

Modelling and machine learning: choosing the right chemistry faster

Choosing the right leaching chemistry for a given black mass composition has traditionally meant extensive lab based trial and error. REVITALISE has built a machine learning framework, developed by the University of Aveiro, and trained on published experimental data for leaching of black mass using different chemical systems.

The model predicts which leaching chemistries and process conditions will deliver the best recovery for NMC cathodic black mass, while weighing up the environmental and economic implications of that choice.

RESULTS IN PRACTICE

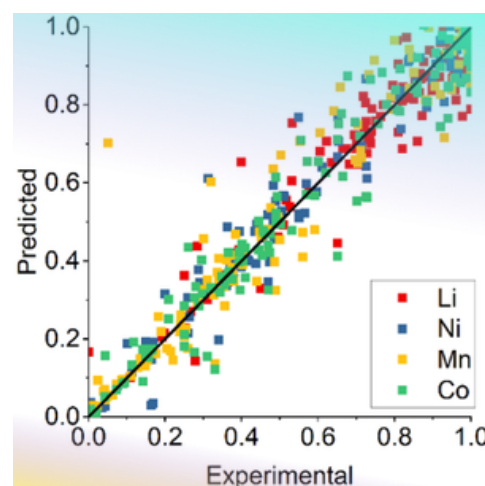
- Data-driven prediction of leaching performance for NMC-based lithium batteries
- Integrated environmental and economic assessment alongside recovery performance
- Data efficient modelling approach successful with relatively small training data sets

PAIN POINTS ADDRESSED

- High cost and time of literature surveys and experimental trial and error when investigating and testing new chemistries on plant
- Difficulty justifying investment in process changes without economic evidence
- Highlight potential environmental hotspots early, to avoid later surprises

$$R^2=0.933$$

Strong predictive accuracy
across 12 acid types



predicted vs experimental
leaching yields

913

underpinning data points

22

independent studies making
up the training data

$\pm 5\%$

typical prediction error

TECHNOLOGY IN DETAIL

How it works

Smarter predictions from limited data. The model combines Gradient Boosting Regression with a Pairwise Difference (PD) data-augmentation technique, which learns from differences between pairs of data points rather than individual points alone - effectively squaring the available training data. Trained on 776 data points and validated on a further 137, the model achieved strong predictive accuracy ($R^2 = 0.933$) on our test data.

What goes in

Built on parameters you already control. Predictions are generated from standard process parameters: acid selection (12 acids are included), leaching temperature, acid selection, acid and hydrogen peroxide concentration, solid-to-liquid ratio, reaction time, and cathode composition (Ni:Mn:Co ratio). No specialised analytical data is required.

What comes out

One model, three insights. For any given set of conditions, the model predicts leaching yields for lithium, nickel, manganese and cobalt, each with an uncertainty estimate. These feed into simplified economic and environmental impact calculations, giving side-by-side comparisons across acids and conditions, and enabling rapid screening of leaching strategies before committing to costly experimental trials.

What sets it apart

From lab validation to plant-ready tool. The model was developed and validated on isolated cathode material under controlled conditions. Ongoing work is extending it to real-world waste streams (including common impurities, mixed-acid systems, and new acids) alongside a growing dataset spanning more cathode chemistries, with the longer-term goal of integration into full process simulation for recycling operations at scale.

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