



AI-Driven Flowsheet Optimization via Multiphysics Surrogate Models

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Context & Objectives: The FIREFLY Project

The project

- European FIREFLY project.
- Developing sustainable, electro-driven recycling flowsheets that combine advanced electrochemical technologies.
- 8 different electro-driven technologies.



The bottleneck

- Sustainable recovery of spent industrial catalysts (e.g. PGMs).
- Variable, complex waste streams require dynamic processing conditions.
- **Multiphysics simulations are highly accurate but computationally heavy and time-intensive.**
- Unsuitable for rapid, system-wide flowsheet optimization.

Our contribution

- AI-driven digital prediction tool.
- Powered by surrogate models trained on high-fidelity datasets.
- Delivers instantaneous predictions for recovery efficiencies and energy consumption.
- Enables rapid optimization of multi-step recycling flowsheets.

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Processes datasets

ETMS

Electrochemical transformation in molten salts

High-fidelity simulation model

725 simulated experiments

133k datapoints

1 experimental setup
1 surrogate model

GDEx

Gas-Diffusion electro-crystallization

COMSOL model

3000 simulated experiments

1.9M datapoints

1 experimental setup
1 surrogate model

COMSOL model in 2025 Amsterdam
“Gas-liquid system in the GDEx process for PGMs recovery.”
by M.I. León Sotelo

ELX

Electro-leaching

COMSOL models

140 simulated experiments

1300 datapoints

5 experimental setups
5 surrogate models

27 experiments, 250 data points
on average per experimental setup

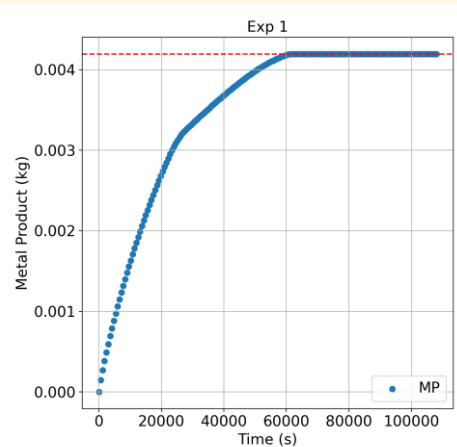
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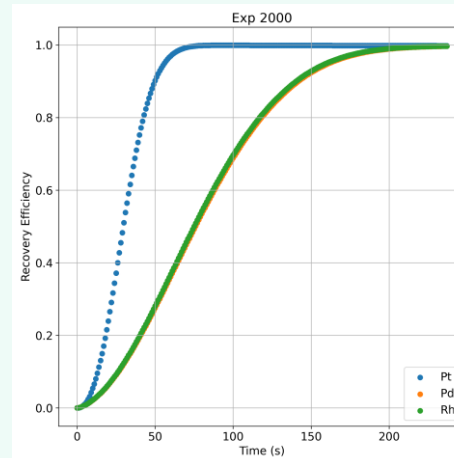
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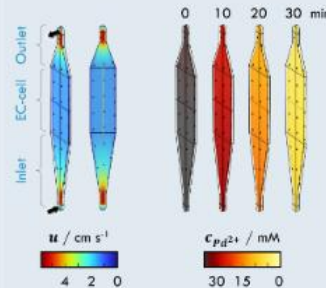
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Gas-liquid system in the GDEx process for PGMs recovery.

Understanding gas-liquid mass transfer barriers unlocks better recovery of elemental PGMs by fine-tuning key transfer parameters.

Maria I. León, Savitha Thayumanasundaram
VITO - Vlaamse Instelling voor Technologisch Onderzoek
Boeretang 200, 2400 Mol, Belgium

Introduction & Goals

Catalysts are essential for efficient chemical processes,

This work focuses on Gas-Diffusion Electrocrystallization

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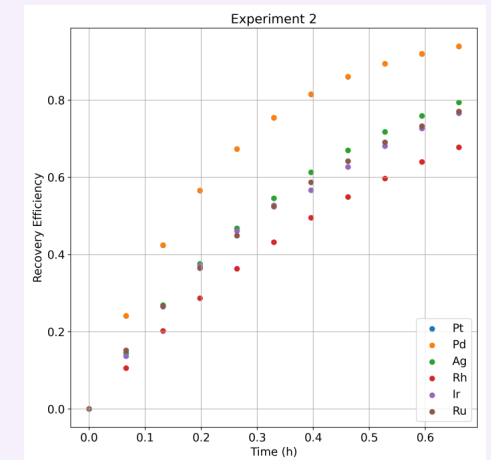
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Surrogate model inputs

