit models are also discussed in the literature. Latest simulation tools for analyzing the solid state batteries like COMSOL also included in the literature. But to extend the EV usage at different application like commercial, domestic and agricultural etc, the need of designing the batteries for different applications with different materials is necessary. Every material has its own proms and corns, but the knowledge of usage of particular materials for particular application is needed. In this review process it is observed that the simulation of solid state batteries for different operating conditions with different cathode materials are not included which is majorly used to understanding the behavior of solid state batteries for EV applications. The direct replacement of commercial vehicles with e-vehicles is also not appreciable. The latest technological developments in the e-vehicle cannot show the right cause of replacing the commercial vehicles with EVs. So by gradually decreasing of commercial vehicles, implementation of EV has to achieve. By implementing the technological developments in electrical energy generation, battery materials, suitable drive system along with battery management system, EV will be the solution for reducing the global environmental pollution. The important challenges faced by the e mobility services are its mileage (Km/ charge), so the performance of the e-vehicle is majorly depended on discharging behavior at different rate conditions. The significance of the C-rate of the battery is the load to the battery.

The practical load of the EV battery is road conditions. So the main aim of this paper is to simulate the solid state battery at different C-rate conditions along with different cathode materials. The complete analysis is carried out in COMSOL multiphysics environment. In COMSOL there is a provision to customize the battery parameters at different C-rate conditions with inbuilt electro-chemical equations

II. Types of Cathode Materials of LI-ion battery

The energy density of the Li-ion battery got attention from the researchers and scientists for implementing in EV application which has severely struggled for energy density for its broad applications. Another motivation for selecting Lithium (Li) is its lightest weight, the design of higher energy density batteries can be possible. Li-ion battery can be designed with different materials like Iron (Fe), Aluminum (Al), Cobalt (Co), Nickel (Ni), Manganese (Mn) and etc. In this work, the battery is designed with LiCoO2 (LCO) as negative electrode Lithium Iron Phosphate (Li3FePO4) (LPO) as an electrolyte and Li metal as a positive electrode is selected.

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Table 1. Half cell and overall chemical reactions of different cathode materials of LI-ion battery.

S.No	Type of Battery	At Anode	At Cathode	Overall Reaction
1.	LCO	$Li \rightarrow Li^{+} + e^{-}$	$CoO_2 + Li^{+} + e^{-} \rightarrow LiCoO_2$	$Li + CoO_2 \rightarrow C_6 + LiCoO_2$
2.	LMO	$Li \rightarrow Li^{+} + e^{-}$	$Mn_2O_4 + Li^{+} + e^{-} \rightarrow LiMn_2O_4$	$Li + Mn_2O_4 \rightarrow C_6 + LiMn_2O_4$
3.	LFP	$Li \rightarrow Li^{+} + e^{-}$	$FePO_4 + Li^{+} + e^{-} \rightarrow LiFePO_4$	$Li + FePO_4 \rightarrow C_6 + LiFePO_4$
4.	NMC	$Li \rightarrow Li^{+} + e^{-}$	$Ni_{1/3}Mn_{1/3}Co_{1/3}O_2 + Li^{+} + e^{-} \rightarrow LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$	$Ni_{1/3}Mn_{1/3}Co_{1/3}O_2 + Li \rightarrow LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$
5.	NCA	$Li \rightarrow Li^{+} + e^{-}$	$Ni_{0.8}Co_{0.15}Al_{0.05}O_2 + Li^{+} + e^{-} \rightarrow LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$	$Ni_{0.8}Co_{0.15}Al_{0.05}O_2 + Li^{+} \rightarrow LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$

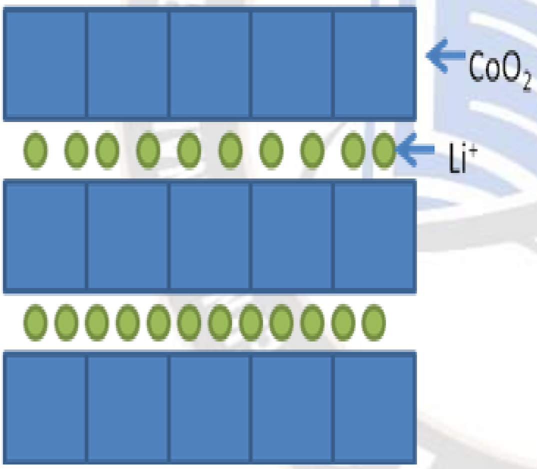


Fig 1: Two Dimensional layered Crystal structure of CoO_2 along with Li ions during Charging of Li-ion battery.

The ionic transportation in the electrolyte is in one dimensional so it is called one-dimensional battery and since positive electrode, negative electrode and electrolyte are solid materials so it is called all solid state batteries. Finally, these type batteries are called one dimensional all-solid-state Li-ion batteries.

