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Review article

Bioleaching of waste-derived rare earth elements: An integrated approach with meta-analysis and predictive analytics for scale-up

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ABSTRACT

This review provides a comprehensive, data-driven perspective on rare earth element (REE) recoveries from various waste streams by bioleaching, integrating mechanistic insights, microbial performance data, advanced statistical and machine learning tools. A total of 77 observations across 10 waste types were analyzed via Bayesian meta-analysis, yielding an average REE recovery of 56.2 % (95 % credible interval: 51.1–61.0 %). Among the waste types, coal fly ash and electronic waste (e-waste) demonstrated the highest recoveries (76 % and 89 %, respectively). Fungi, particularly Aspergillus and Penicillium, performed better than bacteria, despite being less commonly used in bioleaching studies. Fungal-only systems typically achieved 60–76 % recovery, whereas values above 85 % were reported when fungal bioleaching was combined with chemical or physical pretreatments. Acidophilic bacteria exhibited the highest recovery efficiency among the bacterial species (66 %). The microbial consortia (combinations of fungi and bacteria) achieved up to 76 % recovery efficiency due to synergistic interactions. Importantly, many of the highest recoveries ($\geq$90 %) reported in the literature refer to base metals such as Cu, Ni, and Zn, which are more easily solubilized than REEs; harmonizing claims requires distinguishing organism-only effects from organism + pretreatment strategies, and base metal recoveries from REE recoveries. Structural equation modeling (SEM) revealed that factors such as pH, type of waste, and process parameters, played key roles in determining REE recovery success. Among these, process variables (e.g. pH and pulp density) had the strongest direct influence ($\beta = 0.895$). Machine learning models, including support vector machine regression (SVMR) and K-nearest neighbor regression (KNNR), further highlight the importance of metal content, process parameters, and microbial presence. These models performed well, with R^2 values of 0.87 for SVMR and 0.787 for KNNR. Overall, this integrated approach demonstrates the potential for scaling-up bioleaching processes. By combining biological insights with predictive analytics, this integrated framework demonstrates strong foundation for industrial-scale REE recovery and supports shifting toward a more circular and sustainable economy.

1. Introduction

The importance of rare earth elements (REEs) in modern technology, ranging from electronics and renewable energy systems to advanced manufacturing, has increased the urgency for developing sustainable recovery methods [1,2]. Current physicochemical approaches for REE extraction are often energy-intensive, costly, and environmentally disastrous making bioleaching an attractive alternative [1]. Recent

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studies have demonstrated that certain waste streams, such as coal fly ash and e-waste, can contain REE concentrations comparable to or even exceeding those found in primary ores, thus presenting an untapped secondary resource [3]. For instance, experimental data show that bioleaching of coal fly ash using fungal consortia can achieve REE recovery rates (as high as 76%), [4]. Whereas e-waste and acid mine drainage samples have demonstrated recoveries of 89% and 68.8%, respectively. Bioleaching represents a transformative approach to waste valorization, offering a sustainable pathway for the recovery of REEs and other critical metals from diverse waste streams. The integration of microbial biotechnology with data-driven process optimization holds significant promise for overcoming current limitations, advancing bioleaching from experimental setups to practical, scalable solutions that support global sustainability and circular economy objectives. In parallel, machine learning and optimization algorithms have shown strong potential in environmental and engineering domains for predictive modeling and process optimization. For instance, the gradient-based optimizer and the RUN based algorithm demonstrate efficient parameter tuning in nonlinear systems [5,6]. Integrating these approaches with bioleaching is expected to enhance predictive accuracy, enable parameter optimization, and bridge the gap between laboratory findings and scalable applications.

Key operational parameters, such as pH, temperature, aeration, and pulp density, must be meticulously optimized to maximize recovery. For example, the most successful bioleaching experiments were conducted at temperatures between 30 and 40°C, with the pH maintained in the acidic range (1.5 to 3.0), and the reaction times spanning from 20 to 40 days. Laboratory-scale reactors are typically equipped with precise controls for these variables, however, translating these conditions to the industrial-scale remains a challenge due to heterogeneity in waste composition and scale-dependent process dynamics [4]. To address these challenges, the current findings emphasize the integration of bioleaching with advanced data analytics, including statistical modeling, structural equation modeling (SEM), and machine learning approaches. Fig. 1 explains the schematics of the parameters studied in the present review article with datasets and predictive analytics mechanistic approaches, emerging technologies and SEM molding.

