Final Report of WBS 2

Project Description

Lithium precipitation is caused due to several physical conditions during the manufacturing process of Lithium ion batteries. To prevent this, many methods of manufacturing are practised, i.e., controlling temperatures etc. However, precipitation can only be seen by opening batteries after the ageing process, which makes them useless. The goal of this project was to develop an AI based technique to quantify the Lithium precipitation using Neutron scan of the Lithium ion batteries to avoid any damage or waste during the diagnostic process.

For this, we gathered relevant information about lithium precipitation and solutions for its quantification and compiled a review. This review of existing works which explains lithium precipitation, its causes and the application of AI in this regard, is mentioned in the background section. After understanding the dynamics of this problem, we proposed a detailed and well-planned solution which carefully tackles the issues of this project, which are discussed further on. Additionally, we also experimented with provided data for lithium precipitate extraction.

Background

We reviewed several papers and online sources to create a concise and accurate background and literature review. Although, the work done related to this specific problem is negligible, we have searched thoroughly to present a comprehensible review which shows the information present. Firstly, we discuss lithium precipitation and its causes. Then, we provide very recent applications of AI in battery manufacturing.

Lithium Precipitation in Batteries:

When a lithium ion battery is charged, lithium ions travel from the positive electrode to the negative electrode. But when there are some abnormal conditions on the negative electrode, lithium ions fall off from the positive electrode too quickly, but are not inserted into the negative electrode at the same rate. So, electrons only reach the surface of the negative electrode, and form a silver-white metallic lithium deposit, which is called *lithium precipitation*.

Reasons for Lithium Precipitation:

There are several reasons why lithium precipitation occurs [4], which are mentioned below:

- When **the battery is charged at a high rate**, a large amount of lithium ions are extracted from the positive electrode and come to the negative electrode. However, because the impedance of lithium ions inserted into the negative electrode is much greater than that of the positive electrode, the negative electrode get electrons on the surface

- When **the positive electrode coating is too heavy or the negative electrode coating is too light**, there will be insufficient space for lithium insertion in the negative electrode
- **The electrolyte acts as a channel for conducting lithium ions**. If the amount of electrolyte is small or the pole piece (a pole piece directs the flow of ions) is not sufficiently inserted, it will cause lithium precipitation
- Under **low temperature conditions**, following reasons cause lithium precipitation
    - The ionic conductivity of the electrolyte will decrease,
    - The resistance of lithium ions from the positive electrode and the insertion of the negative electrode will be greatly increased
    - The increase in the resistance of the negative electrode will be greater

Artificial Intelligence in Battery Manufacturing

Over time AI has been incorporated into the manufacturing processes, mainly in their improvement and development. This helps in reducing the evaluation times and also to research newer materials and technologies for better battery performance.

For testing performance: A team consisting of Stanford professors and Toyota researchers has developed a machine learning-based method for fast charging which greatly reduced evaluation times for batteries and finding **the best method to charge a battery that maximises the battery's overall lifetime** [2, 3]. This would help prevent the first reason given in the previous section.

For battery materials: is used for material research and reaction energy, as well as finding composites consisting of ordinary chemicals [1]

For capacitor development: study the influence of the structural characteristics of carbon-based electrodes on the capacitance and power density [1]

To summarise, Lithium precipitation is an important issue which severely impacts a battery's performance and usability. Like many other fields, AI has been integrated in battery production to improve existing methods and develop newer technologies. While **AI is** being used to reduce errors in manufacturing, like to find the best method to charge a battery to prevent lithium deposition, it is **not currently being used to detect lithium precipitation after the battery is manufactured**. **This means that we will have to cater to the lack of datasets and existing work by developing everything from scratch and using our own knowledge of AI.**

Proposed Pipeline

To develop the algorithm from point zero, the following tasks would be performed:

- **Data Analysis**
    - Receive Data
    - Data Analysis

Perform an in-depth analysis of the sample scans for knowledge about the material like the pattern of lithium precipitate.

