



AI-Driven Flowsheet Optimization via Multiphysics Surrogate Models

Machine Learning surrogate models trained on high-fidelity simulated datasets were integrated into a digital tool to predict electrochemical processes outputs and optimize metal recovery flowsheets.

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Introduction & Goals

The chemical industry heavily relies on strategic metal catalysts. However, recovering these from waste or off-specification catalysts poses significant challenges. The FIREFLY project addresses this by developing sustainable, electro-driven recycling flowsheets that combine advanced electrochemical technologies such as Gas-Diffusion Electro-crystallization (GDEx), Electroleaching (ELX) and Electrochemical Transformation in Molten Salts (ETMS).

While multiphysics simulations accurately capture the behavior of these electrochemical processes, they are computationally heavy and time-intensive thus, unsuitable for dynamic optimization. This work focuses on bridging that gap by training surrogate models. Integrated into a web application, this AI tool predicts the outputs and energy consumption of each process and optimizes the flowsheets against user-defined criteria and constraints.

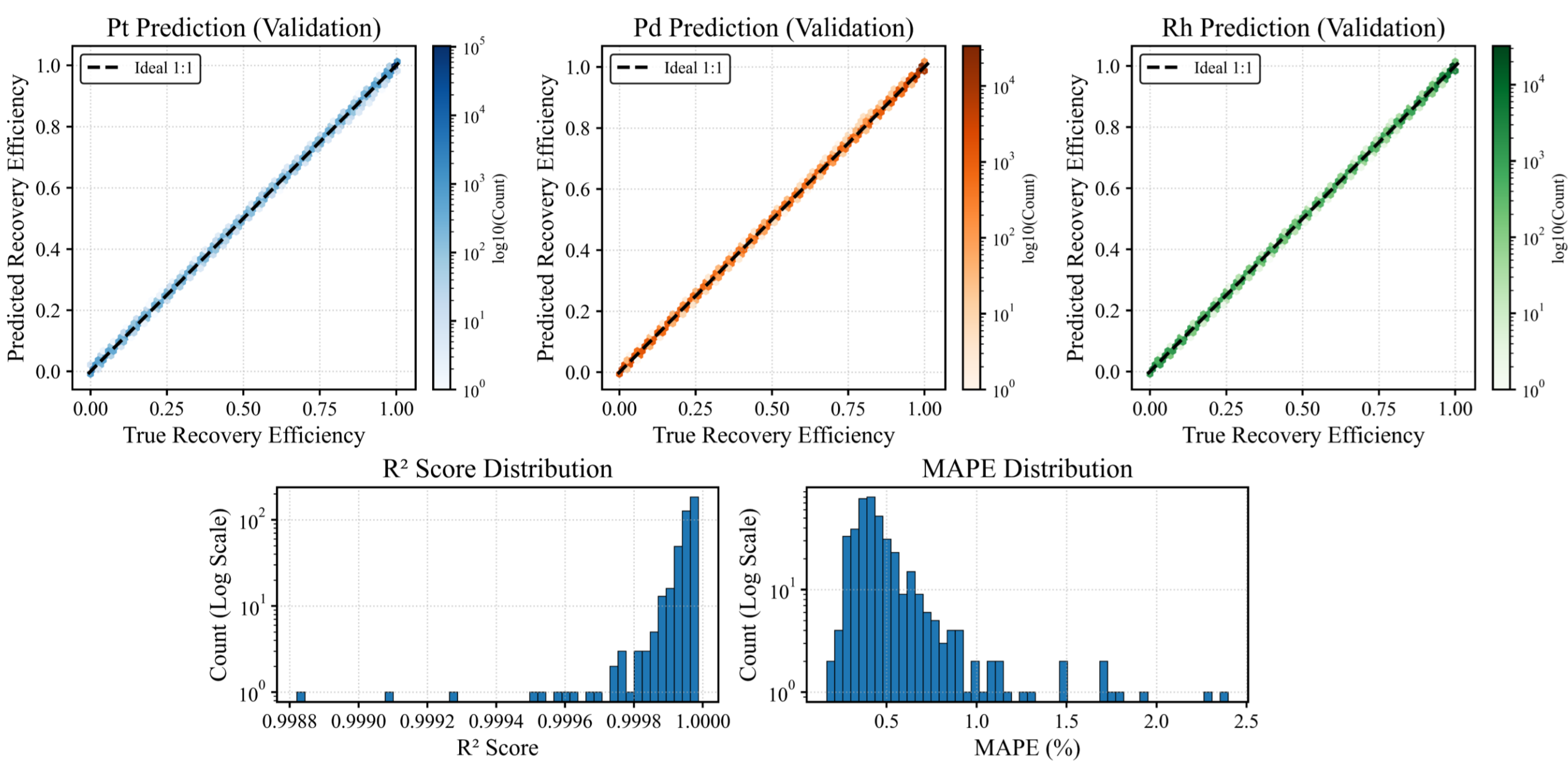


FIGURE 1: Validation performance of the GDEx MLP model. Top: Parity density plots for Pt, Pd, and Rh recovery. Bottom: R^2 score and MAPE distributions across all validation experiments

Methodology

Data Mapping: Operational variables mapped to recovery metrics utilizing high-fidelity COMSOL Multiphysics® datasets.