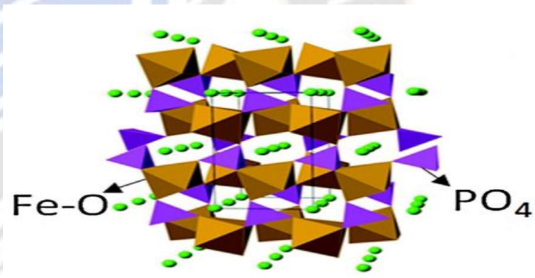


Fig 2: Three Dimensional Olivine Crystal structure of $FePO_4$ with Li ion during Charging of Li-ion battery

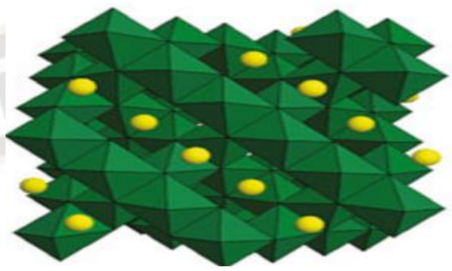


Fig 3: Two Dimensional Spinel Crystal structure of Mn_2O_4 with Li ion during Charging of Li-ion battery.

The important reason behind to select those materials as the electrodes and electrolyte are because of their crystal structure, safety, and availability. LCO has to accumulate the Li^{+} ions in its lattice at the time of charging and it provides the same at discharging process. The half cell reactions of various types of Li-ion batteries are shown in Table1. The lattice structures of different positive electrode are from figure1 to figure 4.The crystal structures and Characteristics of the five different cathode materials of Li-ion battery are given in the Table 2.

Table 2 Comparison of Crystal structures and performance of Li-ion batteries [45]

Materials	Structures	Potential Versus Li/Li^+, average V	Specific Capacity mAh/g	Specific energy, Wh/Kg
$LiCoO_2$(LCO)	Layered	3.9	140	546
$LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$(NCA)	Layered	3.8	180-200	680-760
$LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$(NMC)	Layered	3.8	160-170	610-650
$LiMn_2O_4$(LMO)	Spinel	4.1	100-120	410-492
$LiFePO_4$(LFP)	Olivine	3.45	150-170	518-587

The advantages, disadvantages [25] of different cathode materials of Li-ion batteries along with their spider diagrams [25] which are defined their characteristics are shown in the Table 3.

III. Simulation of Li ion Battery with different Positive electrode materials using COMSOL.

The analysis of the Li-ion battery with the discharge at different C-rates is carried out in COMSOL multi-physics software. The COMSOL set up with geometrical structure is shown in the figure 2.

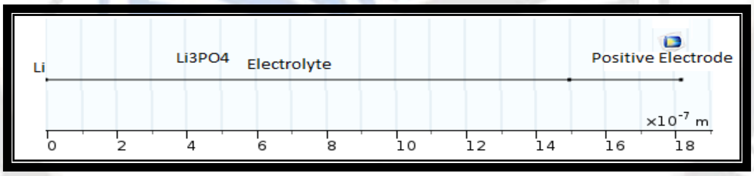
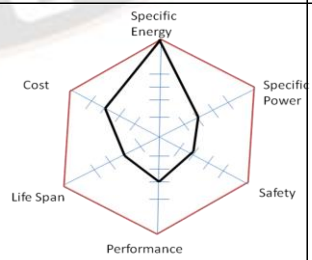


Fig 2: COMSOL structure of one Dimensional solid state battery

Table 3 Comparison of Spider diagrams and performance cathodes of Li-ion batteries

S.No	Cathode Material	Advantages	Disadvantages	Spider Diagram	Applications
1.	$LiCoO_2$(LCO)	Very high specific energy, Market Share is highly stabilized	short life span, paltry thermal stability and constrained load capabilities		Digital cameras, laptops and mobile phones

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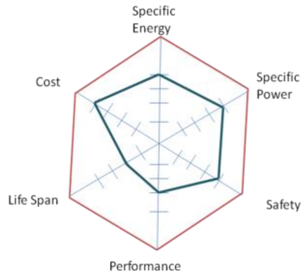
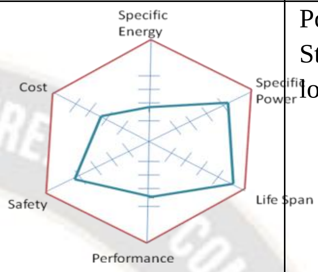
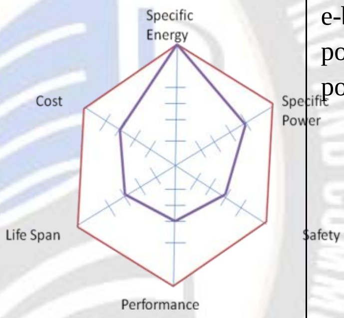
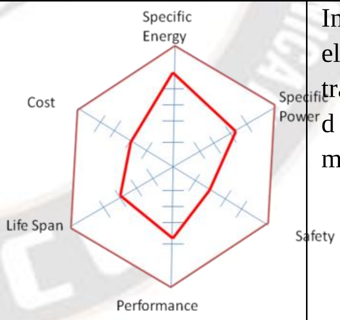
2.	$LiMn_2O_4$(LMO)	Low cost Excellent high rate performance High operating voltage No resource limitations Moderate safety (oxygen release)	Min solubility issue, affecting cycle life Low capacity		electric power trains, medical devices and power tools
3.	$LiFePO_4$(LFP))	Moderately low cost Excellent high rate performance No resource limitations Very slow reaction with electrolyte Excellent safety (no oxygen release)	Low operating voltage Low capacity, especially for substituted variants Controlling patents		Portable and Stationary heavy load currents
4.	$LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$(NMC	High capacity High operating voltage Slow reaction with electrolytes Moderate safety (oxygen release)	High cost of Ni and Co Potential resource limitations Relatively new in performance Controlling patents		e-bikes, portable power tools and power trains
5.	$LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$(NCA)	Performance is well established Slow reaction with electrolytes High capacity High voltage Excellent high rate performance	High cost of Ni and Co Potential resource limitations Controlling saft patents		Industrial , electric power train(TESLA)an d portable medical devices

The geometrical structure which is considered for analyzing the Li-ion battery is one –dimensional structure. As the Li-ions are moved from anode to cathode while charging and cathode to anode while discharge in one dimension, so in this study a one dimensional geometrical structure of Li-ion battery is considered which has Li-metal foil as anode and with different cathode material and Li_3PO_4 as electrolyte.