2. Data analysis and network modeling

Structural equation modeling (SEM) was applied to deepen the understanding of the causal relationships and latent variables influencing system behavior. SEM is a powerful multivariate technique that integrates factor and path analysis to evaluate both direct and indirect effects among observed variables [7]. In the context of bioleaching, SEM helps model the intricate interdependencies between microbial dynamics, environmental conditions, and metal recovery rates, thereby offering a robust predictive tool. Building on the predictive outputs from SEM and other optimization techniques, the framework advances toward developing an innovation roadmap. This roadmap integrates current process capabilities with emerging technologies in microbial engineering, automation, and artificial intelligence (AI)-driven control systems . Such integration is essential to transition from lab-scale experimentation to full-scale industrial applications, enabling more efficient, scalable, and sustainable waste valorization solutions [8]. The integration of bioleaching with real-time data collection, statistical modeling, and predictive analytics offers a transformative approach to waste management. It not only enables resource recovery from otherwise neglected waste streams but also aligns with global objectives for sustainable development and a circular economy [9]. This research aims to operationalize this integrated framework, addressing critical scientific, technological, and operational gaps to increase the feasibility, scalability, and sustainability of biological waste treatment methods [8,10].

PRISMA-style flow diagram detailing the study selection and screening process are presented in Supplementary Fig. 1. The analysis of published research related to bioleaching, metal recovery, and the utilization of microbial agents in waste management was performed by searching the Scopus database via the keywords including “Rare earth elements" or REEs or Metal and bioleaching and "Waste recovery" or Recovery and Waste and Parameters or "process parameters". This search resulted in a total of 156 articles published between 2015 and 2025. To ensure relevance and quality, the bibliometric dataset was refined by including only original research articles and excluding reviews, book chapters, and conference proceedings. After manual screening for topic relevance, 65 research articles were selected for further analysis. The bibliometric data were analyzed via VOSviewer (version 1.6.19). For the generation of keyword co-occurrence maps, a binary counting method was applied with the minimum keyword occurrence threshold set to 6. Out of the 1233 extracted keywords, 53 met the threshold, and among these irrelevant or generic terms ("result" or “paper”) were removed through manual curation, leaving 39 keywords for network and overlay visualization (Fig. 2a & b). The network visualization revealed 3 distinct clusters (with cluster 1 having 16, cluster 2 having 14, and cluster 3 having 9 keywords, respectively). Within each cluster, the most prominent 5 keywords with their co-occurrence included the following: Cluster 1: “controlled study” – 32, “nickel” – 26, “Iron” – 25, “metals” – 24, and “zinc” – 17, Cluster 2: “bioleaching” – 83, “metal recovery” – 64, “copper” – 46, “pH” – 29, and “recovery” – 19, and Cluster 3: “printed circuit boards” – 32, “recycling” – 29, “e-waste” – 26, “concentration (parameter)” – 21, and “timing