ETMS

Electrochemical transformation in molten salts

Input Material Parameters

- Titanium Oxide feed

Input Process parameters

- Cell voltage
- Porosity
- Time

GDEx

Gas-Diffusion electro-crystallization

Input Material Parameters

- PGMs initial concertation (up to 3 elements)

Input Process parameters

- Gas flow rate
- Current density
- Time

ELX

Electro-leaching

Input Material Parameters

- Initial concertation (up to 6 elements)

Input Process parameters

- Current density
- pH
- Time

Surrogate models

ETMS

Electrochemical transformation in molten salts

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133k datapoints

ML surrogate model
Artificial Neural Network

GDEx

Gas-Diffusion electro-crystallization

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ML surrogate model
Artificial Neural Network

ELX

Electro-leaching

per experimental setup
~27 simulated experiments

~250 datapoints

Physics-informed
analytical fitting

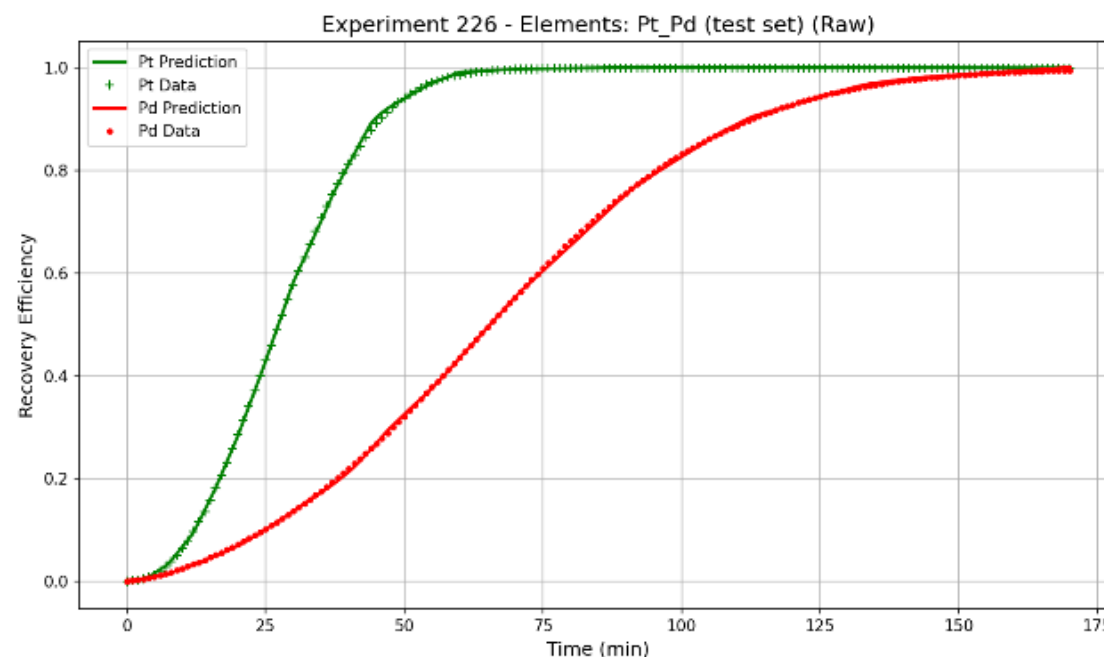
Surrogate models performance – GDEx (ML)

ANN with 2 hidden layers predicting simultaneously Pt, Pd and Rh recovery efficiency