The operating parameters solid state batteries are given in the Table1. The analysis with different C-rates is such that to study the effect of drawing more current from the battery. The analysis is carried out on different aspects by changing the operating parameters such as thickness of the electrode and electrolyte and concentration of the Li at electrolyte. The equations for analyzing the battery performance are included in the COMSOL software tool. Butler-Volmer equation is used for reaction kinetics at positive electrode and negative electrode which is given in equation (1) and (2) respectively [24].

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$$i_{neg} = FK_{neg} \left(\frac{C_{Li^+}}{C_{Li^{+0}}}\right)^{\alpha_{neg}} \left(e^{(\alpha_{neg}Fn)/(RT)} + e^{-((1-\alpha_{neg})Fn)/RT}\right) \tag{1}$$

$$i_{pos} = i_{0.pos} \left(e^{(\alpha_{pos}Fn)/(RT)} + e^{-((1-\alpha_{pos})Fn)/RT}\right) \tag{2}$$

Where $i_{0.pos}$ was calculated by the following equation

$$i_{0.pos} = Fk_{pos} \left(\frac{(c_{Li,\max} - c_{Li})c_{Li^+}}{(c_{Li,\max} - c_{Li,\min})c_{Li^+,0}}\right)^{\alpha_{pos}} \left(\frac{c_{Li} - c_{Li,\min}}{c_{Li,\max} - c_{Li,\min}}\right)^{(1-\alpha_{pos}} \tag{3}$$

The description of each symbol is given in the Table.4

The operating parameters which are used to analyze the performance of batteries are considered from [24], which proved experimentally on LMO Li-ion battery. Hence in this study also the same parameters are used to study the behavioral differences of different Li-ion batteries.

Table 4. Operating Parameters of Li-Ion Solid state battery [24]

S.No	Symbol	Value	Description
1.	L	1500[nm]	Thickness of electrolyte
2.	M	320[nm]	Thickness of electrode
3.	$c_{0\_Li\_ion}$	6.01e4[mol/m^3]	Total concentration of Li ions in Li3PO4 matrix
4.	kr	0.9e-8[m^3/(mol*s)]	Li ion recombination reaction rate
5.	δ	0.18	Fraction of free Li ions in equilibrium
6.	$D_{Li,ion}$	0.9e-15[m^2/s]	Diffusion coefficient for Li ions in electrolyte
7.	D_n	5.1e-15[m^2/s]	Diffusion coefficient for n in electrolyte
8.	$c_{Li,max}$	2.33e4[mol/m^3]	Selected maximal activity of Li, positive electrode
9.	D_{Li}	1.76e-15[m^2/s]	Diffusion coefficient for Li, positive electrode
10.	α_{Pos}	0.6	Charge transfer coefficient
11.	k_{pos}	5.1e-4[mol/m^2/s]	Rate constant charge transfer reaction, positive electrode
12.	T	298.15[K]	Temperature
13.	kd	kr*c0_Li_ion*δ^2/(1-δ)	Dissociation rate constant in electrolyte
14.	$c_{Li,ion,init}$	c0_Li_ion*δ	Initial Li ion electrolyte concentration
15.	i_1C	10e-6[A/cm^2]	1C current
	$c_{Li,init}$	$c_{Li,max}$ /2*1.01	Initial Li concentration, positive electrode
16.	C-rate	1	C rate parameter in parametric sweep
17.	$c_{Li,min}$	$c_{Li,max}$ /2	Minimum Li concentration, positive electrode
18.	α_{neg}	0.5	Charge transfer coefficient, negative electrode
19.	k_{neg}	1e-2[mol/m^2/s]	Rate constant charge transfer reaction, negative electrode

The concentration of the solid lithium as positive electrode will change the equilibrium potential by initializing the negative electrode equilibrium potential to zero. The dissociation/recombination reaction rate at solid electrolyte is given in (4)

$$r_{Li,ion} = kd(c_{0,Li,ion} - c_{Li,ion}) - kr(c_{Li,ion})c_n \tag{4}$$

When the system is at equilibrium the fraction of total lithium dissociated has the following condition is given in (5)

$$c_{Li^+}^{eq} = c_{n-}^{eq} = \delta c_0 \tag{5}$$

The dissociation rate at the electrolyte is provided in (6)

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$$k_d = \frac{k_{rc_{o,Li,ion}} \delta^2}{1-\delta} \qquad (6)$$

The Li+ and n- transportation in the electrolyte can be calculated with Nernst-Planck equation

$$N_i = -D_i \nabla c_i + \left(\frac{z_i F}{RT} \right) D c_i \nabla \phi_l \qquad (7)$$

Electro neutrality was assumed so that $c_{Li+}=c_{n-}$ at all times. Faraday's law was then implemented to couple the flux on the interfaces of the electrolyte. To calculate the transport of solid lithium through the positive electrolyte Fick's law was used

$$N_{Li} = -D_{Li} \nabla c_{Li} \qquad (8)$$

Faraday's law was then used again to couple the flux of the solid lithium at the electrolyte and positive electrode interface with the electrochemical reactions as shown in Table 1. The half cell reactions at positive electrode, negative electrode and overall chemical reactions are shown in the Table1.