- **Development**
  - <u>Feature Extraction</u>
    Develop an algorithm to extract key features (lithium deposits) and perform analysis on their patterns. This will be done by using intensity of pixel values which contain precipitation.
  - <u>Variation Algorithm</u>
    Using the lithium deposit patterns (features) extracted, develop an algorithm to calculate variations in lithium precipitation.
  - <u>Prediction Algorithm and Development</u>
    Design and development of physical properties prediction algorithm and model using the shortlisted features

- **Application Development**
  - Design and develop an architecture which will enable users to use the prediction model
  - Integrate the solution

Tasks Performed

Of the above mentioned pipeline, **we have performed a preliminary visual analysis of the samples provided** to us. Using this analysis and our previous knowledge of a wide variety of datasets used for different tasks, we have **come up with the features for the final dataset that would be beneficial** for the development of AI algorithm. As for the AI algorithm for the quantification of lithium precipitate, we **proposed a carefully planned and detailed solution which consists of two phases**. At the end, we would receive the distribution and percentage of precipitation on the electrode and the changes in precipitate distribution and amount over time

Proposed Algorithm for Quantification of Lithium Precipitation

Detailed implementation of the above steps, data analysis and algorithm development, are discussed here.

Data Analysis:

We observed the samples provided to us earlier and concluded that data with the following characteristics would potentially give good results:

1. Clear samples of Neutron and Electrode (Visual Light (VL)) images which **contain** Lithium precipitate
   a. If the samples contain it, then the **amount of precipitation** is also required
2. Clear samples of Neutron and Electrode (Visual Light (VL)) images which **do not contain** Lithium precipitate

AI for Detection:

Then, we **developed a thoroughly planned, multiphase solution for quantification of Lithium precipitate from neutron images**. There would be two phases for this problem:

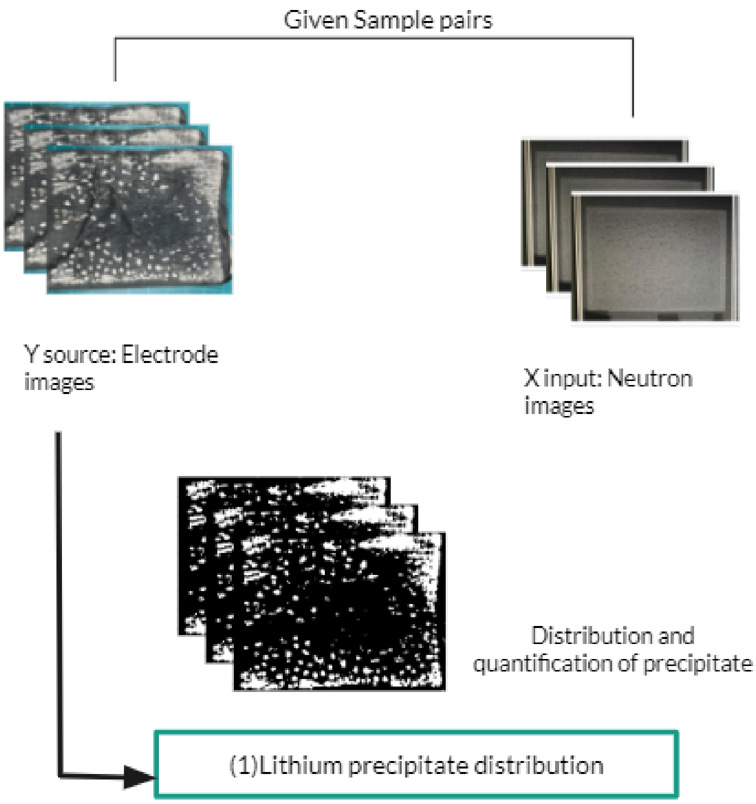
1. Modelling phase
2. Assessment phase

Modelling Phase

In this phase, the first step would be to take neutron images and their corresponding Visual Light images pairs as samples. These pairs will be used to quantify lithium precipitation from Visual Light images.