Excellent performance

$$R^2 = 0.99994 \pm 0.00009$$

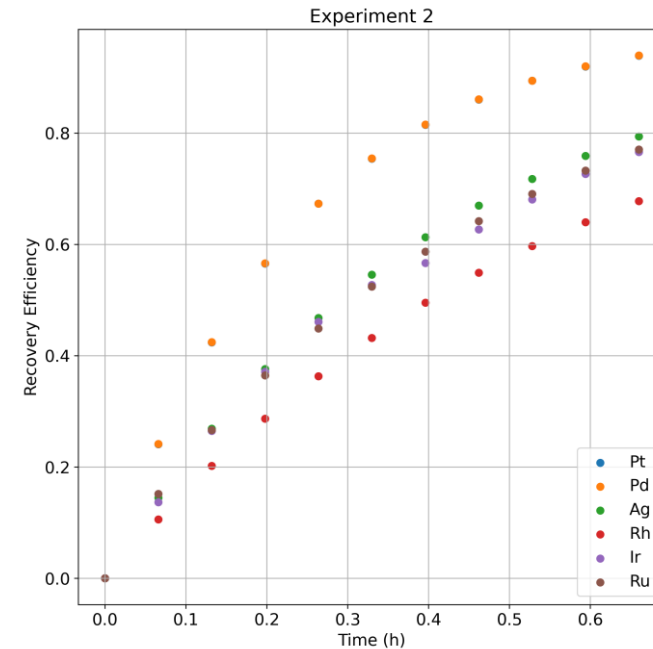
$$\text{MAPE} = 0.56 \pm 0.30 \%$$



One of the worst predicted experiments in the test set

Surrogate models performance – ELX (fitted)

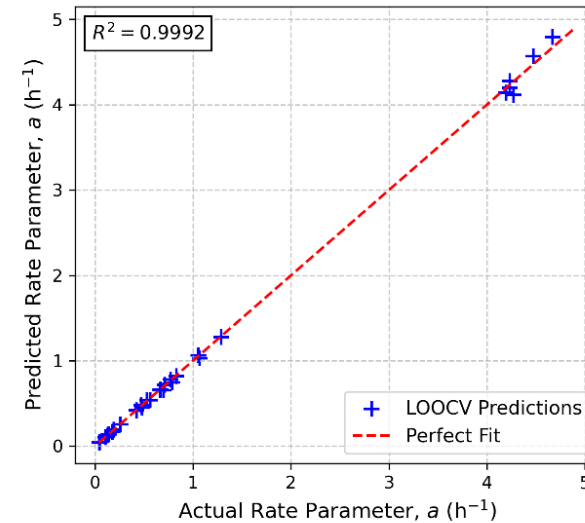
- Time evolution fitted as exponential rise: $1 - e^{-a \cdot t}$
- Exponent (a) fitted with a custom function of two input variables (pH and J)
- Fit per experimental setup and per element



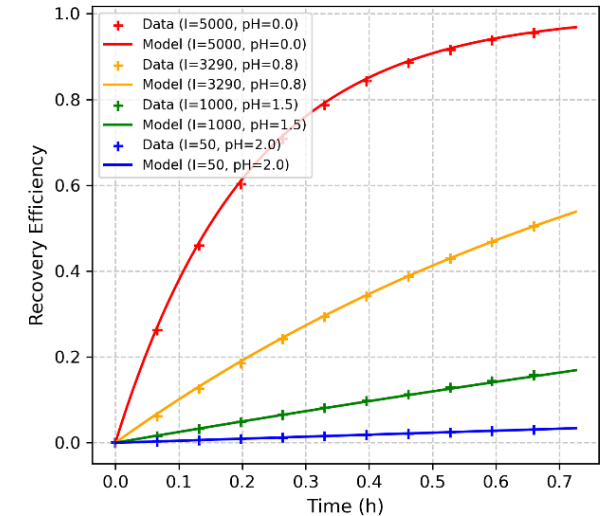
Example of time evolution data of all metals of an experiment

Surrogate models performance – ELX (fitted)

- Time evolution fitted as exponential rise: $1 - e^{-a \cdot t}$
- Exponent (a) fitted with a custom function of two input variables (pH and J)
- Fit per experimental setup and per element
- Excellent performance
 $R^2 = 0.995 \pm 0.011$



Leave-One-Out Cross-Validation (LOOCV) comparing the predicted and actual kinetic rate parameters (a) for Pd and a specific experimental setup



