



Artificial Intelligence in Critical Mineral Recovery: From Beneficiation to Recycling, and a Framework for Validating Deployment-Ready Models

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Abstract : Critical minerals are essential to electrification, renewable energy, advanced electronics, defense systems, and modern manufacturing, but their supply chains are increasingly strained by declining ore grades, geographic concentration, environmental constraints, and the growing volume of complex secondary resources. Artificial intelligence (AI) and machine learning (ML) are being applied across mineral beneficiation, flotation, hydrometallurgy, rare-earth separation, bioleaching, mine-waste recovery, and battery recycling, yet results from these areas are seldom judged using a common standard. This review brings these strands together and examines where AI is already providing credible engineering value, where the evidence is still preliminary, and what is needed for dependable scale-up. Across the literature, ensemble trees, support-vector methods, neural networks, computer vision, and hybrid physics-ML approaches have been used for recovery prediction, soft sensing, operating-condition optimization, froth analysis, leaching design, and rare-earth solvent-extraction screening. The strongest studies go beyond random train/test splits and include external, experimental, or prospective validation. Common limitations include small or proprietary datasets, changing feed characteristics, model drift, limited treatment of uncertainty, weak transferability between ores or waste streams, and insufficient connection to metallurgical fundamentals. On this basis, we propose two practical tools: a nine-test benchmarking framework for judging whether a recovery model has enough validation evidence for pilot or plant use, and a seven-layer architecture that places AI between resource characterization and process decision-making. We further argue that optimization should consider recovery and purity together with energy, water, reagents, emissions, residues, and cost. In this context, AI is most useful as a support layer for adaptive and circular critical-mineral recovery rather than as a substitute for process science.

IndexTerms - artificial intelligence, critical minerals, mineral processing, hydrometallurgy, bioleaching, battery recycling

Abbreviations

AI, artificial intelligence; AMD, acid mine drainage; ANN, artificial neural network; CFD, computational fluid dynamics; CNN, convolutional neural network; DEM, discrete element method; DNN, deep neural network; ECE, expected calibration error; FAIR, findable, accessible, interoperable, reusable; LCA, life-cycle assessment; LIB, lithium-ion battery; LOSO, leave-one-study-out; LSTM, long short-term memory; MAE, mean absolute error; ML, machine learning; MLOps, machine-learning operations; OOD, out of distribution; PDP, partial-dependence plot; PGM, platinum-group metal; REE, rare-earth element; REO, rare-earth oxide; RF, random forest; RL, reinforcement learning; RMSE, root-mean-square error; SHAP, SHapley Additive exPlanations; SVM, support-vector machine; SVR, support-vector regression; TEA, techno-economic assessment; ViT, vision transformer; XRD, X-ray diffraction; XRF, X-ray fluorescence.

I. INTRODUCTION

Critical minerals sit at the center of electrification, low-carbon power generation, energy storage, digital infrastructure, aerospace, and defense. Their strategic importance reflects more than rising demand. Criticality assessments consistently identify a combination of supply concentration, limited substitutability, and economic importance as the defining features of this material class [1,13-16]. Production and, more acutely, refining capacity are concentrated in a small number of jurisdictions, and the governance of that concentration has become a policy question as much as a market one [2,11,20]. National and regional assessments have translated these concerns into formal materials lists and, in the European case, into binding regulation [6,7,9,10]. Projections for clean-energy deployment indicate that material intensity, rather than technology cost alone, may constrain the rate at which low-carbon systems can be built [3-5,12,17,18]. Compounding this, several critical elements are recovered only as by-products of major metal production, so their supply responds weakly to their own price signals [19]. Mine waste, historically treated as a liability, is now recognized as a further reservoir of the same elements [8]. Meeting future demand will therefore require more than opening new deposits. The more immediate opportunity is to recover greater value from increasingly heterogeneous feedstocks while reducing energy use, water demand, reagent consumption, emissions, and residue generation. The rare-earth literature illustrates the shift most clearly: recovery from end-of-life products, industrial residues, and urban-mining feedstocks has been reviewed repeatedly over the past decade [21,24,25,30,31,44,45]. Individual streams have developed their own process literatures, including NdFeB permanent magnets [33-35,41-43], fluorescent-lamp phosphors [36-38], nickel-metal-hydride batteries [39,40], and rare-earth-bearing industrial process residues [32]. In parallel, tailings and mineral-processing wastes are being reassessed as resources rather than liabilities [46-48]; acid mine drainage (AMD) has been shown to carry recoverable rare earths and cobalt [50,113]; and separation technologies aimed specifically at dilute and heterogeneous secondary feeds are an active development area [49]. In practice, this broadens critical-mineral recovery from a mining problem into a resource-circulation problem, and it does so in a way that makes feed variability the central engineering difficulty. Mechanistic models remain the foundation of mineral processing and extractive metallurgy because they represent mass balance, thermodynamics, kinetics, interfacial chemistry, particle behavior, and reactor physics [97]. Their limitation is not scientific validity but the difficulty of describing every interaction in operations that are nonlinear, time-varying, and multiscale; comminution modeling has long been constrained by exactly this problem, and progress in energy-efficient comminution has been correspondingly slow [98,99]. Machine learning (ML) is useful in this setting when it complements, rather than replaces, metallurgical understanding by extracting relationships from complex process data. The methods now in routine use are mature and well documented outside metallurgy: ensemble trees [51,53,54], kernel methods [52], and deep networks [55,56], together with tools for post hoc interpretation [57,58], sample-efficient experimentation [62,63], and the embedding of physical law into learned models [59,60]. Their transfer into recovery engineering also imports a known failure mode. Leakage between correlated observations has been shown to inflate reported accuracy across ML-based science [64], and, as Sections 4 to 7 show, recovery datasets are unusually prone to it because neighboring records so often originate from the same ore campaign, image sequence, or published study. The role of AI in this field has also changed markedly. Earlier applications were dominated by classification, fault detection, and inferential measurement, and successive reviews of minerals-processing ML document the steady widening of that scope [67,68,73,74]. More recent surveys extend it to flotation optimization [69], pyrometallurgy [75], cross-process optimization in copper metallurgy [76], and general trends across minerals engineering [70-72]. Current studies use ML to guide experiments, screen extractants and adsorbents, predict leaching behavior from large literature-derived datasets, interpret froth images, and support optimization under changing process conditions. This movement from observation toward decision support is what makes a cross-domain assessment necessary now: the claims being made are no longer about measurement accuracy alone but about what a plant should do. Several capable reviews already cover mineral concentration [68], flotation froth analysis [78,92], pyrometallurgy [75], and individual secondary-resource streams [21,33,39]. What remains less developed is a unified view of AI across the full critical-mineral recovery chain, together with a common standard against which claims originating in these different domains can be compared. A model reported for froth imaging and a model reported for solvent-extraction screening are currently evaluated by conventions that have little in common, which makes it difficult for an engineer to judge which results are close to deployment. This review makes three contributions. First, it synthesizes the AI evidence across seven process domains – feed characterization, beneficiation and sorting, comminution, flotation, hydrometallurgy and rare-earth separation, bioleaching, and battery and secondary-resource recycling – within a single evaluative frame, so that a result reported in one domain can be judged against practice in another. Second, it proposes a nine-test benchmarking framework (Section 10, Table 6) that specifies the validation evidence an AI model should present before it is offered for pilot or plant use, in place of the headline accuracy metrics that currently dominate the literature. Third, it sets out a seven-layer architecture (Section 9, Fig. 2) in which AI sits between resource characterization and decision execution rather than operating as a stand-alone predictive module, and it identifies the research gaps that must close for that architecture to be realized (Table 7). The organizing question throughout is practical: where does AI already add defensible value, where is the evidence still preliminary, and what is required for reliable plant-scale adoption?

II. REVIEW SCOPE AND METHODOLOGY

We used a critical narrative-review design rather than a formal PRISMA systematic-review protocol. The aim is to compare and appraise evidence across domains rather than to produce an exhaustive count, because the constituent literatures use incompatible reporting conventions and a pooled quantitative synthesis across them would not be meaningful. For transparency, Table 1 gives the search and appraisal protocol used for the review.

Table 1. Search and appraisal protocol.

