Materials and meta-data for thermochemical electrolysis.

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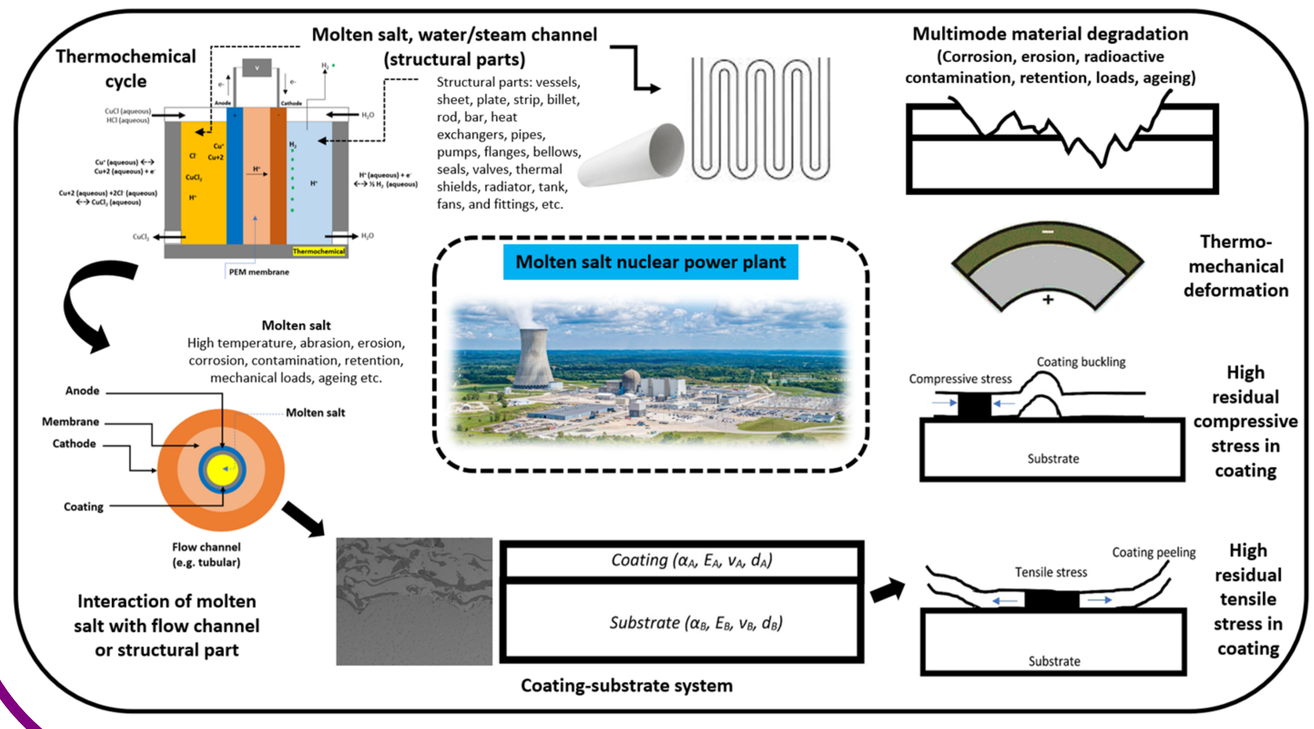
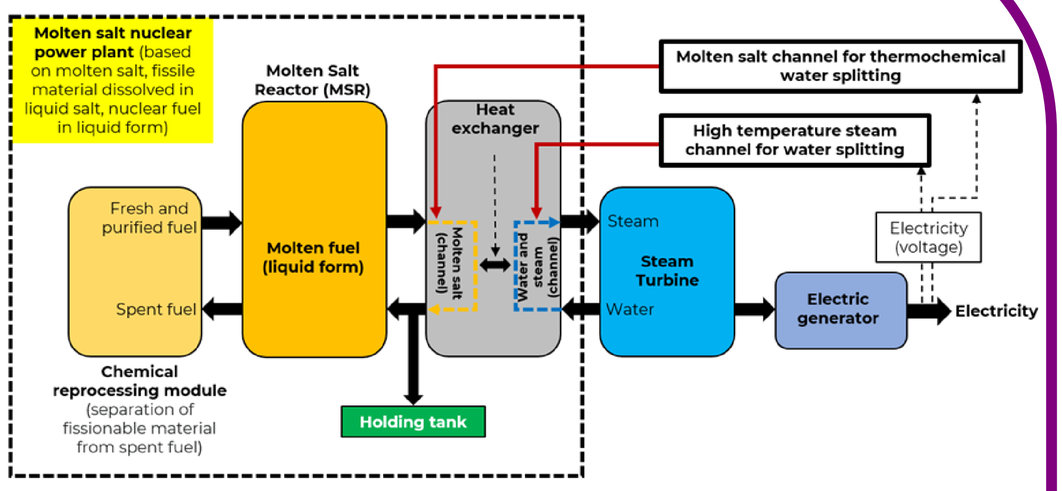
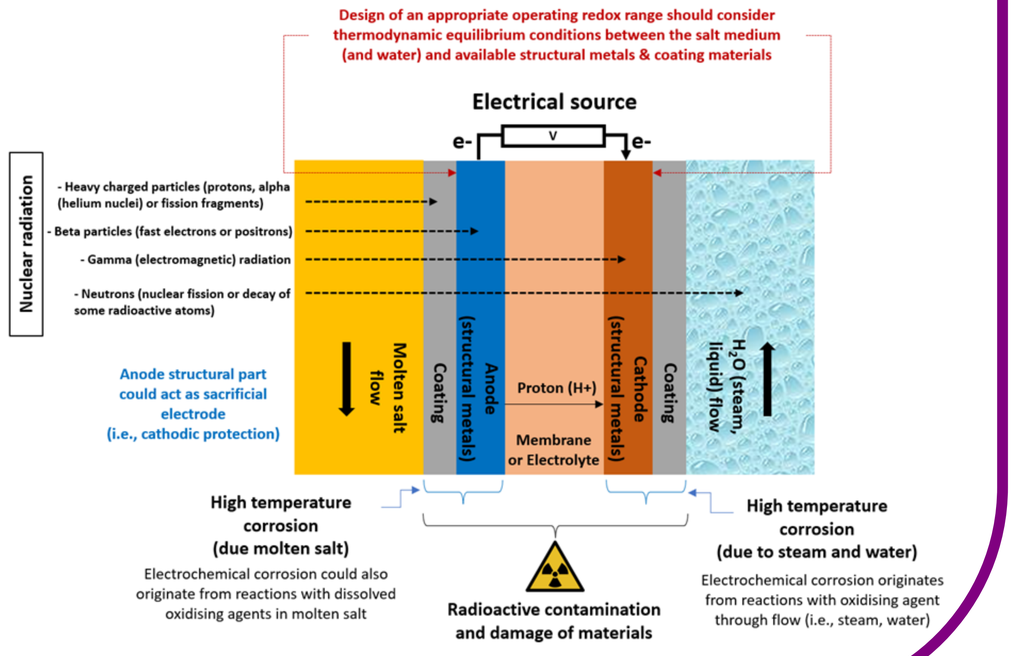
Problem Statement & Opportunity