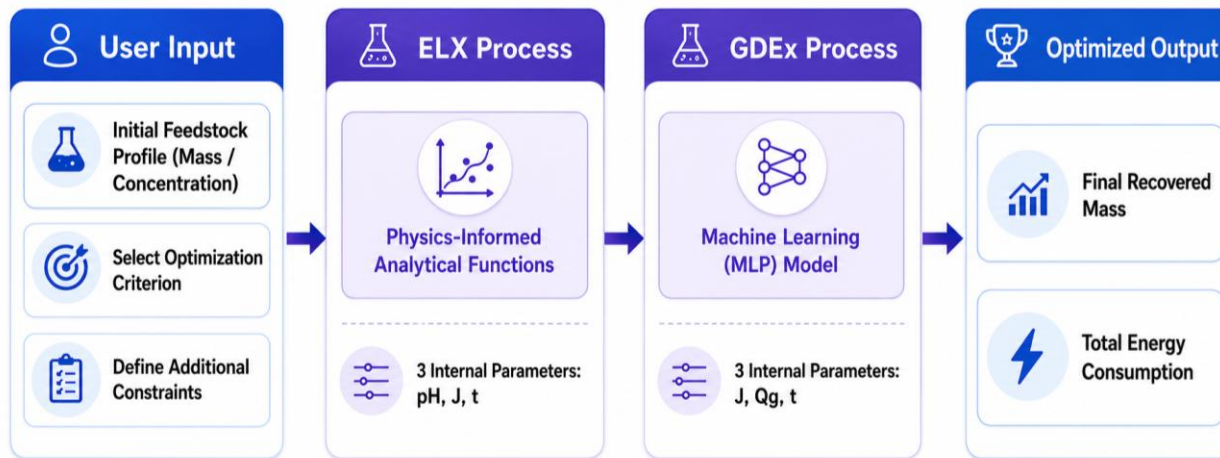
Analytical surrogate model predictions versus simulation data for the temporal evolution of Pd recovery efficiency across representative experiments

Flowsheet creation and optimization

Four flowsheets were created

Pt recovery flowsheet example

- To recycle Pt, one possible way is to combine ELX and GDEx processes!
- Phase space of 6 processed variables (3 for ELX and 3 for GDEx)



Flowsheet Optimization

- Answer: “What is the optimal flowsheet setup?”
- What is “Optimal”?
 - Highest efficiency?
 - Lowest energy consumption?
 - Running ELX in a less acidic environment (e.g. pH ≥ 1) and minimizing the energy consumption while having a recovery efficiency of the target metal $\geq 85\%$?

Flowsheet optimization designed for speed

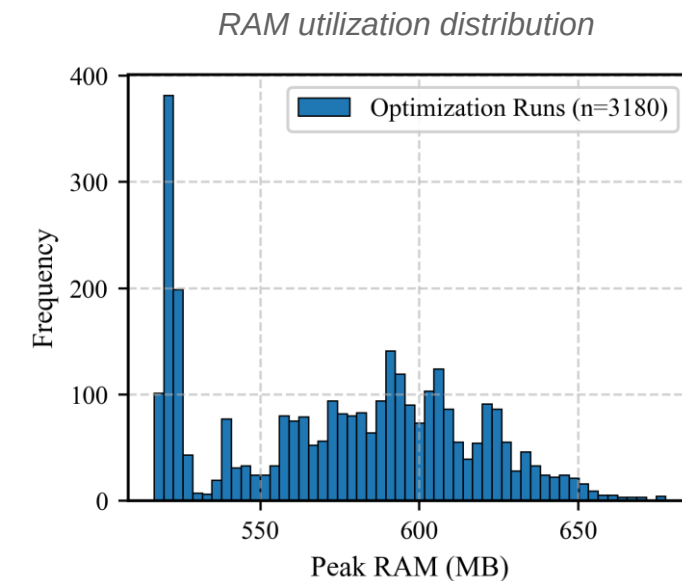
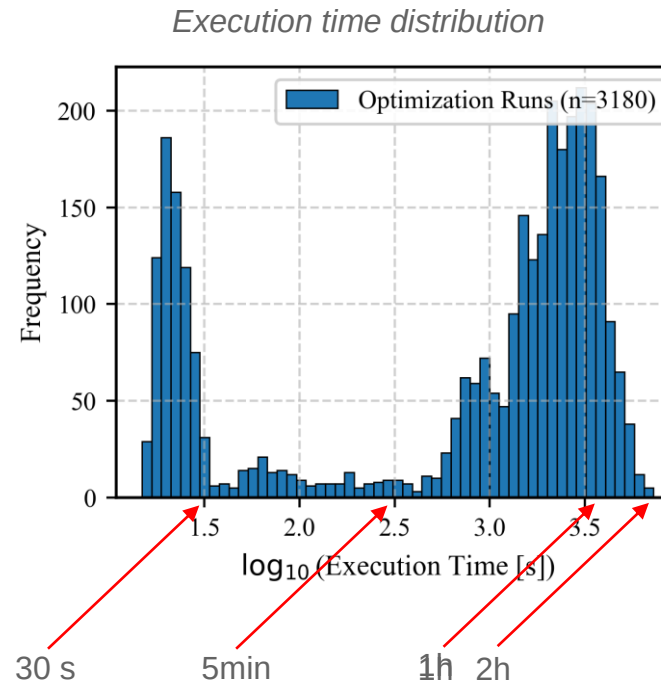
Single technology flowsheets