Protocol element	Detail
Review design	Critical narrative review with structured appraisal. No PRISMA protocol was registered. The original search was not logged as a systematic-review flow, so retrospective identification, screening, and full-text counts are not reported.
Databases searched	Targeted searches of scholarly discovery/indexing services and publisher databases, supplemented by backward reference chaining. A database-by-database search log was not retained in the original narrative-review workflow; specific databases are therefore not asserted retrospectively.
Search period	Literature available online through September 2026; final literature search and bibliographic verification completed 3 September 2026.
Core search strings	("artificial intelligence" OR "machine learning" OR "deep learning") AND ("critical minerals" OR "rare earth elements" OR flotation OR comminution OR hydrometallurgy OR leaching OR "solvent extraction" OR bioleaching OR "battery recycling" OR "mine waste" OR tailings OR "acid mine drainage").
Records identified	Not recorded during the original narrative-review workflow; not retrospectively reconstructed.
Records screened on title and abstract	Not recorded during the original narrative-review workflow; not retrospectively reconstructed.
Full texts assessed	Not recorded during the original narrative-review workflow; not retrospectively reconstructed.
Sources included in the synthesis	146 cited sources in the final synthesis, including peer-reviewed studies, foundational process sources, and authoritative institutional reports.
Inclusion criteria	Peer-reviewed studies reporting the recovery problem, feed or process context, model inputs, validation strategy, and predictive performance; foundational process literature required for metallurgical interpretation; authoritative institutional assessments of criticality and supply.
Exclusion criteria	Publications not available in English; conference abstracts without methodological detail; studies reporting no validation approach; AI applications outside the recovery chain (for example exploration targeting or fleet logistics).
Appraisal criteria	(i) Data representativeness; (ii) validation rigor; (iii) mechanistic plausibility and interpretability; (iv) evidence of prospective, experimental, pilot, or industrial utility.

Literature was assembled through targeted searches of scholarly discovery/indexing services and publisher databases using combinations of the terms listed in Table 1, supplemented by backward reference chaining from relevant reviews and primary studies. The evidence base spans foundational process literature and peer-reviewed AI/ML studies available online through September 2026; the final search and bibliographic verification were completed on 3 September 2026. Because the original narrative-review workflow did not retain a database-by-database search log, identification, title/abstract screening, and full-text assessment counts are not reconstructed retrospectively. Bibliographic details and DOI status were cross-checked against publisher pages, DOI-resolver records, or authoritative institutional records where available, with particular attention to recent and article-number-based entries; sources for which no DOI is assigned are cited without one. For the structured validation audit reported in Section 10, the 30 primary model-development studies were coded against the nine-test framework using binary indicators only when the relevant evidence was explicitly reported; the structured coding was retained by the authors and is available from the corresponding author upon reasonable request. Figures 3 and 4 were generated directly from this coding using reproducible Python plotting workflows. ChatGPT (OpenAI, GPT-5.6 Sol) assisted with tabulation-consistency checks and with drafting Python code used for the visualizations; it was not used to fabricate or alter source-study results. The authors reviewed the final coding and visualizations and take responsibility for the classifications and presentation. Studies were prioritized when they reported the recovery problem, the feed or process context, the model inputs, the validation strategy, the predictive performance, and any experimental confirmation or evidence of industrial relevance. AI-focused papers were interpreted alongside established literature in mineral processing, hydrometallurgy, bioprocessing, and recycling so that algorithmic results could be judged against mineralogy, chemistry, scale, and flowsheet constraints. During synthesis, evidence was organized by process stage and evaluated against four criteria: (i) data representativeness, meaning whether the training data plausibly span the feed and operating variability the model would face; (ii) validation rigor, meaning whether the evaluation design resembles deployment rather than a random resampling of one dataset; (iii) mechanistic plausibility and interpretability, meaning whether the learned relationships are consistent with known chemistry and process behavior; and (iv) evidence of prospective, experimental, pilot, or industrial utility. These four criteria are the basis of the critical-interpretation columns in Tables 4 and 5 and are formalized as testable requirements in Section 10. Three limitations follow from this design and should be borne in mind

throughout. The review does not claim a complete systematic search, and no PRISMA-style identification, screening, or full-text flow count is reported because those counts were not retained during the original narrative-review workflow. Studies published in languages other than English, and proprietary plant results that are not published at all, are under-represented; the latter is a systematic bias because the most operationally mature AI deployments may be the least likely to appear in the open literature. Finally, the appraisal of individual studies rests on what each paper reports, and reported validation design cannot be independently audited from a published account alone.

III. AI METHODS MOST RELEVANT TO RECOVERY ENGINEERING

The methods used most often in Sections 4 to 8 are summarized here, together with the situations in which they are most useful. Table 2 provides a compact selection guide and lists the reporting information needed for each method.

3.1 Supervised learning for tabular metallurgical data

Most recovery datasets are tabular rather than image based. Typical inputs include feed composition, particle size, pulp density, pH, redox potential, temperature, reagent dosage, residence time, and sensor measurements, with final grade, recovery, or extraction as the target. Random forests [51], support-vector regression [52], gradient-boosting methods such as XGBoost

[53] and CatBoost [54], and multilayer neural networks are therefore the workhorses of the field. Their appeal is the ability to capture nonlinear interactions without requiring an explicit closed-form process equation, and the evidence base for their use in leaching and extraction prediction is now substantial [107-109,114]. Two cautions apply throughout. First, tree ensembles interpolate well but extrapolate poorly: predictions outside the convex hull of the training conditions revert toward the training mean rather than following the underlying chemistry, which is precisely the wrong behavior when a plant moves to an unfamiliar feed. Second, tabular metallurgical data are rarely independent. Rows frequently share an experimental campaign, a sample, or a source publication, and treating them as independent during resampling produces optimistic error estimates of the kind documented across ML-based science [64]. Both issues argue for grouped rather than random validation, a point developed in Section 10.

3.2 Deep learning and computer vision

Processes that generate images or spectra have opened a different pathway. In ore sorting and flotation, convolutional neural networks, transfer learning, segmentation methods, and more recently vision-transformer architectures can extract information that is difficult to encode by hand [55,56]. Froth images, for example, contain cues related to bubble size, texture, color, stability, mineral loading, and dynamic behavior, and a decade of froth-image work has progressively replaced hand-crafted descriptors with learned representations [79,80,85-87]. The central risk is that the model learns process-irrelevant features. Lighting, camera position, lens fouling, and background conditions all correlate with plant state in a single-site dataset, and a model can achieve excellent held-out accuracy by exploiting those correlations rather than the froth itself. Testing on imagery from a different camera installation, or at minimum from a different campaign, is the only reliable way to distinguish the two cases.

3.3 Explainable AI and uncertainty

For recovery engineering a point prediction is rarely sufficient. An engineer also needs to know whether the model is operating inside its domain of experience and which variables are driving a recommendation. Shapley-value attribution [57], local surrogate explanations [58], permutation importance, and partial-dependence analysis can be used to test whether learned relationships are consistent with known chemistry. Used carefully, these are diagnostic instruments rather than substitutes for mechanistic interpretation: an attribution that contradicts established solution chemistry is evidence of a data artifact, not the discovery of new chemistry. Uncertainty deserves equal weight and receives far less. Prediction intervals, calibration checks, and out-of-distribution detection determine whether a recommendation is safe to act on, and their absence is one of the clearest markers separating a demonstration from a deployable tool. Structured documentation practices developed in the wider ML community, notably datasheets for datasets [65] and model cards [66], provide a ready template for reporting these properties in metallurgical work.

3.4 Hybrid and physics-informed approaches

Purely data-driven models are especially vulnerable when mineralogy, solution chemistry, or battery composition moves beyond the training range. Hybrid and physics-informed approaches offer a more robust alternative by coupling ML with mass balances, kinetic equations, thermodynamic relationships, CFD or DEM simulations, or known monotonic trends [59,60]. Such constraints reduce nonphysical predictions and, in favorable cases, lower the quantity of data required for useful calibration – an important consideration when each additional data point is a leaching experiment rather than a database query. Related methods address the cost of experimentation directly: Bayesian optimization selects the next most informative condition rather than sampling a grid [62], active learning does the same for labeling effort [63], and reinforcement learning offers a framework for sequential set-point policy once a sufficiently trustworthy process model exists [61]. This sequence is important. Reinforcement learning applied directly to a high-value plant is a safety question rather than a modeling question, which is why Section 9 places digital-twin verification ahead of closed-loop autonomy.

Table 2. AI methods and their suitability for critical-mineral recovery.