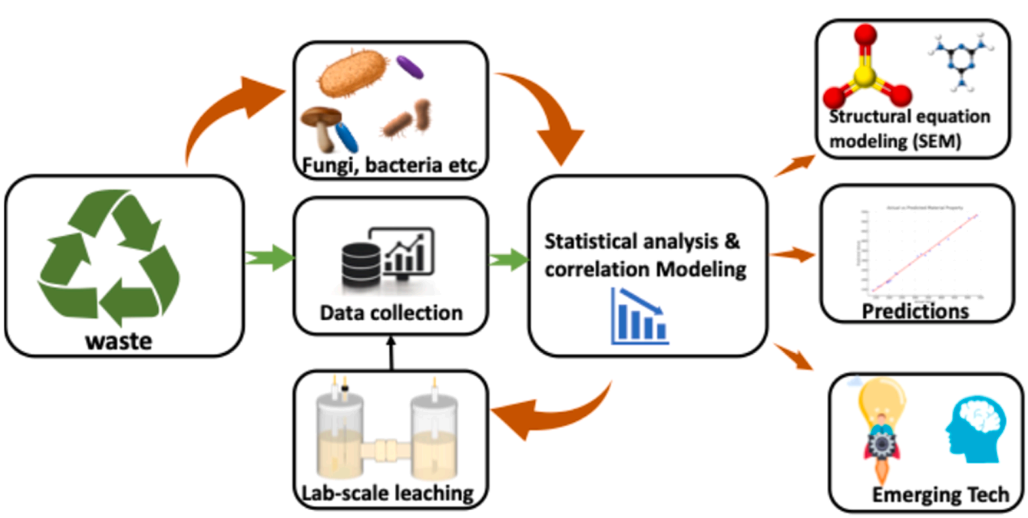

Fig. 1. The schematics of the parameters studied in the present review article, a flow diagram.