- Optimization algorithm runs in ~1 minute or less

Flowsheets with two technologies

- Simple tasks (e.g. minimize energy, or maximize recovery efficiency) run in a few minutes
- Complex tasks with strict additional criteria (e.g. minimize the energy while target element efficiency is more than 95%) can take up to 2h.
- Multi-start gradient descent approach.
 - Intrinsic randomness mitigates risk of convergence to local minima.

Execution time and Peak RAM utilization plots (Pt recovery flowsheet)
3180 runs / 318 distinct scenarios executed 10 times each.



FIREFLY APP

- Web based app
- Core Components
 - Knowledge Graph (Neo4j)
 - Backend orchestrator (Fast API)
 - Keycloak authentication service
 - User Interface (React.js & Chakra UI)
- Includes:
 - Single process prediction (running of surrogate models)
 - Flowsheet optimization
 - Interactive map of a GIS inventory of relevant resources.



Conclusions & Impact

Solution

AI surrogate models successfully bridged the gap between computationally heavy multiphysics simulations and rapid decision-making.

Performance

The dual-approach strategy (MLP & Analytical fitting) achieved exceptional predictive accuracy ($R^2 > 0.99$, low MAPE) without overfitting

Speed

Optimization of complex, up to 6-variable flowsheets achieved in minutes up to hours, keeping peak RAM utilization under 700 MB.

Impact

The digital tool provides a lightweight, highly reliable ecosystem ready for real-time industrial process optimization.





Thank You / Q&A



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A photograph of a large industrial facility, possibly a refinery or chemical plant, with numerous tall distillation columns and complex piping. The scene is set against a dramatic sky with orange and purple hues from a sunset or sunrise. The foreground shows some greenery and a blue-roofed building.