IV. Results:

Li-ion cell with Li metal as negative electrode, LCO, LMO, LFP, NMC and NCA as negative electrodes and Li_3PO_4 is simulated in the COMSOL multi physics simulation tool. The COMSOL one-dimensional solid state Li-ion battery is shown in the figure 2. The simulation is conducted in different cathode materials for analyzing the discharge curves, variation of the concentration along electrolyte and electrode and electrolyte voltage drop along the thickness of the electrolyte. The total results have been presented with different cathode materials which are LCO, LMO, LFP, NMC and NCA respectively. The results of each material have discharge characteristics, Li-ion concentration distribution along the thickness of the electrolyte, electrolyte potential along the thickness of the electrolyte and concentration variation along the thickness of electrode. The mentioned plots are analyzed at different C-rates which are 1.6, 3.2, 6.4, 12.8, 25.6 and 51.2. The reason behind selecting the different C-rates is to analyze the battery behavior with different load conditions. C-rates for consumer electronics, C-rates for EVS C-rates (add the Table column)especially with the consideration of EV.

IV.I Study of discharge curves of different cathode Li-ion battery under different C-rates: The plots of discharge characteristics of LCO cathode Li-ion battery is shown in the figure 8(a). It starts from 4.2V and due to migration of the Li^+ ions and Solid Li species. At 1.6 C-rate, it discharges to its minimum voltage of 2.5 V in 2200 s which prefers at normal discharge condition of any battery application used at high power accessories. But 51.2 C-rate is the extreme discharging condition of the battery which needs to study for EV applications at different load conditions. At this C-rate it discharges to 2.2 V in 50 seconds which differs the ampere hour rating of the battery with 1.6 C-rate. The remaining charge is utilized in the form of heat which affects the performance and life span of the battery. Similarly for other cathode material Li-ion battery is also followed same operation. LMO cathode material Li-ion battery discharge characteristics are shown in the figure 8(b). It discharges from 4.1V to its minimum voltage of 3.5V at 1.6 C-rate in 2200 sec. when compare to minimum voltage of LCO the minimum voltage of LMO is higher at 1.6 C-rate. With the highest C-rate condition i.e. 51.2 it discharges to 3.31V in 50 seconds, which is also higher than LCO.

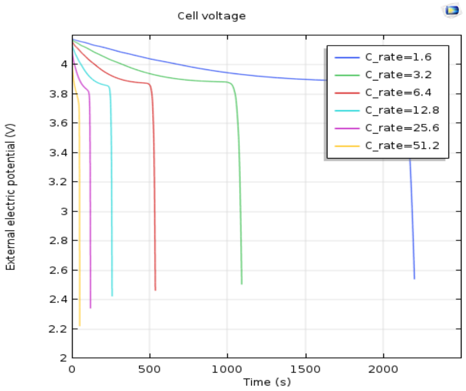

Fig 8(a). Discharge Curves of LCO Li-ion battery

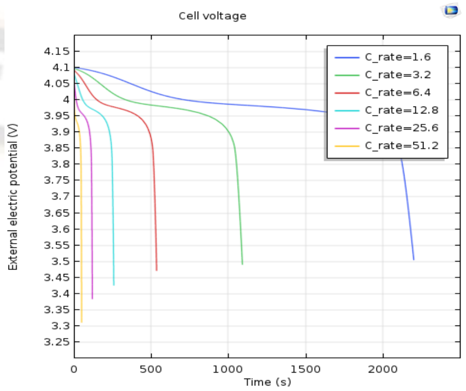

Fig 8(b). Discharge Curves of LMO Li-ion battery

LFP cathode materials Li-ion battery discharge characteristics are shown in the figure 8(c). At 1.6 C-rate it discharges from 3.4V to 1.8V in 2200 seconds, which is lesser than both with LCO and LMO Li-ion batteries. At 51.2 C-rate it discharges to 1.4V in 68 seconds. With NMC Li-ion battery it discharges from 3.9V to 0.8V in 2202 seconds which is lesser than LCO, LMO and LFP. But at 51.2 C –rate it discharges to 0.54V at 50 seconds which is shown in figure (d). The variation from 1.6 C-rate to 51.2 C-rate is lesser when compare to LCO, LMO and LFP. With NCA cathode material, it discharges from 3.8 V to 2.1V in 2200 seconds at 1.6 C-rate and at 51.2 C-rate it discharges to 1.82 V in 50 seconds which is given in figure (e). The comparison of complete discharge characteristics are shown in the Table 4.