Neutron Transmission Image (left) and Actual Electrode (Visual Light (VL)) *(right)*

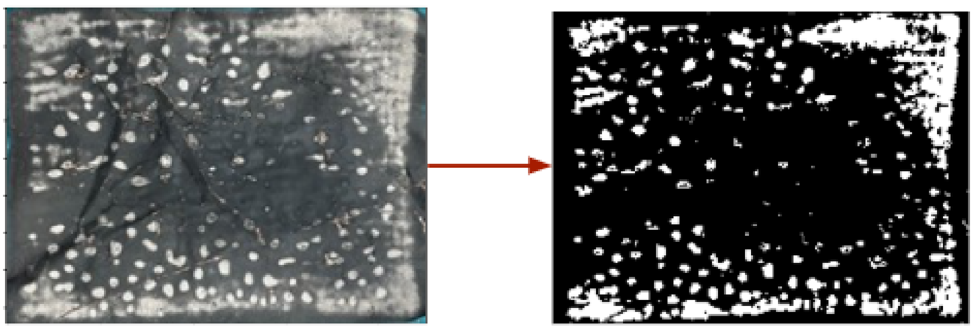
Take these sample images as input and apply AI techniques on them to predict the distribution of lithium precipitate..A diagram of this methodology is shown below:



Using the output, the quantification of lithium deposit will be obtained using the following method:

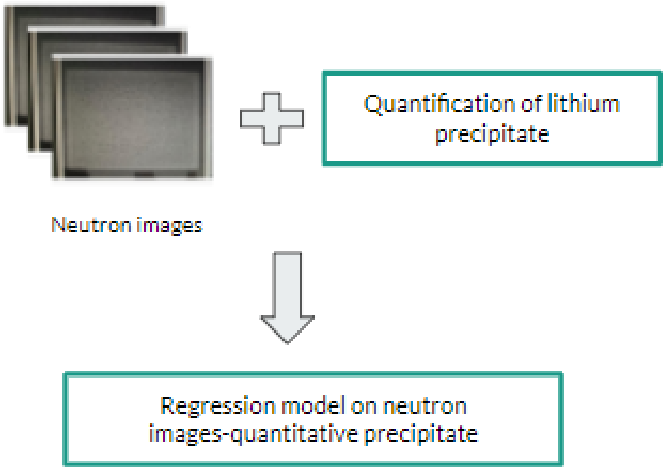
We have **worked on the extraction of lithium precipitate algorithm** as shown below. Battery area is equal to the total area and lithium area is the area covered by white spots. Using these values:

$$\%\text{ of lithium precipitate} = \frac{\textit{Area covered by white lithium spots}}{\textit{Total area}}$$