Data-Rich Processes (GDEx): Multi-Layer Perceptron (MLP) neural network trained on >1.9M simulated data points (~3k experimental conditions).

Validation Strategy: Data split by entire experimental runs.

Exceptional Model Performance: Reaching an average R^2 of 0.99995 ± 0.00009 and a MAPE of 0.56 ± 0.30 on the validation sets.

Smaller Data Processes (ELX): Modeled using physics-informed analytical functions, utilizing an average of 250 data points across 5 different setups.

Results

Model Integration: Seven surrogate models developed six of which based exclusively on COMSOL Multiphysics® simulations.

Flowsheet Construction: Four distinct recycling flowsheets were constructed using the above models.

Optimization Speed: Single-model flowsheets evaluated in seconds to minutes & complex flowsheets (coupling models, up to 6 parameters) evaluated in seconds to a few hours, depending on constraint strictness.

Practical Impact: Lightweight tool delivering fast and trustworthy results in dynamic tasks where heavy simulations are impractical.

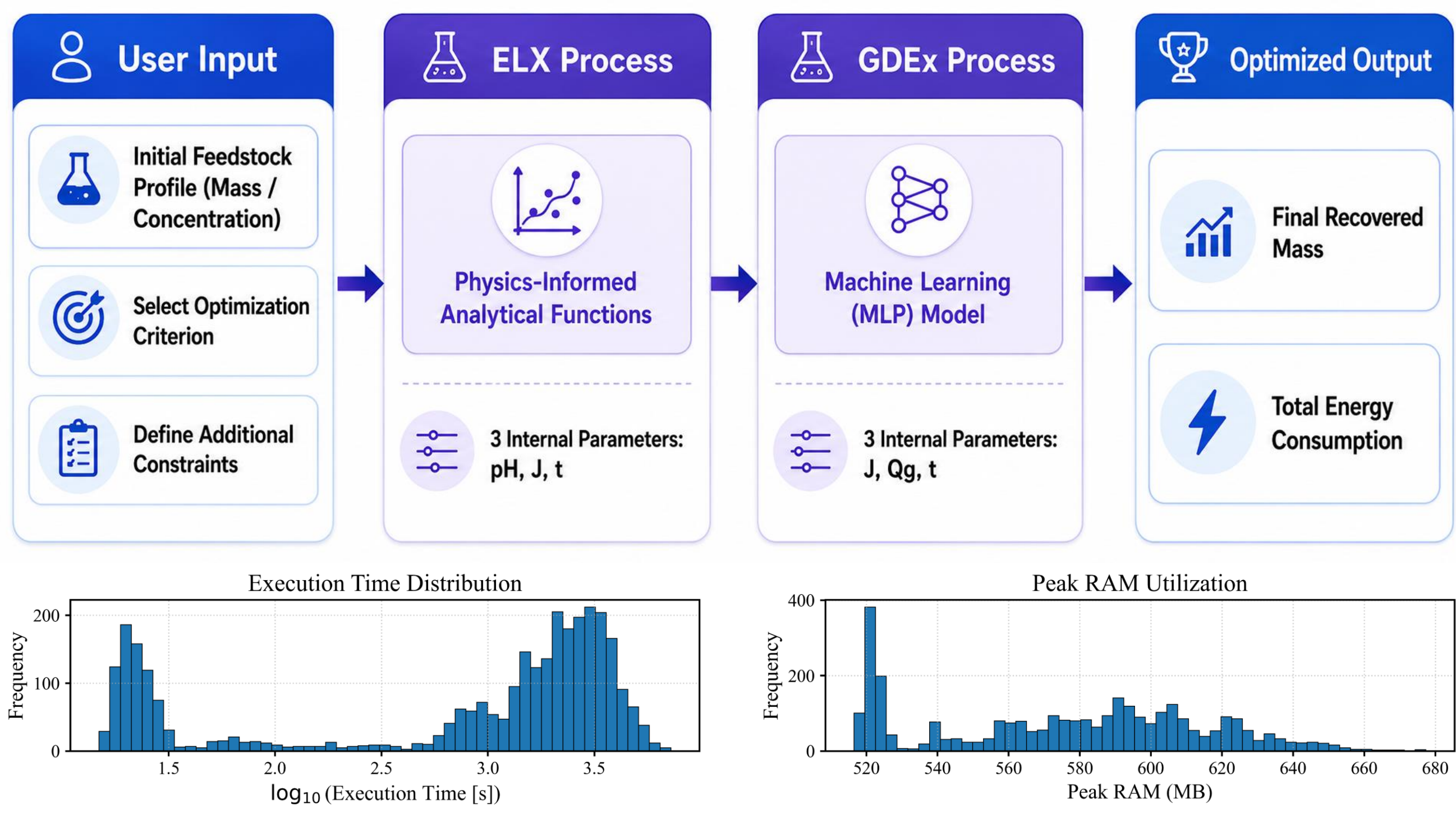


FIGURE 2: Example AI-driven optimization workflow (top) with time and RAM distributions for 3180 flowsheet evaluations under varying initial conditions.

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