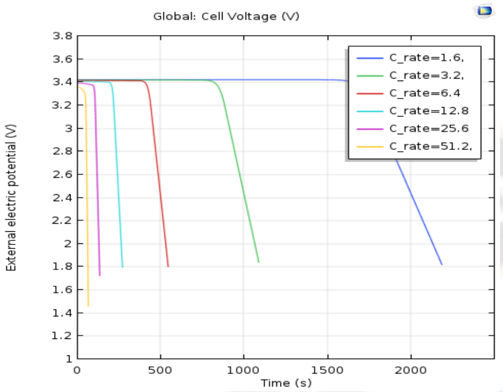

Fig 8(c). Discharge Curves of LFP Li-ion battery

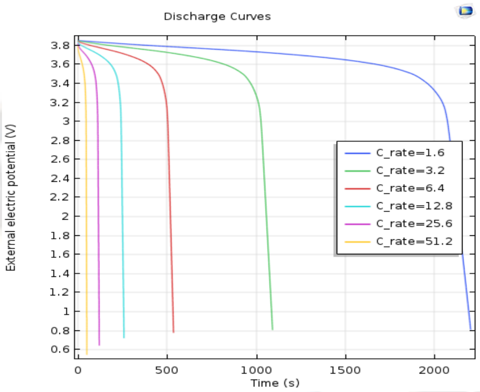

Fig 8(d). Discharge Curves of NMC Li-ion battery

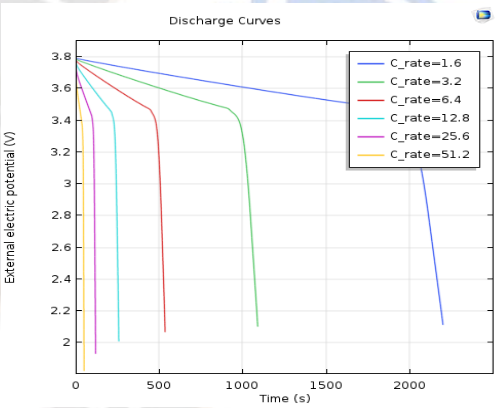

Fig 8(e). Discharge Curves of NCA Li-ion battery

Table 5. Comparative analysis of discharge voltages of Different cathode materials at 1.6 and 51.2 C-rate

S.No	Cathode material of Li-ion battery	Discharges from (V)	Minimum voltage at 1.6 C-rate (V)	Minimum voltage at 51.2 C-rate (V)	Difference between 1.6 C-rate to 51.2 C-rate (V)
1	$LiCoO_2$(LCO)	4.2	2.5	2.2	0.3
2	$LiMn_2O_4$(LMO)	4.1	3.5	3.3	0.2
3	$LiFePO_4$(LFP))	3.4	1.8	1.4	0.4
4	$LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$(NMC	3.9	0.8	0.54	0.26

5	$LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$(NCA)	3.8	2.1	1.82	0.28

IV.II Variation of Concentration in the electrolyte:

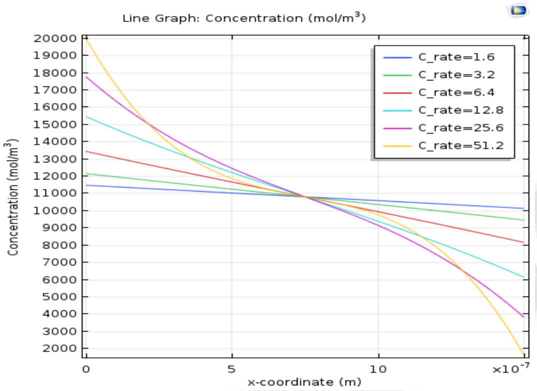

Fig 9(a) Concentration Variation in electrolyte for LCO

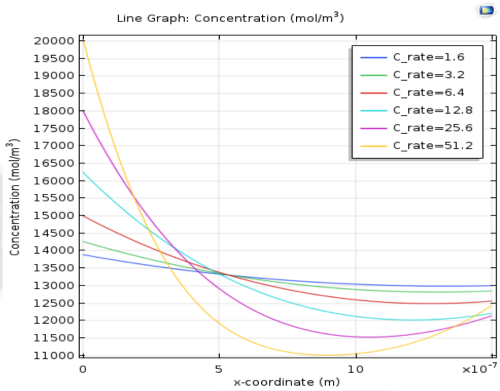

Fig 9(b) Concentration Variation in electrolyte for LMO

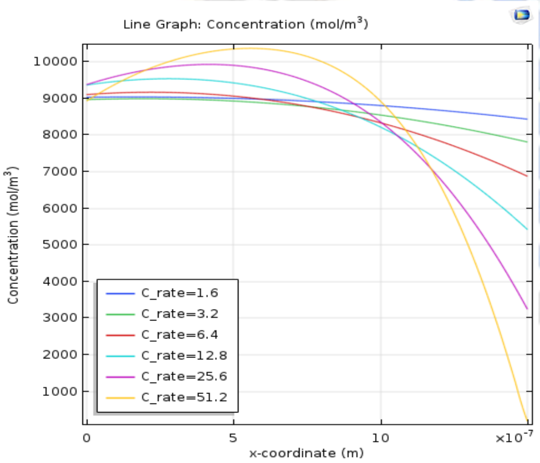

Fig 9(c) Concentration Variation in electrolyte for LFP

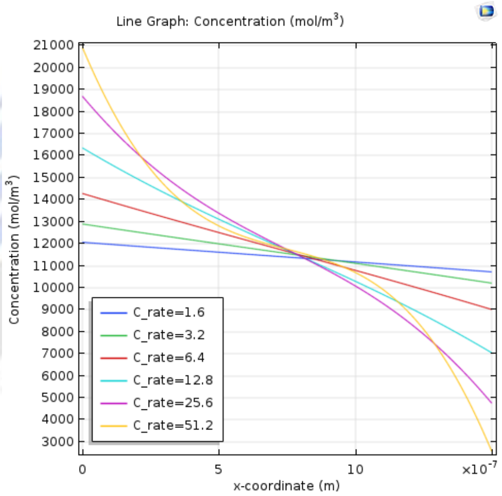

Fig 9(d) Concentration Variation in electrolyte for NMC

The variation of Li concentration along the thickness of the electrolyte for different cathode materials is given from fig 9(a) to fig 9(e) which is referred to different cathode materials. For LCO cathode material the variation of concentration is shown in the fig 9(a) at different C-rate conditions. At 1.6 C-rate variation of the Li concentration is almost constant at 11000 mol/m^3. But variation is increases with increasing of C-rate. At 51.2 C-rate the variation is from 20000 mol/m^3 to 1635 mol/m^3 along the thickness of the electrolyte. The change of variation is linear for all C-rates except 51.2C-rate. Fig 9(b) shows the variation of Li concentration along the thickness of the elctrolyte for LMO cathode. Variation is constant at 14000 mol/m^3 for 1.6 C-rate. Like in LCO for LMO also , variation increases with the increase of C-rate. The large variation is for 51.2 C-rate from 20000 mol/m^3 to 12500 mol/m^3, which is a nonlinear variation. Fig 9(c) shows the variation of Li concentration along the thickness of the elctrolyte for LFP cathode. Variation is constant at 9000 mol/m^3 for 1.6 C-rate. Like in LCO and LMO in LFP also , variation increases with the increase of C-rate. The large variation is for 51.2 C-rate from 9000 mol/m^3 to 900 mol/m^3, which is a nonlinear variation. Similarly for NMC and NCA also. Table 5. Shows the comparative analysis on variation of Li concetration in the thickness of solid electrolyte(Li_3PO_4).

International Journal on Recent and Innovation Trends in Computing and Communication
ISSN: 2321-8169 Volume: 11 Issue: 11
***Article Received:** 10 September 2023 **Revised:** 20 October 2023 **Accepted:** 30 October 2023*

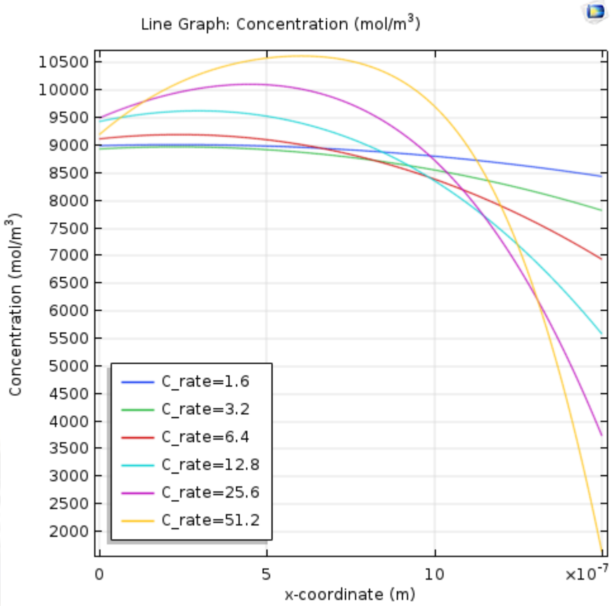

Fig 9(e) Concentration Variation in electrolyte for NCA

Table 6. comparative analysis on variation of Li concetration in the thickness of solid electrolyte(Li_3PO_4) for 51.2 C-rate

S.No	Cathode material of Li-ion battery	Concentration at front end of the electrolyte(mol/m^3)	Concentration at trail end of the electrolyte (mol/m^3)	Variation of concentration between the two ends (mol/m^3)
1	$LiCoO_2$(LCO)	20,000	1635	18365
2	$LiMn_2O_4$(LMO)	20,000	12500	7500
3	$LiFePO_4$(LFP))	9000	900	8100
4	$LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$(NMC	21000	2800	18200
5	$LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$(NCA)	9000	1800	7200

IV.III Variation of Concentration in the Cathode: Plots from 10(a) to 10(e) are shown the variation of concentration of Li along the thickness of the electrode at different C-rates. Except LFP cathode, all other materials have the concentration of 23500 mol/m^3 at starting end of the electrode. The concentration of the Li is almost constant along the electrode for 1.6 C-rate for all electrodes but it is reduces along the thickness of the electrode as C-rate increases. Table 6 shows the comparative analysis on variation of the concentration along the thickness of the electrode for different electrode at 51.2 C-rate.