- One of the important challenges is to develop coating materials for thermochemical containment vessels and pipes that encounters the highly corrosive and harsh environment produced by the molten salt at high temperature.
- Overall assessment based on the evidence from previous investigations in this area is that none of the high-performance structural materials (coating, substrates) are likely to survive for an extended period in the high temperature corrosive environment.
- There are innovative means and methods which could be considered to have sustainable coating-substrate assembly and extended lifetime.

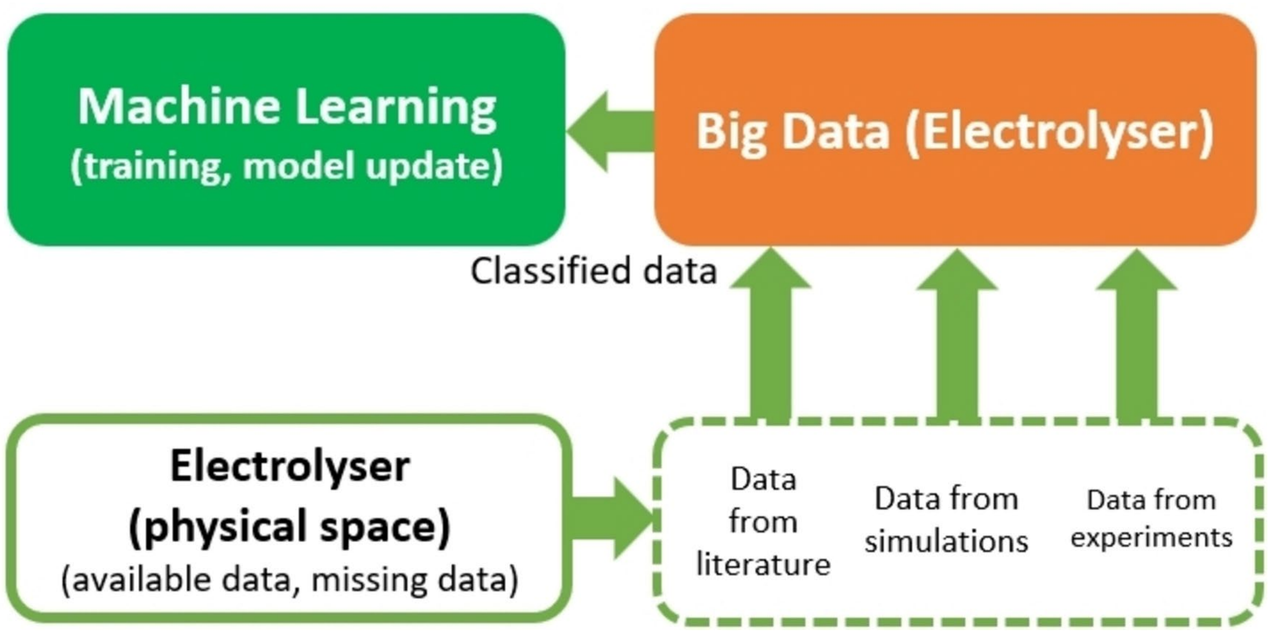




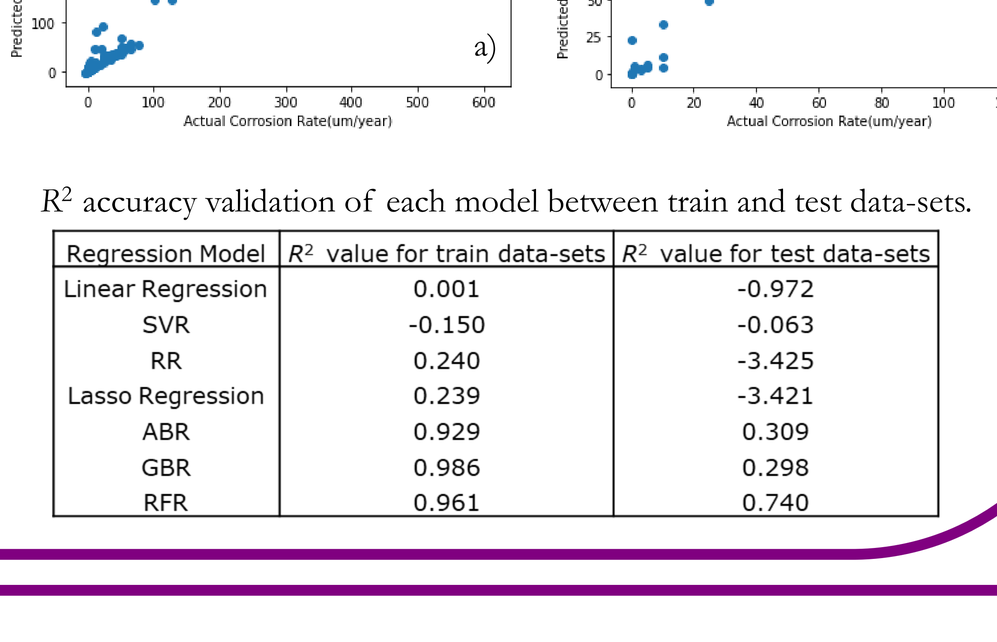


Data Analytics Approach

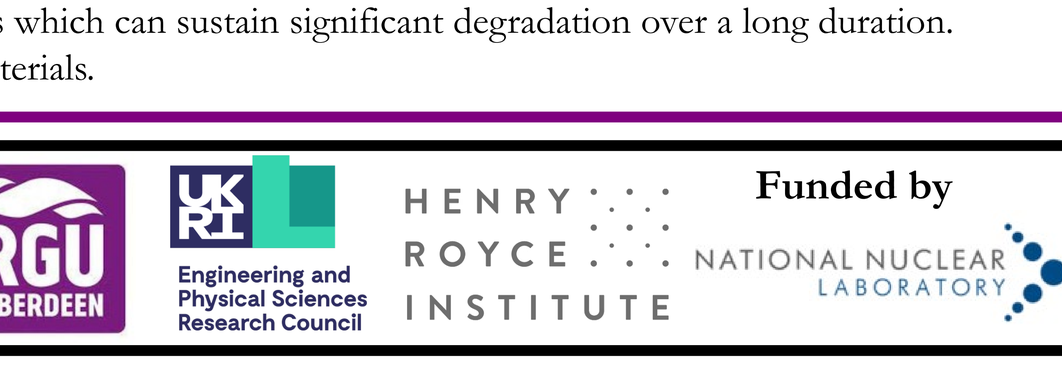
- Gathered accessible datasets on substrate corrosion caused by thermochemical processes for a variety of coating-substrate systems and developed a machine-learning (ML) approach for estimating the corrosion rates.
- Seven machine learning (ML) regressor models were used: Gradient Boosting Regression (GBR), Ada Boost Regression (ABR), Support Vector Regression (SVR), Random Forest (RF), Lasso Regression (LR), and Linear Regression (LR).
- RFR employs a method that integrates estimations from various machine learning models to provide forecasts that are quite precise than those from an individual model.



(Faisal et al., ChemNanoMat , 8(12), 2022, e202200384)



a) Prediction accuracy of RFR model in train data-sets, b) Prediction accuracy of RFR model in test data-sets.



R^2 accuracy validation of each model between train and test data-sets.

Regression Model	R^2 value for train data-sets	R^2 value for test data-sets
Linear Regression	0.001	-0.972
SVR	-0.150	-0.063
RR	0.240	-3.425
Lasso Regression	0.239	-3.421
ABR	0.929	0.309
GBR	0.986	0.298
RFR	0.961	0.740

Summary

- None of the high-performance structural materials (substrates) are likely to survive for an extended period in the high temperature chloride-based environment.
- One possible solution is to use special metals coated with metallic or ceramic coatings which can sustain significant degradation over a long duration.
- Data analysis approach could be useful to predict the degradation of coatings and materials.

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