Method	Strength	Best suited data	Typical recovery use	Weakness	Recommended reporting
Random forest	Robust nonlinear baseline; feature importance	Small to medium tabular	Recovery/grade prediction; soft sensing; baseline modeling	Poor smooth extrapolation	Cross-validation, external test, feature stability
XGBoost / CatBoost	Strong tabular accuracy; captures interactions	Heterogeneous tabular	Leaching/extraction prediction; heterogeneous process optimization	Hyperparameter sensitivity	Nested tuning, SHAP, calibration
SVM / SVR	Effective on small nonlinear datasets	Small standardized datasets	Small-data recovery and leaching prediction	Scaling and kernel choice	Sensitivity analysis across kernels
ANN / DNN	Flexible nonlinear approximation	Medium to large datasets	Nonlinear recovery, purity, and process-state prediction	Opaque and data-hungry	Architecture, regularization, uncertainty
CNN	Automated spatial feature learning	Images and spectra	Froth/particle image analysis; ore sorting; visual soft sensing	Requires labels; domain shift	Independent-site testing
Vision transformer	Captures global image relationships	Large image datasets	High-capacity froth and process-image monitoring	High data and compute demand	Benchmark against CNN baselines
Bayesian optimization	Sample-efficient experimental selection	Expensive experiments	Sample-efficient selection of experimental conditions	Depends on surrogate validity	Report search bounds and constraints
Reinforcement learning	Sequential decision optimization	Dynamic process environment	Sequential set-point and control-policy optimization	Safety and sample efficiency	Train in a validated digital twin first
Physics-informed ML	Embeds process knowledge	Mixed physics and data	Physics-constrained recovery prediction and process optimization	Model- development complexity	Ablation against pure physics and pure ML

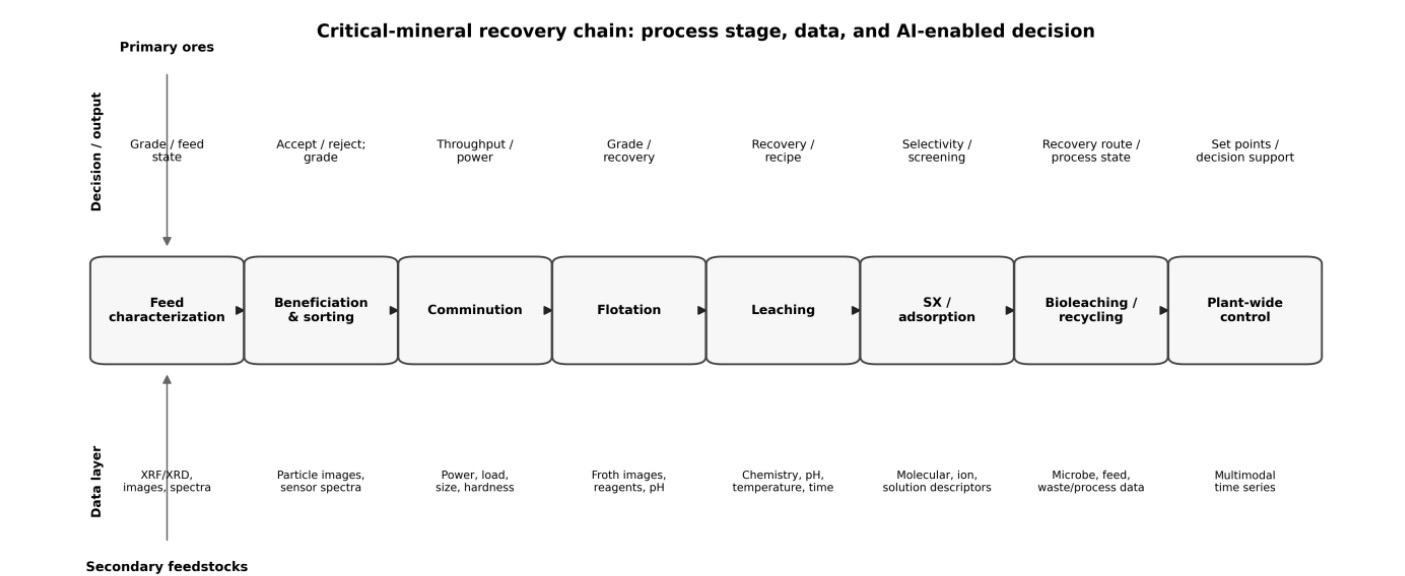


Fig. 1. The critical-mineral recovery chain and the AI task layer mapped onto each stage, for primary ores and secondary feedstocks. Data sources are shown below each stage and the corresponding decision output above it. Python was used to prepare the plotting and layout code, with assistance from ChatGPT (OpenAI, GPT-5.6 Sol). The authors reviewed and verified the final schematic.

Table 3. Functional role of AI across the critical-mineral recovery chain.

Stage	Typical data	AI task	Representative algorithms	Primary value	Key risk
Feed characterization	Mineralogy, XRF/XRD, images, hyperspectral data	Classification; grade estimation; anomaly detection	RF; SVM; CNN; ViT	Rapid feed decisions	Domain shift between deposits
Beneficiation and sorting	Particle images, sensor spectra, operating data	Ore/waste discrimination; recovery prediction	CNN; transfer learning; RF; SVM	Reject barren material early	Biased labels; changing ore texture
Comminution	Power, load, size distribution, hardness	Throughput and power prediction; optimization	RF; ANN; Bayesian networks; hybrid ML	Energy and throughput control	Sensor drift; causal ambiguity

Stage	Typical data	AI task	Representative algorithms	Primary value	Key risk
Flotation	Froth images, reagents, air, pH, mineralogy	Grade and recovery soft sensing; control	RF; ANN/DNN; CNN; ViT	Real-time monitoring	Lighting and feed variability
Leaching	Feed chemistry, pH, temperature, time, reagent dosage	Recovery prediction; recipe optimization	SVR; gradient boosting; XGBoost; ANN	Reduced experimental burden	Extrapolation outside training range
Solvent extraction and adsorption	Molecular descriptors, pH, concentration, ion properties	Distribution and selectivity prediction; material screening	FCNN; CatBoost; gradient boosting; SHAP-assisted ML	Accelerated separation design	Data sparsity for new chemistries
Bioleaching	Microbe, pH, temperature, pulp density, feed	Recovery prediction; factor ranking	RF; gradient boosting; ensemble ML; ANN	Handles nonlinear bioprocesses	Temporal biological dynamics
Recycling and secondary resources	Battery chemistry, waste composition, sensor and process data	Sorting; disassembly; leaching optimization	XGBoost; RF; SVM; CNN	Adaptive processing of heterogeneous waste	Uncertain feed provenance
Plant-wide control	Multimodal time series and process-model states	Optimization; forecasting; decision support	Hybrid/physics-informed ML; forecasting models; RL	Closed-loop autonomy	Safety, interpretability, cybersecurity

IV. AI IN BENEFICIATION, ORE SORTING, COMMINATION, AND FLOTATION

Beneficiation is an attractive point for AI intervention because decisions made early in the flowsheet propagate downstream. Rejecting barren material before fine grinding reduces comminution energy, water use, reagent demand, and tailings generation simultaneously, so a modest improvement in early discrimination is worth more than a comparable improvement later. Reviews by McCoy and Auret and by Gomez-Flores et al. show that AI has been applied across sensing, ore classification, concentration, comminution, and flotation [67,68]. The practical value is greatest when a prediction is tied to a specific operating decision rather than treated as an isolated classification exercise.

4.1 Sensor-based sorting and characterization

Sensor-based sorting combines optical, X-ray, laser, hyperspectral, or related measurements with a classification decision. The harder problem is not usually achieving high accuracy on the original dataset, but maintaining that accuracy when moisture, particle size, surface condition, lighting, or mineral texture changes. Ore texture in particular varies systematically with position in a deposit, so a classifier trained on one bench can encounter a genuinely different input distribution a few months later without any change in the sensor or the algorithm. Models intended for deployment should therefore be challenged with material from different campaigns or deposits rather than evaluated only through random train/test splits drawn from a single sample population, and the resulting degradation should be reported rather than suppressed.

4.2 Comminution

Comminution remains one of the largest energy consumers in mineral processing, and its behavior depends on ore hardness, feed size, mill load, water addition, liner condition, and liberation requirements [98,99]. AI can provide soft sensors for states that are difficult or expensive to measure continuously, and it can support probabilistic rather than point estimates of throughput, power, or product size; Bayesian network models of semi-autogenous milling illustrate this probabilistic framing in an industrial copper context [100]. The more credible applications preserve physical constraints and are tested across meaningful changes in ore characteristics. A model that predicts mill power accurately within one ore type but cannot be transferred to the next blend has demonstrated curve fitting rather than process understanding, and the distinction is invisible unless the transfer is actually attempted.