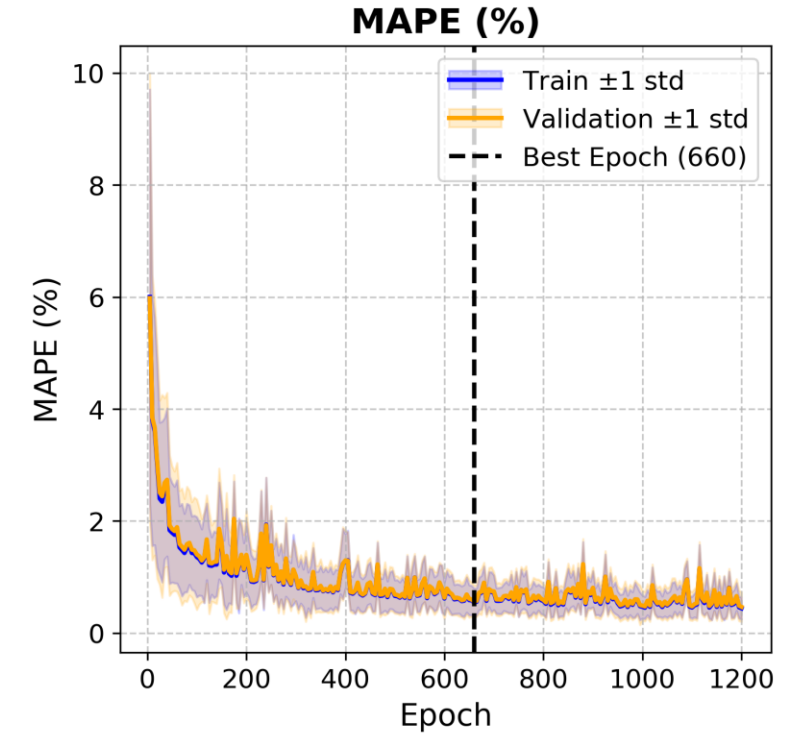
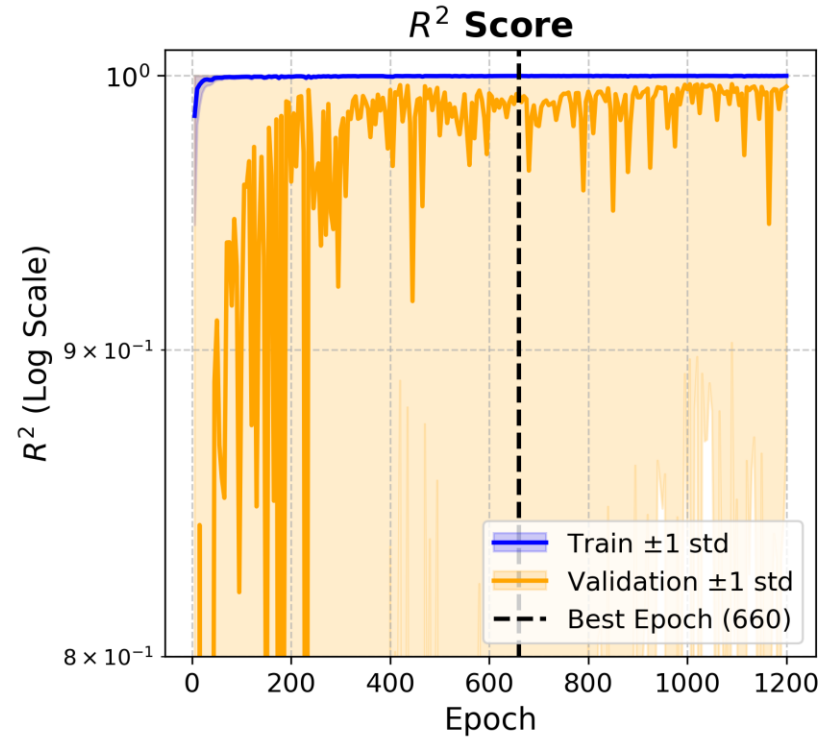
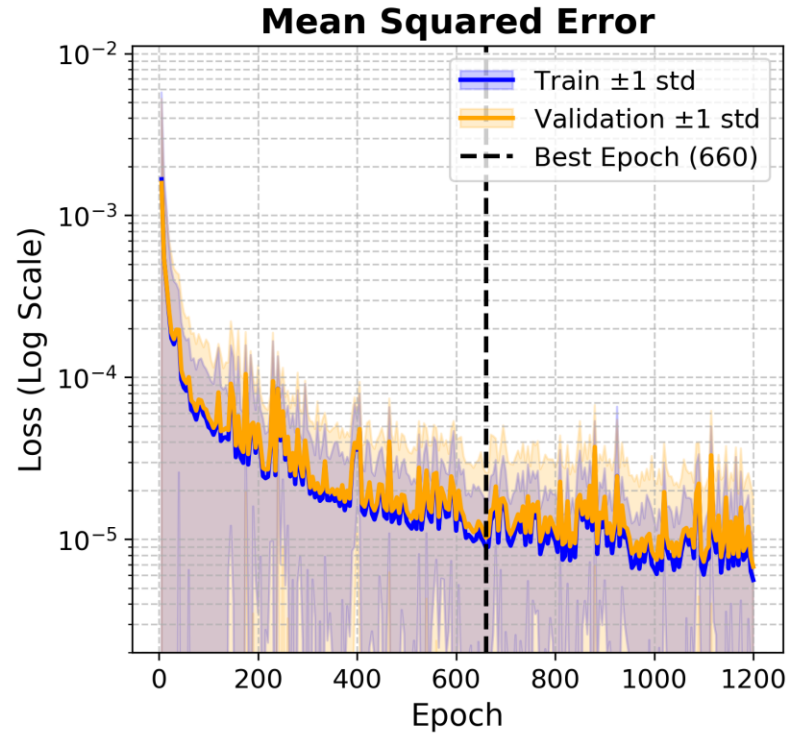
Back up