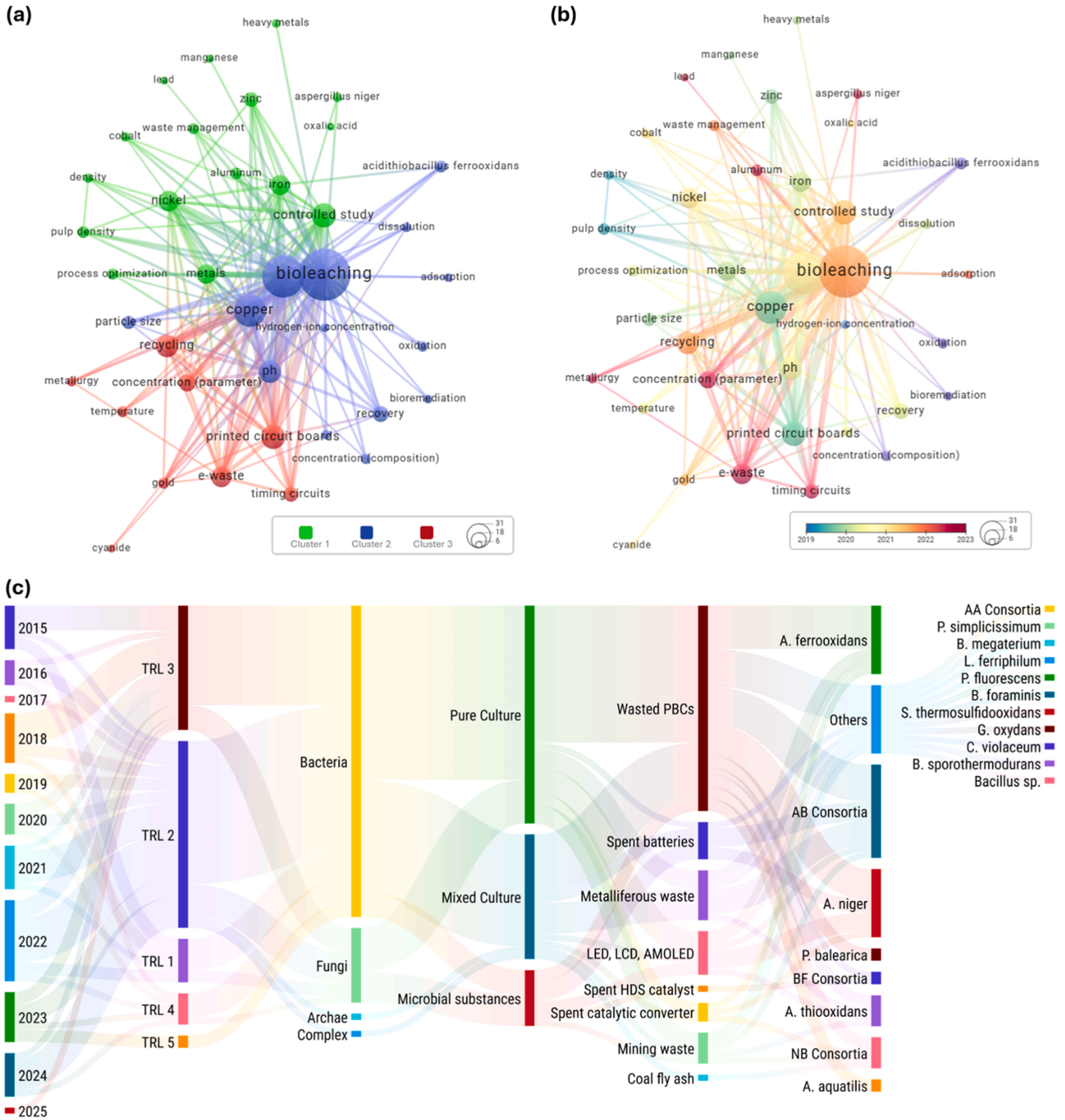

Fig. 2. Graphical representation of literature trends, data classification, and system relationships in bioleaching-based REE recovery. a) Keywords network visualization (clustered in green, blue, and red themes; node size ∝ keyword count; line thickness ∝ co-occurrence) b) Keyword overlay visualization (olor gradient 2015 to 2024; node size ∝ keyword count; VOSviewer-generated), and c) Sankey diagram showing the relation of publication (2015 to 2025) with different TRLs (Technology Readiness Levels) of studies, microbial model used, Application method (pure culture, mixed culture, or microbial derived substances including siderophore, extracellular substances, biosurfactant), Extraction matrices (solid waste, leachate, sludge), and microorganisms used for REEs and metals recovery.

circuits" – 17. A total of 687 links were observed, with a combined link strength of 3593 established between keywords. An overlay visualization (Fig. 2b) was created to analyze the temporal evolution of the research focus based on the average publication year of each keyword occurrence, highlighting the shift toward integrated microbial consortia applications, process optimization, and specific choice of metal and metal recovery techniques after 2020.

To illustrate the interrelationships among microbial types, waste categories, research stages, and technology readiness levels (TRLs), data modelling was performed (using Flourish studio – accessible on https://app.flourish.studio/) and presented in the form of a Sankey diagram (Fig. 2c). The dataset used for this analysis was manually extracted from the screened research articles and compiled into a structured format detailing with the year of publication, TRL level (1 to 5), type of microorganism model (bacteria, fungi, archaea, and complex), application method type (pure culture, mixed culture, or microbial-derived substances - including enzyme, extracellular polymeric substances, biosurfactant, siderophore, and organic acids), the waste type (mining waste, spent batteries, metalliferous waste, and other), microbial strains or consortia used in the studies. The different types of consortia were abbreviated as AA consortia for acidophilic archaeon consortia, AB consortia for acidophilic bacterial consortia, BF consortia for bacterial-fungal mixed consortia, and NB consortia for non-acidophilic bacterial consortia. The width of the flows in the Sankey diagram corresponds to the number of studies linked between categories, offering a visual representation of the research focus and development trajectory in this field.