4.3 Flotation

Flotation has one of the most mature AI literatures in mineral processing because both operating variables and froth appearance carry information about process state. Early machine-vision studies established links between froth texture, bubble size, color, velocity, and metallurgical response, and several were implemented industrially [77,94-96]. The control literature that developed alongside them clarified what a froth sensor is actually for: stabilizing a loop, not producing an estimate in isolation [93]. Newer deep-learning approaches learn these relationships directly from images rather than from engineered descriptors [78,92], which makes flotation a useful test bed for the wider transition from offline prediction to real-time sensing and control. Several recent results bear directly on critical minerals. Gomez-Flores et al. compared multivariable regression, k-nearest neighbors, decision trees, and random forests using physicochemical and operational flotation variables, and found that random forests best captured the tested behavior [82]. Pu et al. developed a hierarchical network, FlotationNet, using 3,498 industrial observations to predict iron and silica product purities, with noticeably weaker performance on silica than on iron [81]. Industrial work combining hybrid image features with deep learning reported prediction of Zn, Pb, Fe, and Cu concentrate grades with real-process errors below approximately 4.53% [90]. Neural-network models built on batch and pilot-column image data established comparable relationships earlier and at smaller scale [83,84], and segmentation approaches such as Mask R-CNN have been applied to resolve individual bubbles rather than treat the froth as a texture [87]. Vision-transformer studies, including CNN-versus-transformer comparisons on platinum-group-metal flotation imagery, mark the continued movement toward high-capacity

image models [88,89], while work on unstable flotation conditions addresses the case that matters most operationally, namely the froth that is not behaving normally [91]. Transferability remains the principal weakness across this body of work. Many flotation models are developed within a narrow ore blend, reagent regime, camera geometry, or lighting condition. Excellent performance on held-out images from the same campaign does not establish that behavior will persist after a change in mineralogy or reagent chemistry, and because froth appearance is a downstream consequence of both, the failure can be silent: the model continues to produce confident, plausible, and wrong estimates. More credible studies should use temporal or campaign-wise validation, report drift explicitly, and state how the model is to be recalibrated when the operating domain moves.

Table 4. Representative AI studies in mineral processing and flotation.

Study	Process / feed	Data validation and	AI method	Target	Key result	Main limitation
McCoy & Auret (2019) [67]	Mineral processing review	Review literature; no single validation dataset	Multiple ML methods	State of the field	Identified modeling, diagnosis, and machine vision as core areas	Heterogeneous evidence base
Gomez-Flores et al. (2022) [68]	Mineral concentration	Review literature; no single validation dataset	Supervised and unsupervised AI	Technology mapping	Reviewed gravity, density, magnetic, and sensor-based separations	Limited industrial standardization
Fu & Aldrich (2018) [79]	Flotation froth	Flotation-froth image dataset; transfer-learning evaluation	Transfer learning with CNN	Froth feature extraction	Pretrained CNN outperformed conventional features	Site-specific image domain
Pu et al. (2020) [81]	Iron flotation plant	3,498 industrial observations; comparative predictive evaluation	Hierarchical DNN	Fe and silica prediction	Best iron prediction among baselines; silica prediction weaker	Uneven performance across outputs
Gomez-Flores et al. (2022) [82]	Flotation	Physicochemical and operating variables; comparative model evaluation	RF, KNN, DT, regression	Grade and recovery	RF performed best among the compared methods	Cross-ore generalization not established
Aldrich et al. (2022) [78]	Froth image analysis	Review of froth-image analysis studies; no single validation dataset	CNN and transfer learning	Soft sensing	Deep learning increasingly dominant	Label scarcity and domain shift
Bendaouia et al. (2024) [90]	Polymetallic flotation	Industrial polymetallic-flotation data; application-test evaluation	CNN with ML/ANN	Zn, Pb, Fe, Cu grade	Application-test error below 4.53% for concentrate grade prediction	Single-site deployment
Liu & Aldrich (2024) [89]	PGM flotation	Industrial PGM flotation images; ViT/CNN comparison	ViT and CNN	Process monitoring	ViT and CNN features compared on industrial images	Needs broader cross-site validation
Qu et al. (2025) [92]	Flotation froth	Review of multimodal/deep-learning studies; no single validation dataset	Multimodal and deep learning	Monitoring and control	Identified multimodal and physics-informed directions	Future concepts exceed present deployment

V. AI-DRIVEN HYDROMETALLURGY AND RARE-EARTH SEPARATION

Hydrometallurgy is particularly well suited to ML because extraction outcomes depend on many interacting variables: feed composition, particle size, lixiviant concentration, pH, redox potential, temperature, time, solid-to-liquid ratio, extractant structure, phase ratio, and competing ions. The foundational process literature for rare earths documents how tightly these variables are coupled and how narrow the operating windows can be [22,23,26-29]. Experimental campaigns therefore become expensive as dimensionality increases, and a well-validated surrogate model can narrow the search space provided that its applicability limits are stated explicitly.

5.1 Leaching prediction and optimization

The pyrolusite leaching study by Zhang et al. demonstrated that support-vector regression could predict manganese leaching with $R^2 = 0.92$ under the investigated conditions [107]. For ion-adsorption rare-earth ore, a literature-derived dataset of 2,365 entries with 14 input variables was used to train ML models; an optimized gradient-boosting regressor achieved a test-set $R^2 = 0.9063$, and partial-dependence analysis was used to interpret parameter interactions [108]. Machine-learning-guided recovery from NdFeB magnet waste has combined model development with parameter-influence analysis and experimental validation, which is a materially stronger evidential position than model comparison alone [109]. Related work extends data-driven methods to process measurement rather than process prediction, using spectro-colorimetric analysis with ML to infer concentrations during automated solvent extraction [106]. Such approaches are valuable as surrogate models, but they should be treated as interpolation tools operating within a documented process envelope rather than as general descriptions of leaching chemistry. Battery recycling provides the clearest example of literature-scale learning. Niu et al. assembled 17,588 data points from published hydrometallurgical studies and evaluated XGBoost, random forest, support-vector, and AdaBoost models across 20 input features to predict four metal-leaching outputs (Li, Co, Mn, Ni), with a graphical interface and additional experiments used to demonstrate practical guidance [114]. The scale of the dataset is a genuine strength. It also introduces hidden heterogeneity, because literature-derived records differ in analytical method, pretreatment, cathode history, and reporting convention, and these differences are

correlated within source publications rather than distributed randomly across them. The appropriate response is not to discard such datasets but to validate them by holding out entire studies, as discussed in Section 10.

5.2 Rare-earth solvent extraction

Rare-earth solvent extraction is one area where AI is beginning to move beyond process prediction toward the design of separation materials. Liu et al. trained fully connected neural networks on molecular descriptors, extended-connectivity fingerprints, rare-earth properties, and extraction conditions, then synthesized and tested new ligands experimentally [101]. That combination of prediction and laboratory confirmation is more persuasive than accuracy alone, because it demonstrates that the learned relationships can guide experiments the model has not seen. By 2026 the evidence base had expanded substantially. A curated dataset of 3,343 extraction points was used to train a CatBoost model that achieved $R^2 = 0.96$ and $MAE = 0.14$ for distribution-ratio prediction, with laboratory validation across fourteen lanthanides [102]. A separate organophosphorus-ligand study used more than 3,500 measurements and reported R^2 values of approximately 0.98 for training and 0.83 for testing, linking pH, molecular fragments, partial charges, ionic radii, and topology to extraction behavior [103]. The gap between those two figures is informative because it quantifies how much of the apparent performance depends on ligands the model has already seen. Collectively, these studies suggest that chemically informed descriptors combined with explainable boosting are becoming practical screening tools for solvent-extraction development, with the important qualification that screening narrows a candidate list and does not replace the experimental program that follows it. AI is also entering adsorbent design and selective recovery from dilute solutions. Feature-engineering approaches have predicted rare-earth adsorption capacity from molecular and material descriptors [104], while newer work applies leave-one-study-out validation together with SHAP analysis to identify the nanomaterial features that control selective REE capture [105]. The leave-one-study-out design is particularly useful here because it directly addresses the heterogeneity problem described above. This line of work is particularly relevant to mine water, phosphogypsum leachates, and process effluents, where concentrations are often too low for conventional bulk separation [110-112].

Table 5. Representative AI-enabled hydrometallurgical and rare-earth recovery studies.