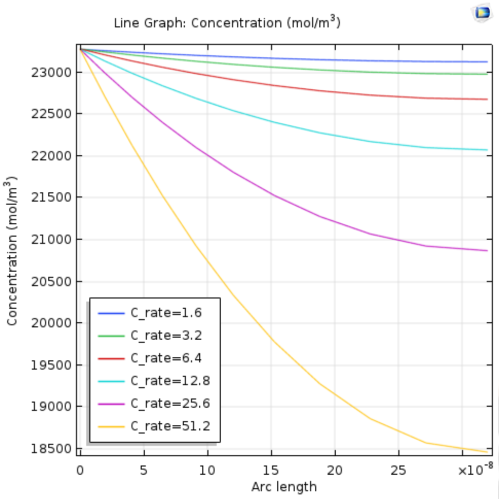

Fig 10(a) Concentration Variation in LCO

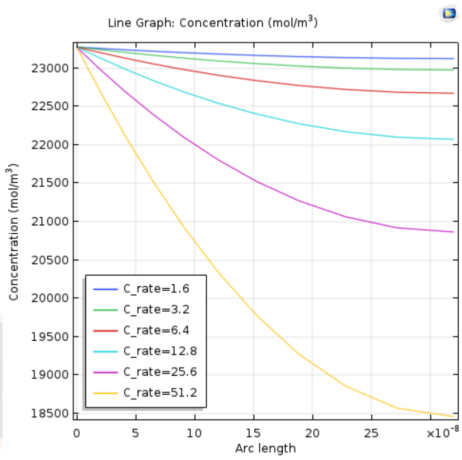

Fig 10(b) Concentration Variation in LMO

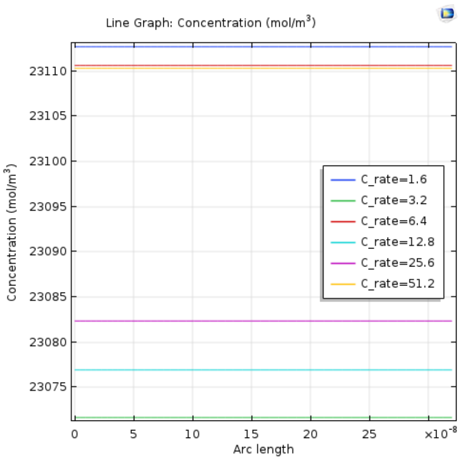

Fig 10(c) Concentration Variation in LFP

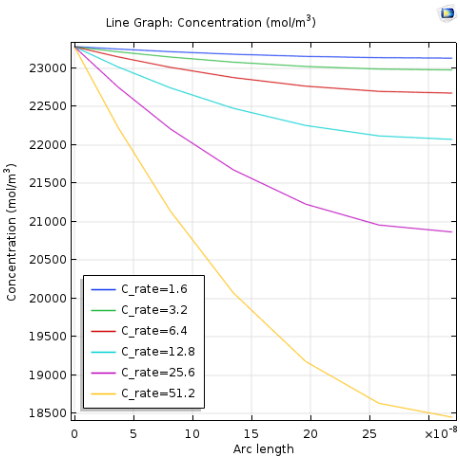

Fig 10(a) Concentration Variation in NMC

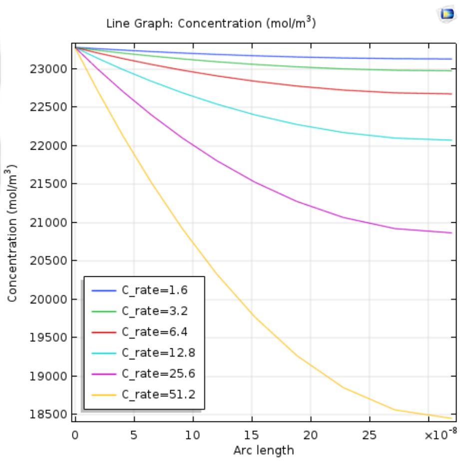

Fig 10(e) Concentration Variation in NCA

Table 7. comparative analysis on variation of Li concetration in the thickness of Cathode for 51.2 C-rate

S.No	Cathode material of Li-ion battery	Concentration at front end of the Electrode(mol/m^3)	Concentration at trail end of the Electrode(mol/m^3)	Variation of concentration between the two ends (mol/m^3)
1	$LiCoO_2$(LCO)	23280	18450	4830
2	$LiMn_2O_4$(LMO)	23280	18450	4830
3	$LiFePO_4$(LFP))	23110	23110	0
4	$LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$(NMC	23280	18450	4830
5	$LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$(NCA)	23280	18450	4830

Electrolyte potential :