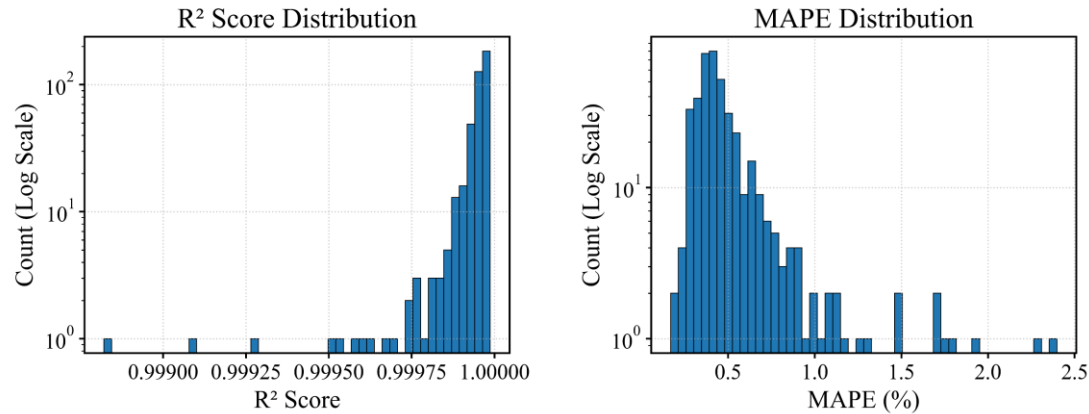
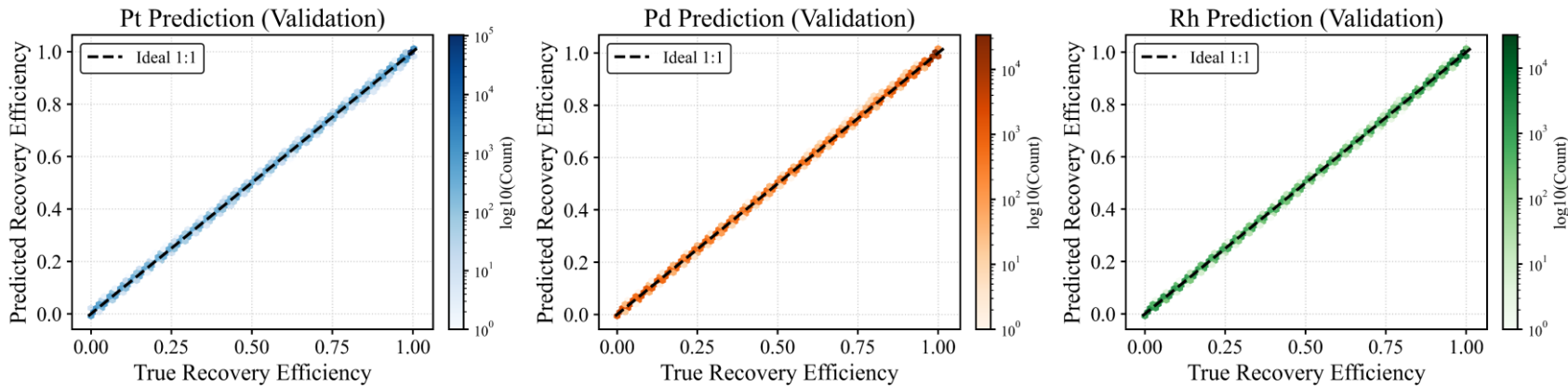
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GDEx surrogate model convergence plots



GDEx surrogate model metrics



Metric	Training Set	Validation Set	Test Set
R^2	0.99995 ± 0.00005	0.99994 ± 0.00007	0.99994 ± 0.00009
MAPE	0.55 ± 0.25	0.56 ± 0.30	0.56 ± 0.30