Study	Feed / process	Dataset validation and	Model	Inputs	Output performance and	Critical interpretation
Liu et al. (2022) [101]	REE solvent extraction	Extraction data using molecular descriptors, REE properties, and process conditions; newly designed ligands were synthesized and tested experimentally	FCNN	Ligand fingerprints and descriptors plus conditions	Predicted separation/extraction behavior and guided ligand screening; laboratory confirmation of model-guided candidates	Experimental follow-up provides stronger evidence than model comparison alone; broader chemistry transfer still requires testing
Zhang et al. (2022) [107]	Pyrolusite leaching	Pyrolusite-leaching experimental data evaluated under the investigated operating conditions	SVR, GBR and others	Leaching conditions	Manganese-leaching prediction with reported $R^2 = 0.92$	Good within-domain predictive performance; transfer beyond the investigated process envelope is not established
Niu et al. (2023) [114]	Spent LIB acid leaching	17,588 literature-derived data points; 20 input features; additional experiments used for practical demonstration	XGB, RF, SVM, AdaBoost	20 feed and process features	Predicted Li, Co, Mn, and Ni leaching; XGBoost/RF/SVM/AdaBoost compared and a graphical interface demonstrated	Large evidence base, but study-level heterogeneity and correlated source records create leakage/transfer risks
Bashiri et al. (2024) [104]	REE adsorption	REE-adsorption data represented with engineered molecular/material descriptors	Feature- engineered ML	Adsorbent and REE descriptors	Predicted rare-earth adsorption capacity from adsorbent and REE features	Useful for screening, but extrapolation to new materials and chemistries requires external validation
Xu et al. (2025) [109]	NdFeB magnet waste	NdFeB-magnet-waste leaching data with parameter-influence analysis and experimental validation	XGBoost best among four algorithms	Leaching and process variables	XGBoost performed best among the compared algorithms and was used to guide recovery conditions	Model development plus laboratory validation provides stronger deployment evidence than retrospective comparison alone
Liu et al. (2025) [108]	Ion-adsorption RE ore	Literature-derived dataset of 2,365 entries with 14 input variables; test-set evaluation and partial-dependence analysis	Gradient boosting	14 variables	Optimized gradient-boosting regressor achieved test-set $R^2 = 0.9063$	Strong predictive result for the compiled domain; source-wise transfer should be tested because literature records are correlated
Luo et al. (2025) [105]	Wastewater adsorption	Literature-derived wastewater/adsorption data evaluated with leave-one-study-out validation and SHAP analysis	ML with SHAP	Material and operating variables	Predicted selective REE capture and identified influential material/operating features	Leave-one-study-out validation directly addresses between-study heterogeneity and is stronger than random row splitting

Study	Feed / process	Dataset and validation	Model	Inputs	Output performance and	Critical interpretation
Liu et al. (2026) [102]	REE solvent extraction	Curated dataset of 3,343 extraction points; laboratory validation across fourteen lanthanides	CatBoost with SHAP	Extractant, conditions, and REE properties	CatBoost achieved $R^2 = 0.96$ and $MAE = 0.14$ for distribution-ratio prediction	High reported accuracy plus multi-lanthanide laboratory validation supports screening use within the documented domain
Zhang et al. (2026) [103]	REE solvent extraction	More than 3,500 solvent-extraction measurements with separate training and test evaluation	CNN and data-driven model	Ligand, ion, and conditions	Reported $R^2 \approx 0.98$ for training and ≈ 0.83 for testing	Train-test gap indicates reduced performance on less-familiar ligands and highlights the importance of external chemistry validation

VI. AI-ASSISTED BIOLEACHING AND BIORECOVERY

Bioleaching is attractive for low-grade ores and wastes because microorganisms and their metabolites mobilize metals through acidolysis, redox reactions, complexation, and related mechanisms, often under ambient conditions and without concentrated mineral acids [115-119]. The technology is established at commercial scale for sulfide ores, particularly in copper heap leaching, where decades of operating experience have clarified both its economics and its rate limitations [128,129]. Applying the same logic to critical minerals is a more recent development. Phosphate-solubilizing bacteria have been used to leach rare earths from monazite-bearing ore

[120]; element yield and community structure have been examined for high-grade monazite under different carbon sources [121]; fungal systems such as *Penicillium expansum* have been applied to rare earths in electronic waste [122]; and direct bioleaching has been demonstrated on coal fly ash

[123]. Downstream, biosorption offers a complementary route for preconcentrating rare earths from dilute solution [111,112]. The same biological complexity that makes these systems versatile makes them difficult to optimize. Recovery depends on feed mineralogy, microbial community composition, pH, temperature, nutrient supply, pulp density, aeration, particle size, and time, with strong interactions among these variables and with several of them under partial biological control rather than direct operator control. This is a setting where empirical modeling has clear value, because the coupled biology and chemistry are not yet described well enough mechanistically to support first-principles optimization. A major ML study compiled 871 experimental observations from 206 papers and evaluated 40 regression algorithms; random forest gave the strongest performance among those tested, and resource type, particle size and density, temperature, and microorganism emerged among the most influential predictors [124]. A later meta-analysis of waste-derived REE bioleaching combined statistical synthesis with predictive analytics, reporting an average recovery of approximately 56% with support-vector regression reaching $R^2 \approx 0.87$ [125]. More recent work on spent-battery bioleaching applied ensemble learning, SHAP attribution, and Bayesian optimization: XGBoost alone reported $R^2 = 0.885$, the stacked XGBoost-XGBoost model reported $R^2 = 0.949$, and an inverse-prediction example increased modeled recovery from approximately 60% to 99% when pulp density was raised from 0.5% to 5% for *Acidithiobacillus thiooxidans* [126]. Reviews of microbial routes for spent lithium-ion batteries place these results in the context of a still-emerging process literature [127]. Two limitations recur. First, the ranking of influential variables across these studies reflects what the source experiments chose to vary, not what governs bioleaching in general; a factor held constant throughout a literature cannot be identified as important by a model trained on it. Second, and more consequentially, most current models treat bioleaching as a static input-output problem, predicting final extraction from endpoint variables. Biological recovery is inherently dynamic. Microbial populations shift, metabolite production rises and falls, passivation layers form, oxygen transfer becomes limiting, and metal toxicity accumulates, all on timescales comparable to the leach itself. A model that maps initial conditions to final recovery cannot represent a system in which the same initial conditions can follow different trajectories, and it therefore cannot support intervention partway through a leach, which is precisely where operational value lies. Future work should incorporate time-series measurements, population dynamics, or mechanistic biokinetic constraints, and should report performance at intermediate times rather than at the endpoint alone.

VII. AI AND INTELLIGENT RECYCLING OF LITHIUM-ION BATTERIES

Spent lithium-ion batteries (LIBs) are a strategically important secondary source of Li, Ni, Co, Mn, Cu, Al, graphite, and, depending on chemistry, phosphate-bearing material. The recycling literature spans mechanical pretreatment, pyrometallurgy, hydrometallurgy, direct recycling, deep-eutectic-solvent processing, and bioleaching [130-136,141,142], and the field has been mapped in enough detail that the remaining difficulties are largely operational rather than conceptual. AI can intervene before, during, and after metallurgical recovery, and the three points differ in maturity.

7.1 Identification, sorting, and disassembly

Battery recycling begins with uncertainty about cell format, chemistry, state of charge, state of health, damage history, and manufacturer-specific design [130]. Computer vision and other sensor models can support automated sorting and robotic or semi-autonomous disassembly, while state-of-health assessment helps distinguish cells suitable for reuse or repurposing from those requiring material recovery [137]. These front-end decisions carry disproportionate weight: they improve safety, and they reduce

the feed variability that every downstream unit operation must otherwise absorb. A sorting error is not merely a lost unit of value but a perturbation propagated into leaching chemistry.

7.2 Data-driven leaching and downstream separation

Hydrometallurgical operations have attracted the most direct ML attention because they expose measurable input-output relationships and are already central to industrial battery recycling. Literature-scale models can estimate metal dissolution across many combinations of acid, reductant, temperature, time, and particle size [114]. A recent framework goes further by integrating preliminary environmental and economic assessment directly into the modeling workflow, so that candidate leaching conditions are screened against cost and impact rather than extraction alone [138]. That integration is the direction the field should take. The remaining step is to connect leaching prediction with selective precipitation, solvent extraction, membranes, electrowinning, or direct precursor synthesis, so that optimization targets product quality and total flowsheet performance instead of a single extraction figure that may be achieved at the expense of everything downstream.

7.3 Emerging AI opportunities in direct recycling

Direct recycling aims to preserve or regenerate electrode materials rather than reduce them fully to elemental or salt products, and its process fundamentals and scale-up constraints are now reasonably well characterized [139,140]. This creates an emerging rather than established AI opportunity in material diagnosis: models could infer degradation mode, lithium deficiency, transition-metal disorder, contamination, or particle damage from characterization data and help select an appropriate regeneration pathway. Automated characterization coupled with AI-guided decision support could eventually enable chemistry-aware recycling lines. Current evidence, however, is considerably stronger for direct-recycling process development and for AI-assisted front-end operations than for closed-loop AI deployment [137,139,140], and this section is included as a research direction rather than a summary of demonstrated results.