This visualization provides insights into progressive trends and highlights emerging research domains within the scope of microbial metal recovery and bioleaching technologies (Fig. 2c). It can be clearly seen that there is an increase in investigations related to bioleaching in recent years, while most of the studies are performed at TRL 1 to 3, representing that bioleaching as a technology has evolved from basic research into early proof-of-concept, while few recent studies also report for pilot-scale implementation (TRL 4 and 5). By far the most commonly used model organism is bacteria, while the application methods are pure and mixed type. Among the most used extraction matrices include wasted printed circuit boards (PCBs). This is because precious metals (such as Au) are used in the preparation of PCBs, specifically during plating on connectors and contacts. Among the most commonly used microbial strains for bioleaching studies include *A. thiooxidans, A. ferrooxidans,* and *A. niger*, while consortia-based applications most commonly reported in research studies are linked with acidophilic bacterial consortia. To allow quantitative synthesis across heterogeneous studies, the present work applied a consistent set of harmonization rules. REE recovery values were extracted as reported, but where studies measured only a subset of elements, recoveries were expressed as the proportion of recovered REEs relative to the reported input set. This ensured comparability, but means that "total REE recovery" refers to the subset analyzed in each study rather than a fixed global panel. Time scales were harmonized by recording both the reported endpoint recovery and the time to that endpoint. When necessary, values were normalized to a common unit of days; in cases with multiple sampling points, the maximum recovery within the study time frame was used. Pretreatments (e.g., roasting, grinding, acid pre-leaching) were documented explicitly, and results were coded as "organism-only" versus "organism + pretreatment" for subgroup analyses. For consistency, rare earth elements are abbreviated as REEs, with light (LREEs: La–Sm) and heavy (HREEs: Eu–Lu + *Y*) groups explicitly defined. Concentrations are expressed in mg/kg for solids and g/L for aqueous phases. All temperatures are reported in °C, pulp densities in % w/v, and statistical intervals as confidence intervals (CI). Standard statistical notation is applied: regression coefficients (β), explained variance (R^2), Bayes factors (BF_{10}), and Kendall's tau (τ). These conventions are applied consistently throughout the manuscript, figures, and supplementary materials.

2.1. Variation in extraction efficiency by microbial community

A comprehensive analysis of 34 peer-reviewed studies (49 data points) revealed that fungi generally outperform both heterotrophic and chemolithotrophic microorganisms in terms of their bioleaching efficiency. Although fungi technically fall under the heterotroph category, their unique bioleaching capabilities lead to separate classifications in research [11]. Among the 11 fungal studies, the most frequently used strains include *Aspergillus niger, Aspergillus ficuum, Penicillium simplicissimum*, and *Penicillium tricolor*. Notably, combining multiple fungal strains in co-cultures rather than relying on single strains has proven more effective, likely due to synergistic interactions or resource-sharing between species [12]. Fungi also have practical advantages over bacteria: they leach materials faster, adapt quickly (shorter lag phase), tolerate toxic environments, and thrive across a wider pH range [12]. Their ability to survive alkaline conditions makes them particularly suited for treating alkaline waste [11,13]. However, a few studies contradict these findings, suggesting that fungi are not universally consider superior for bioleaching [14]. Heterotrophic bacteria, while less efficient than fungi, still outperform chemolithoautotrophs. The most common strains in 14 heterotroph studies included *Acidobacilius* and *Acidithiobacillus, Pseudomonas aeruginosa*, and *Acetobacter methanolicus.* These bacteria rely on organic carbon for energy, which can be a logistical hurdle. Despite this, their metabolic byproducts often hold greater commercial value, making them more economically viable than chemolithoautotrophs in certain contexts. They also adapt better to neutral or alkaline pH levels compared to their chemolithotrophic counterparts [15]. Chemolithoautotrophs, though highly resistant to heavy metal toxicity, show the lowest leaching efficiency overall. Their activity is largely confined to extreme acidity ($pH \leq 2.0$), limiting their applicability [15]. Among 26 studies on these microbes, the most tested strains include *Acidithiobacillus thiooxidans, Leptospirillum ferrooxidans, acidophilic consortia, Sulphobacilius thermosulfidooxidans*, and *Acidithiobacillus ferrooxidans*. Fungi and *Acidithiobacillus* led the pack, heterotrophs held their ground, and chemolithotrophs trailed behind. However, as with any biological process, the best option depends on the waste type, pH, and end goals. Fungal-only bioleaching typically yields 60–76 % recovery, but higher values (85–95 %) appear in cases where fungi are combined with chemical or physical pretreatments [16] Similarly, bacterial systems alone may achieve moderate efficiencies but can exceed 90 % under optimized or hybrid conditions [12]. Moreover, most high-yield values in the literature refer to base metals (Cu, Ni, Zn), which are generally more easily solubilized than REEs. Therefore organism-only effects from organism with pretreatment combinations is distinguished, and REE-focused recoveries from those targeting base metals [16]. However, as with any biological process, the best option depends on the waste type, pH, and end goals. This combined analysis indicates a general trend of fungal superiority; it is important to note that this conclusion is drawn from heterogeneous studies with varying waste matrices and process conditions. To provide a more controlled comparison, a secondary analysis was conducted focusing on studies involving similar waste types (e-waste, coal fly ash) within a comparable acidic pH range ($pH < 5.0$). In these more direct contrasts, fungal treatments consistently maintained their performance advantage [16] However, the optimal microbial choice remains highly dependent on specific waste composition and process parameters, therefore, the generalization of fungal superiority may be applied contextually [16]