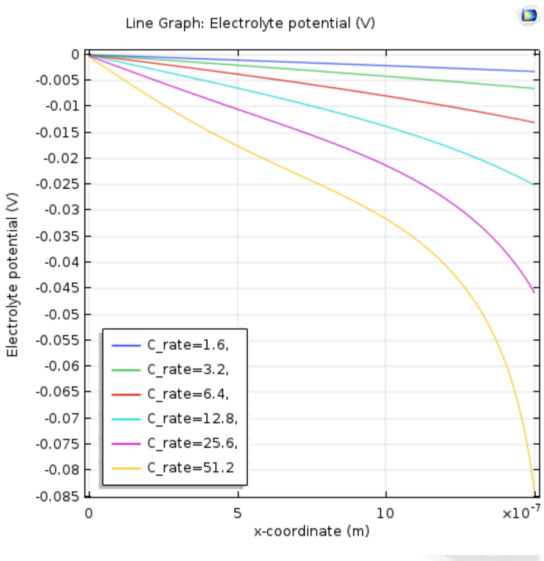

Fig 11(a) Electrolyte potential drop for LCO

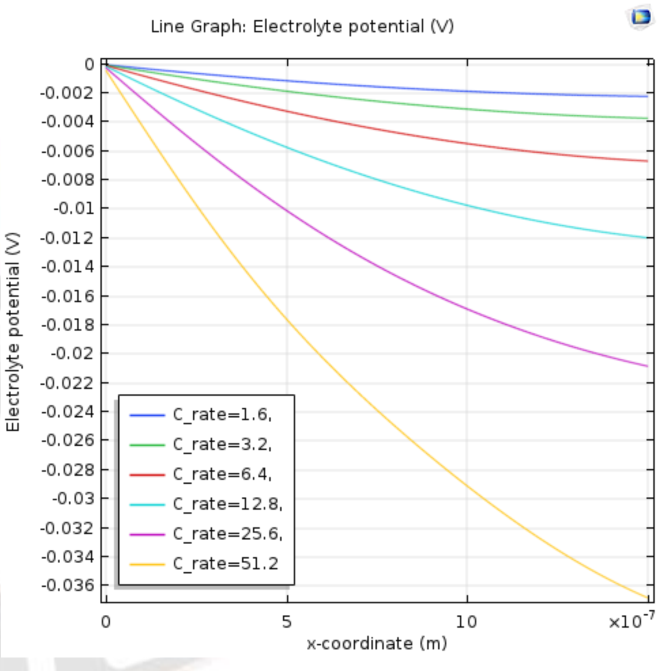

Fig 11(b) Electrolyte potential drop for LMO

Electrolyte is electrically insulator, it does not allows the electrons through if , but due to diffusion action there is a probability of electron leakage along the elctrolyte. Due to this a small voltage drop can be seen across the electrolyte. If the C-rate increases the chances of leakage of electrons also increases which raises the voltage drop. Plots from fig 11(a) to fig 11(e) shows the voltage drop of the same elctrolyte with different cathode materials at differnet C-rates. The voltage drop is almost zero for 1.6 C-rate and as C-rate increases the volatge drop across the electrolyte also increases for all the eletrode materials.

International Journal on Recent and Innovation Trends in Computing and Communication
ISSN: 2321-8169 Volume: 11 Issue: 11
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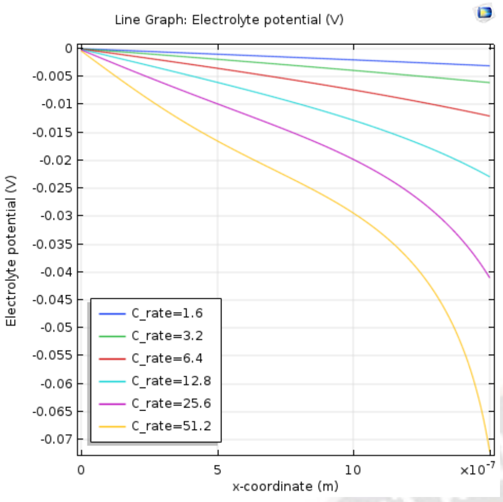

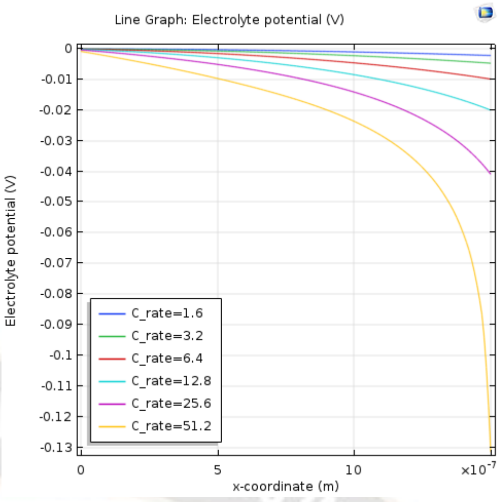

Fig 11(c) Electrolyte potential drop for LFP Fig 11(d) Electrolyte potential drop for NMC

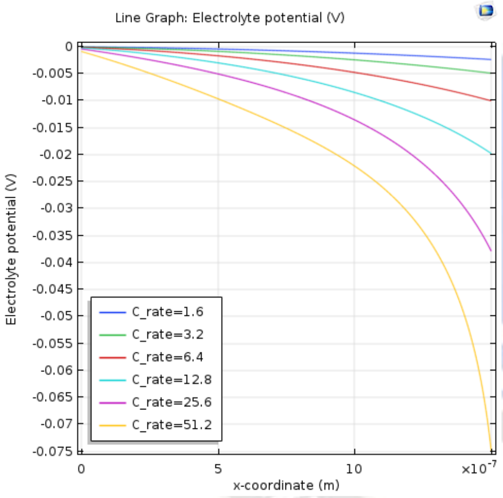

Fig 11(e) Electrolyte potential drop for NCA

Conclusions: A comparative analysis of different cathode materials with different C-rates is studied in this paper. With the above analysis, it is very helpful to analyze the behavior of Li-ion batteries at different load conditions with different Cathode materials. The characteristics of variation of Li-ion concentration along the thickness of the electrolyte and variation of Li ion concentration along the thickness of cathodes are used to select the required cathode materials for different applications of EV. The discharge curve characteristics are used to understand the behavior of the battery at different materials and used to estimate the energy density at those C-rates.

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