VIII. MINE WASTE, ACID MINE DRAINAGE, AND SECONDARY-RESOURCE RECOVERY

Mine wastes are increasingly viewed not only as environmental liabilities but also as secondary mineral resources. Tailings may retain REEs, Li, Co, Ni, Ti, Zr, Nb, W, and Sb, and their reprocessing has been assessed both as a supply opportunity and as a route to reducing the environmental burden of legacy sites [8,46-48]. AMD can carry dissolved rare earths and cobalt, and adsorption to precipitated manganese(IV) oxides has been shown to offer a high-grade recovery route from such waters [50,113]. Phosphogypsum represents a further large-volume stream from which rare earths can be leached [110]. Advanced separation technologies aimed specifically at dilute and heterogeneous secondary feeds are developing alongside these resource assessments [49]. These resources are difficult for reasons that differ from those of primary ores. Composition varies across space and across time, grades are low, and the recovery process must frequently satisfy water-treatment or residue-management constraints simultaneously with a metallurgical objective. In an AMD system the feed is not merely variable but externally driven, responding to rainfall, seasonal water table movement, and the internal chemistry of the waste body, none of which the operator controls. A fixed flowsheet tuned to a nominal composition is therefore structurally mismatched to the problem. This is precisely where adaptive models are useful. Continuous measurements of pH, conductivity, spectroscopy, flow, and metal concentration can be combined with predictive models to adjust precipitation, adsorption, ion-exchange, membrane, or solvent-extraction conditions as the feed moves. The value of AI here lies less in replacing treatment chemistry than in helping a process respond consistently to a feed that does not stay constant, and in doing so with a stated confidence, since a recommendation made on an unusual water composition should be flagged rather than executed silently. Biosorption and related biological preconcentration routes may extend the accessible concentration range further [111,112]. The same logic applies to tailings reprocessing, where the opportunity is to link geometallurgy directly to operating decisions. Spatial mineralogical models can support selective excavation so that the reprocessing plant sees a deliberately blended feed rather than whatever the excavator encountered; sensor-based sorting can reject low-value material before it consumes reagent; hydrometallurgical models can adjust conditions to changing mineralogy; and plant-wide optimization can balance recovery against acid consumption, neutralization demand, and residue stability. Two features distinguish this setting from conventional processing and should shape how models are built for it. Environmental performance is a constraint rather than a co-benefit, because a reprocessing operation that destabilizes a residue has failed regardless of its recovery. And the resource is finite and non-renewable in a stricter sense than an orebody, since a tailings facility can only be reprocessed once, which raises the cost of a poorly optimized first pass.

IX. FROM PREDICTION TO DIGITAL TWINS AND CLOSED-LOOP CONTROL

Many published AI studies in this field still remain offline exercises: a dataset is assembled, split, modeled, and evaluated. Industrial value rises substantially when the model becomes part of a feedback loop, and the engineering requirements change with it. A practical recovery digital twin combines mechanistic equations, learned surrogates, sensor reconciliation, process constraints, and optimization, so that candidate actions can be evaluated before they are applied to the physical plant. A digital twin is therefore more than a prediction tool: it provides a controlled environment in which unsafe or ineffective actions can be identified before they are applied to the plant. The reviewed studies therefore support a unified architecture in which AI sits between characterization and decision execution rather than operating as a stand-alone predictive module. Seven layers are involved (Fig. 2):

- Resource characterization: mineralogy, chemistry, particle information, battery identity, waste provenance, and the variability of each.

- Data fusion: laboratory assays, online sensors, images, spectra, time series, and mechanistic-model states combined into a single process state estimate.
- Prediction: grade, recovery, extraction kinetics, selectivity, product purity, and equipment or process condition.
- Explainability and uncertainty: feature attribution, applicability-domain assessment, prediction intervals, and anomaly detection.
- Multi-objective optimization: recovery and purity subject to reagent, energy, water, emissions, residue, and economic constraints.
- Digital-twin verification: candidate actions tested against a hybrid model before plant implementation.
- Closed-loop learning: realized process outcomes update model calibration and operating policy. The essential property is that these layers communicate continuously rather than in a single pass. A predictive model disconnected from sensing, process constraints, and decision logic has limited value as a plant tool no matter how accurate it is, because accuracy in the absence of an actionable interface is not an operating capability. The uncertainty layer is what makes the loop safe to close: it determines whether a given recommendation is executed automatically, presented for operator approval, or rejected as outside the model's domain of experience. The same architecture serves primary ores and secondary resources, and its principal advantage is adaptability. When the feed changes, characterization and model updating occur before the operating policy is altered, rather than after a period of degraded performance has revealed the change through lost recovery. That ordering is better suited to the variability of critical-mineral feedstocks – and especially to secondary feedstocks, whose composition is set upstream by consumption and collection rather than by geology – than a fixed flowsheet tuned to a single nominal composition. Two governance requirements follow from closing the loop and are easily overlooked at the pilot stage. High-consequence actions must remain bounded by hard process and safety constraints that the optimizer cannot relax, and a validated fallback policy must exist for the case in which the model becomes unavailable or is detected to be operating out of domain. Reinforcement learning, which is attractive precisely because it can discover non-obvious sequential policies, should be trained inside a validated twin rather than on a live high-value circuit [61].

Related work in other industrial domains provides transferable - not mineral-specific - examples of the sensing, forecasting, anomaly-detection, and cybersecurity functions that can surround such a control loop. Hybrid SSA-VAE-BiLSTM and adaptive SSA-LSTM models have been used for industrial energy forecasting and anomaly detection under noisy, non-stationary operating data [143,144]. Separately, instruction-level fine-tuning of Gemma-2B aligned with MITRE ATT&CK has been used for synthetic adversarial-log generation and threat-informed defense [145]. These studies are cited here as contextual design evidence for plant-wide AI reliability and cyber stress-testing, not as evidence of critical-mineral recovery performance.

Seven-layer architecture for deployment-oriented AI recovery systems

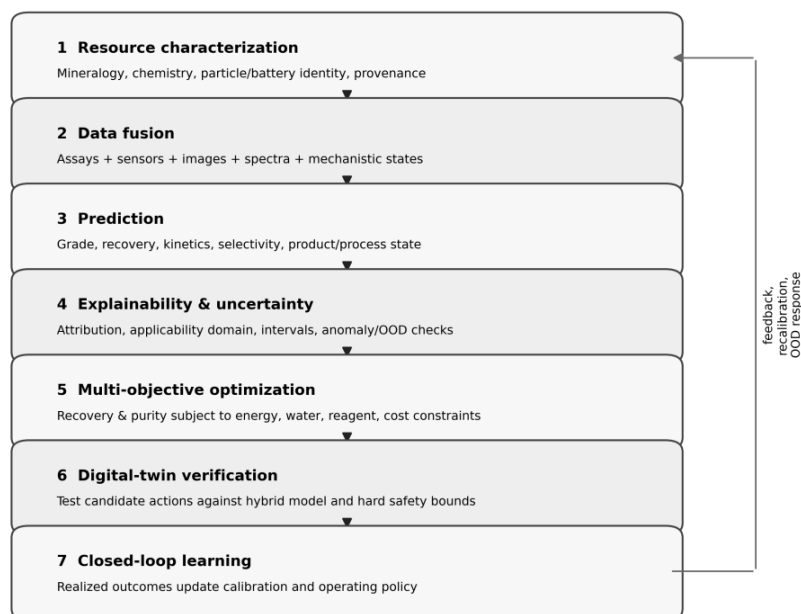


Fig. 2. Proposed seven-layer architecture for AI-driven critical-mineral recovery, showing the closed-loop path

from resource characterization through digital-twin verification to operating-policy update. Dashed arrows indicate model recalibration triggered by out-of-domain detection. Python was used to prepare the plotting and layout code, with assistance from ChatGPT (OpenAI, GPT-5.6 Sol). The authors reviewed and verified the final schematic.