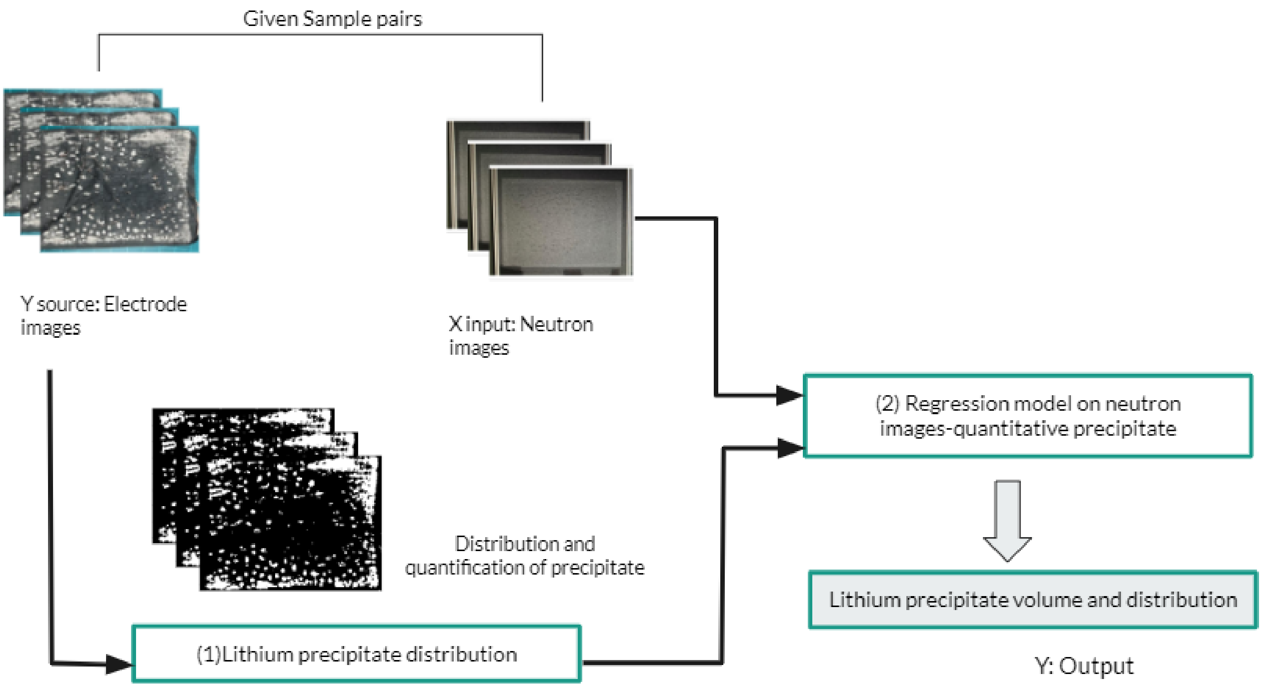


Original Electrode Image *Predicted White Lithium precipitate on Electrode*

The next step would be to take neutron image and the corresponding quantification of precipitate as pairs as input for a regression model, as shown below:



The final work flow would be as follows:



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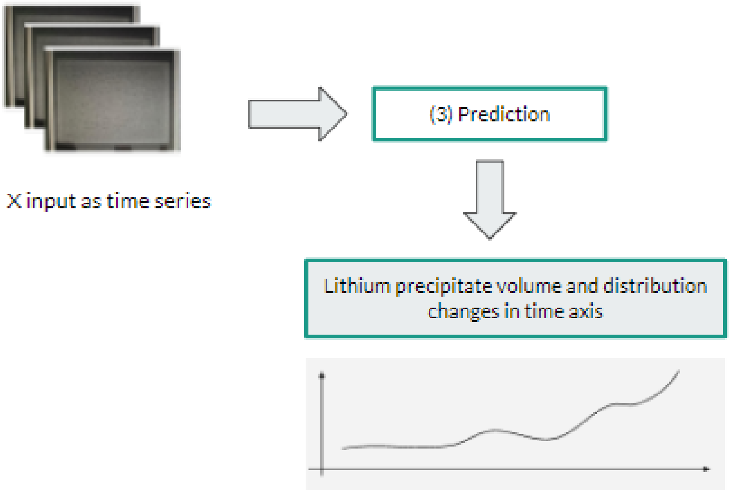
Assessment Phase

In the assessment phase, this regression model will be used to quantify precipitation from neutron images only and also analyse them on time axis.

If there are several methods of making batteries and different times are required for checking the quality of each method,this will be especially useful to visualise precipitation trends over time.



Conclusion

For this project, we have performed a literature review with regards to lithium precipitation and any existing methods for its quantification. However, since there are no existing AI solutions or datasets for this, we would have to develop the algorithm from scratch ourselves using our knowledge of AI and the data that would be provided by Hyundai. We narrowed down the type of dataset which could potentially give us good results by observing the samples provided to us earlier. Moreover, we also started experimentation on these samples and developed an algorithm for lithium precipitate segmentation. We also proposed a multi-step solution for lithium quantification. The solution consists of two phases, modelling and assessment, through which we could predict the following information:

1. The distribution and percentage of precipitation on the electrode
2. The changes in precipitate distribution and amount over time

References

[1] Luo, Z., Yang, X., Wang, Y., Liu, W., Liu, S., Zhu, Y., Huang, Z., Zhang, H., Dou, S., Xu, J. and Tian, J., 2020. A survey of artificial intelligence techniques applied in energy storage materials R&D. *Frontiers in Energy Research*, *8*, p.116.

[2] Attia, P.M., Grover, A., Jin, N., Severson, K.A., Markov, T.M., Liao, Y.H., Chen, M.H., Cheong, B., Perkins, N., Yang, Z. and Herring, P.K., 2020. Closed-loop optimization of fast-charging protocols for batteries with machine learning. *Nature*, *578*(7795), pp.397-402.

[3] Useful link

[4] Useful link