X. BENCHMARKING, VALIDATION, AND A TEST FRAMEWORK FOR FUTURE STUDIES

A recurring problem in AI-for-metallurgy studies is that strong performance metrics are often reported using validation schemes that differ substantially from real deployment. Random train/test splitting is optimistic whenever neighboring observations share an experiment, an ore campaign, an image sequence, or a source publication, and every major data type in this

review has that structure. The resulting bias can be substantial. Where records are strongly clustered, a random split can effectively test a model on paraphrases of its own training data, and the reported error then describes memorization rather than generalization [64]. Validation should instead reflect how the model will encounter genuinely new material, through blocked, temporal, leave-one-campaign-out, leave-one-study-out, or external-feed testing. Table 6 therefore sets out nine tests that can be used to judge the evidence supporting an AI model proposed for critical-mineral recovery. The tests are ordered by increasing evidential strength, but individual studies can report more than one test. To ground the maturity assessment empirically, we conducted a structured audit of 30 primary model-development studies cited in Sections 4–7 [79–91,94–96,100–109,114,124–126]. All 30 reported an internal predictive evaluation; one explicitly used leave-one-study-out validation [105]; five included model-linked experimental validation [101,102,105,109,114]; and one demonstrated live plant-control deployment [95]. Under the strict definitions in Table 6, none of the 30 explicitly reported an external-feedstock test, a temporal holdout test, calibrated uncertainty/OOD testing, a formal ablation test, or a mechanistic-consistency test. These counts are test-coverage counts rather than mutually exclusive study categories and are shown in Fig. 3.

Table 6. Minimum test framework for AI models proposed for critical-mineral recovery, ordered by increasing evidential strength.

Test	Purpose	Preferred split	Metric examples	Pass criterion	Why it matters
1. Internal predictive test	Check basic fit	Blocked or grouped holdout	R2, MAE, RMSE, F1, AUC	Beats simple and mechanistic baselines	Avoids reporting a complex model with no real gain
2. External feedstock test	Check transferability	Different ore, waste, or source	Error plus calibration	Performance remains within engineering tolerance	Tests mineralogical and compositional shift
3. Temporal test	Check plant drift	Future campaign or time block	MAE, drift statistics	Stable performance after time shift	Approximates real deployment
4. Leave-one- study-out	Check literature- model robustness	Entire paper or source held out	R2 and MAE by study	No collapse on unseen studies	Essential for literature-derived datasets
5. Uncertainty test	Assess confidence	Calibration set plus OOD samples	Coverage, ECE, interval width	Intervals are calibrated	Supports safe operation
6. Ablation test	Identify the value of features and physics	Remove groups of inputs	Change in metric	Material gain from key data sources	Prevents unnecessary sensor complexity
7. Mechanistic consistency	Check scientific plausibility	Constraint and edge cases	Mass balance, monotonic trends	No physically impossible recommendations	Builds operator trust
8. Model-linked experimental validation	Test real-world experimental validity	Model-guided or post-model experiments	Recovery/purity or prediction error versus experiment	Confirms or improves real experimental outcomes	Strong evidence short of a plant trial
9. Pilot or plant trial	Test deployment	Live operating campaign	Recovery, grade, stability, cost	Net operational benefit	Determines technology readiness

Note: The test framework and pass criteria in Table 6 represent the authors' synthesis and recommended evaluation criteria based on the reviewed literature. They are not formal regulatory or industry-standard thresholds, and the pass criteria are deliberately expressed in engineering rather than statistical terms, since the operative question is whether a model is good enough for a specific decision rather than whether it is good in the abstract. Table 7 maps the principal research gaps identified across Sections 4 to 9 onto recommended responses and an indicative priority. The gaps are not independent: inadequate dataset description makes grouped validation impossible, and the absence of grouped validation conceals domain-shift failure, which in turn makes uncertainty reporting appear unnecessary. Progress on data description is therefore prerequisite to most of the rest.

Table 7. Principal research gaps and recommended responses.

Gap	Current symptom	Consequence	Recommended response	Priority
Small and nonstandard datasets	Differing units and incomplete feed description	Poor reproducibility	FAIR data templates and raw-data repositories	Very high
Random data leakage	Rows or images from the same campaign split across sets	Inflated accuracy	Grouped, temporal, or source- based splits	Very high
Feedstock domain shift	Model trained on one ore or battery chemistry	Deployment failure	External validation and transfer learning	Very high
Optimization of recovery only	Ignores purity, reagents, water, and energy	Unsustainable optimum	Multi-objective, TEA- and LCA- constrained optimization	Very high
Sparse pilot validation	Laboratory or retrospective results dominate	Unknown industrial value	Prospective pilot campaigns	Very high
Weak uncertainty reporting	Single deterministic prediction	Unsafe optimization	Prediction intervals and OOD detection	High

Gap	Current symptom	Consequence	Recommended response	Priority
Limited mechanistic integration	Black-box correlations	Nonphysical recommendations	Hybrid and physics-informed models	High
Static bioleaching models	Endpoint prediction only	Misses microbial dynamics	Time-series and biokinetic models	High
Cybersecurity and governance gaps	AI coupled to plant systems	Operational risk	Role-based control, audit logs, safe fallback	High
Poor model maintenance plans	No retraining or drift strategy	Performance decay	MLOps and calibration protocols	Medium-high

Note: The priority ratings in Table 7 represent the authors' synthesis based on the reviewed literature and are not formal regulatory or industry-standard rankings.

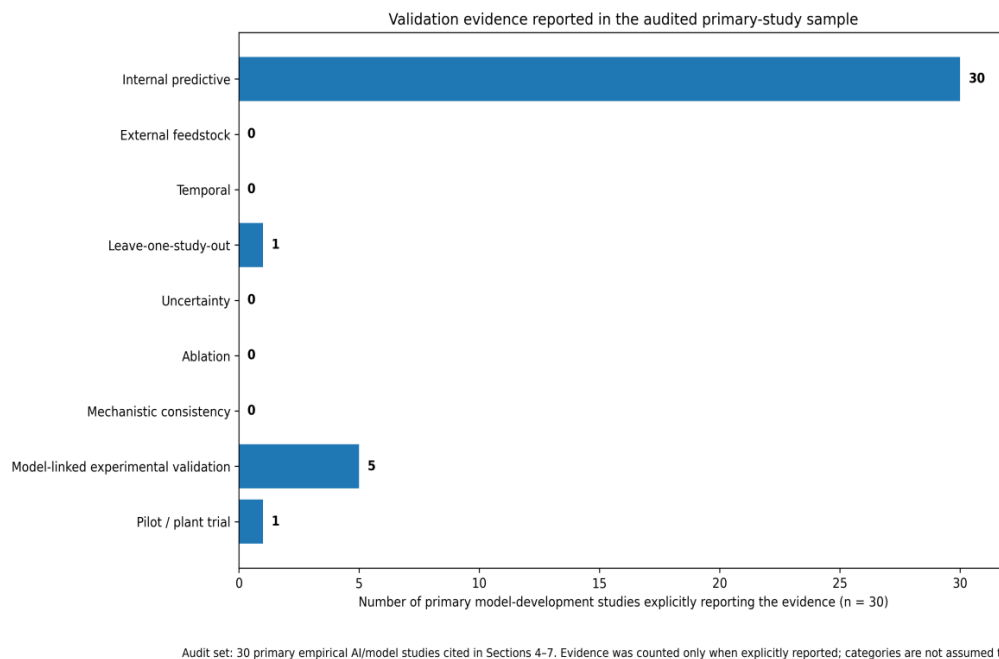


Fig. 3. Validation evidence reported in a structured audit of 30 primary model-development studies [79–91,94–96,100–109,114,124–126]. Bars show the number of studies explicitly reporting each validation-evidence category. Counts are not mutually exclusive or assumed to be cumulative. The underlying structured coding was retained by the authors and is available from the corresponding author upon reasonable request. The figure was generated in Python directly from that structured coding. ChatGPT (OpenAI, GPT-5.6 Sol) assisted with drafting plotting code, and the authors verified both the coding and the final visualization.

XI. SUSTAINABILITY, TECHNO-ECONOMICS, AND RESPONSIBLE AI

AI-driven optimization is not necessarily sustainable by itself. A model can raise recovery while simultaneously increasing acid consumption, heating demand, water use, neutralization requirements, or impurity loading in the product. For example, a leaching model optimized only for extraction will often favor higher acidity, higher temperature, and longer residence time, because those conditions almost always raise extraction. Each also raises reagent cost, energy demand, downstream neutralization load, and the co-dissolution of impurities that the purification circuit must subsequently remove. Such a result may be mathematically optimal for extraction, yet it can simply shift the burden from the leaching step to downstream treatment. For critical-mineral recovery the objective function should therefore include metallurgical and environmental terms together: recovery, purity, throughput, energy, water, reagents, emissions, residues, and cost. Where formal techno-economic and life-cycle indicators are available they should enter the optimization directly rather than being computed afterward as a justification, and recent battery-leaching work integrating preliminary environmental and economic assessment into the modeling workflow shows that this is practicable at the screening stage [138]. Where such indicators are not available, proxy constraints on reagent and energy intensity are preferable to their omission. Responsible deployment also requires traceable data provenance, version-controlled models, operator oversight, and explicit treatment of uncertain recommendations. Documentation practices from the wider ML community translate directly: a dataset description recording provenance, collection conditions, and known gaps [65], and a model record stating intended use, validation design, and performance boundaries [66]. Explainability matters here not because every nonlinear model can be reduced to a simple rule, but because engineers need sufficient transparency to recognize implausible behavior and to decide when a prediction should not be trusted. Where AI is coupled to plant control systems, role-based access, audit logging, and a tested manual fallback are operational-safety requirements rather than administrative additions.

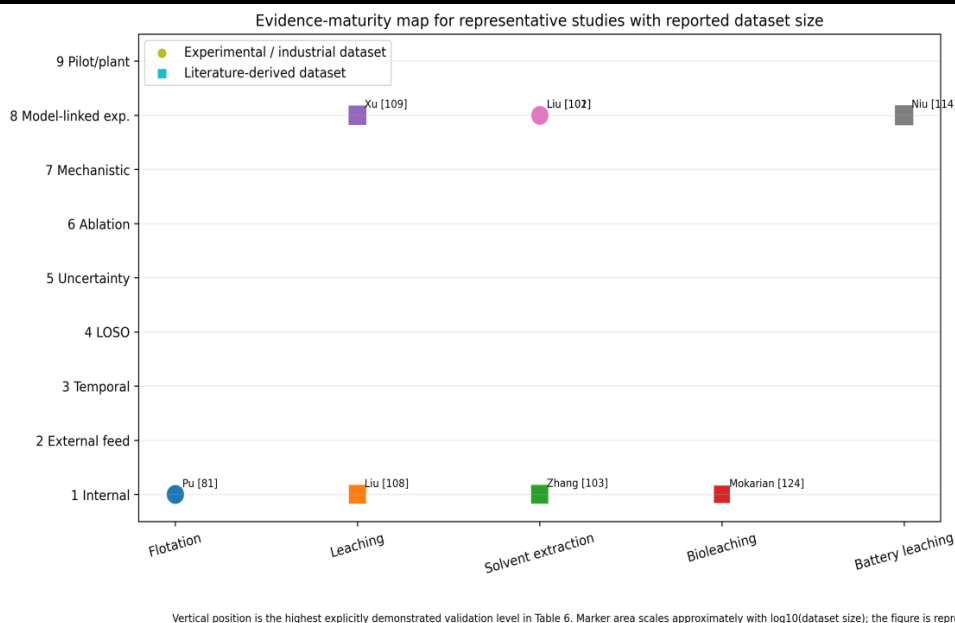


Fig. 4. Representative evidence-maturity map for studies with explicitly reported dataset sizes. Process stage is

shown on the horizontal axis and the highest explicitly demonstrated validation level from Table 6 on the vertical axis. Marker area scales approximately with $\log_{10}(\text{dataset size})$; circles denote experimental or industrial datasets and squares denote literature-derived datasets. The map is representative rather than exhaustive. The underlying 30-study validation coding was retained by the authors and is available from the corresponding author upon reasonable request. The figure was generated in Python directly from that structured coding. ChatGPT (OpenAI, GPT-5.6 Sol) assisted with drafting plotting code, and the authors verified both the coding and the final visualization.

XII. RESEARCH AGENDA

Based on the gaps summarized in Table 7, the following priorities are arranged from basic data needs through to deployment.

- Create benchmark datasets that report complete feed mineralogy and composition, process conditions, analytical methods, and negative or failed experiments, using FAIR-compliant templates and open repositories.
- Adopt blocked, temporal, leave-one-study-out, and external-feed validation in place of random splitting alone, and report the performance difference between the two rather than only the more favorable figure.
- Develop physics-informed models that enforce mass balance, chemical consistency, and kinetic or thermodynamic constraints, and benchmark them against both pure-physics and pure-ML baselines.
- Prioritize multimodal sensing that combines process variables with images, spectra, mineralogy, and solution chemistry, and report ablations showing what each modality contributes.
- Apply uncertainty-aware Bayesian optimization and active learning to select the next most informative experiment, particularly where each data point is a leaching or bioleaching campaign.
- Move from single-metal recovery prediction to flowsheet-level multi-output models that include impurities and downstream product specifications.
- Represent bioleaching and other biologically mediated processes dynamically, using time-series or biokinetic formulations rather than endpoint regression.
- Integrate techno-economic and life-cycle indicators directly into optimization objectives instead of evaluating them after the fact.
- Build and validate digital twins before reinforcement learning or autonomous control is deployed on high-value industrial systems.
- Demonstrate models prospectively at pilot and plant scale, and report model drift and recalibration frequency over time.
- Adopt interoperable data and model governance so that AI results can be audited, maintained, and transferred across facilities.
- For operator-facing generative-AI assistants, evaluate parameter-efficient domain adaptation under realistic compute constraints; LoRA- and adapter-based fine-tuning have been investigated as lower-resource options for domain-specific LLM adaptation [146]. Such interfaces should remain separated from unconstrained process actuation until reliability, authorization, and audit requirements are demonstrated.

XIII. CONCLUSIONS

Artificial intelligence is taking on a larger role in critical-mineral recovery, moving beyond a mainly analytical function toward process support and decision-making. The most developed evidence currently comes from flotation machine vision and soft sensing, ML-guided hydrometallurgical leaching, rare-earth solvent-extraction models supported by experimental validation, and increasingly sophisticated battery-recycling applications. These examples show that AI can reduce the experimental search space, improve process visibility, and support better operating decisions when the underlying data are representative and the

validation is rigorous. However, a high R^2 value alone does not demonstrate industrial readiness. Many published models are trained on narrow datasets, evaluated with random splits, or built from literature compilations in which feedstock and experimental heterogeneity are difficult to control and are correlated within source studies. External validation, uncertainty quantification, mechanistic consistency, and prospective testing under changing operating conditions are more informative than any single headline accuracy metric. In the audited 30-study primary-model sample described in Section 10, all studies reported internal predictive evaluation, whereas only five reported prospective experimental validation and one demonstrated live plant-control deployment. The nine-test framework is intended as a practical benchmark for strengthening future studies, not as a claim that the current literature already satisfies every step. Further progress is likely to depend more on integration than on adding algorithmic complexity. Physics-informed ML can link metallurgical fundamentals with plant data; multimodal sensing can improve state estimation in variable feedstocks; active learning can make experimental programs more efficient; and digital twins can provide a safe environment in which optimization and control strategies are tested before they reach a circuit. Coupled with techno-economic and life-cycle objectives, and deployed within the architecture set out in Section 9, AI can become a practical enabler of more adaptive, circular, and resource-efficient critical-mineral recovery systems. In practical terms, the main constraint is increasingly the quality and relevance of the supporting evidence rather than the availability of more complex algorithms.

CREDIT AUTHORSHIP CONTRIBUTION STATEMENT

Vamshikrishna Challa: Conceptualization, Methodology, Investigation, Data curation, Formal analysis, Visualization, Writing - original draft, Writing - review & editing. Sudhir Sitaram Amritphale: Conceptualization, Validation, Supervision, Project administration, Writing - review & editing. J. S. Chouhan: Writing - review & editing. All authors contributed to the critical evaluation of the literature, the development of the review framework, the interpretation of findings, and the approval of the final manuscript.

FUNDING

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

DATA AVAILABILITY

No new experimental data were generated for this review. The structured 30-study validation coding used for Figs. 3 and 4 is available from the corresponding author upon reasonable request; all other data discussed are contained in the cited publications and remain with the original sources.

ACKNOWLEDGEMENTS

Vamshikrishna Challa acknowledges the Computational Analysis and Modeling program at Louisiana Tech University for providing an interdisciplinary research environment supporting work at the interface of artificial intelligence, computational modeling, and critical-mineral recovery. Sudhir Sitaram Amritphale acknowledges Science Investments LLC for supporting research perspectives in materials science, resource recovery, and sustainable technologies. J. S. Chouhan acknowledges the Department of Civil Engineering, Samrat Ashok Technological Institute, Vidisha, Madhya Pradesh, India, for providing an academic environment supportive of his scholarly contribution to this review. The authors also acknowledge the researchers whose published studies form the scientific foundation of this review.

DECLARATION OF GENERATIVE AI AND AI-ASSISTED TECHNOLOGIES IN THE MANUSCRIPT PREPARATION PROCESS

During the preparation of this work, the authors used ChatGPT (OpenAI, GPT-5.6 Sol) to improve language and readability, assist with reference-consistency checks, support tabulation-consistency checks for the structured validation audit, and assist in drafting Python code used to generate explanatory schematics and data visualizations. The tool was not used to fabricate or alter source-study results or underlying data. After using the tool, the authors reviewed and edited the text, coding, and figures as needed and take full responsibility for the content of the publication.

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