2.2. Bayesian meta-analysis of the effectiveness of bioleaching

To quantitatively synthesize evidence on Rare Earth Element (REE) recovery via bioleaching, a Bayesian meta-analysis was conducted using data from 50 observations across 10 waste types, including coal fly ash, electronic waste (e-waste), acid mine drainage, red mud, sulfur-bearing materials, and various industrial residues.

2.2.1. Data harmonization and model specification

Reported recovery values were harmonized to a consistent endpoint: the percentage of REEs recovered at the conclusion of the experimental period. When studies provided raw counts, these were converted to proportional recovery rates to ensure cross-study comparability. For studies reporting multiple REEs individually, a mean recovery was calculated to represent the overall 'REE recovery' for that observation. The analysis was performed using JASP (version 0.95.2). A Bayesian normal-normal hierarchical model was employed, where observed recoveries y_i for study i are modeled as $y_i \sim N(\theta_i, \sigma_i^2)$, with each study's true effect θ_i distributed as $\theta_i \sim N(\mu, \tau^2)$. Here, μ represents the overall mean recovery, and τ the between-study heterogeneity. Present work used weakly informative priors: a Normal(0, 1) prior for the overall mean μ, and a Half-Cauchy(0, 1) prior for the heterogeneity parameter τ. Model convergence was confirmed with $\hat{R} < 1.01$ and effective sample sizes (ESS) > 200 for all parameters. Posterior predictive checks indicated a good model fit to the data.

2.2.2. Assessment of heterogeneity and primary results

The primary analysis used a random-effects model, which is conceptually the most appropriate for our heterogeneous dataset. The model yielded a group-level average REE recovery (μ) of 52.4 % (95 % Credible Interval: 40.1 % to 64.9 %), as shown in Fig. 3a. The corresponding Bayes Factor ($BF_{10} > 100,000$) provides decisive evidence for a non-zero average recovery rate, confirming the efficacy of bioleaching across diverse waste substrates (Fig. 3b). Assessment of heterogeneity revealed a posterior mean for τ of 2.685 (95 % CI: 0.048 to 11.021), confirming substantial between-study variability (Fig. 3c). This heterogeneity is expected, given the diversity in microbial consortia, operating pH, temperature, and waste matrix characteristics across the included studies. Although the Bayes Factor comparing random- to fixed-effects models ($BF_{r/1}$ = 1.726) offered only anecdotal support, and the random-effects model was prioritized on theoretical grounds. A sensitivity analysis using alternative priors for τ (Uniform and Half-Normal) produced overlapping credible intervals for μ (range: 51.8 % - 53.1 %), confirming the robustness of our primary finding.

2.2.3. Meta-Regression and heterogeneity drivers

To investigate the sources of heterogeneity, a Bayesian meta-regression was conducted with the following moderators: pH (continuous), pulp density (% w/v, continuous), temperature (°C, continuous), waste class (categorical), and microbe type (categorical: fungi, acidophilic bacteria, heterotrophic bacteria, chemolithoautotrophs). The models used weakly informative priors (Normal [0,1] for slopes; half-Cauchy[0,1] for τ). The results identified pH and pulp density as the strongest moderators, each substantially reducing the residual between-study variance (τ decreased from 2.69 to 1.11 when both were included in the model). Higher pulp densities were consistently associated with lower recovery, while more acidic conditions (lower pH) favored higher recovery. Concerning microbe type, fungal treatments demonstrated a decisive positive effect, with a mean increase in recovery of +34.2 % (95 % CrI: 21.5, 46.9) compared to the reference category (Chemolithoautotrophs). Waste class was also a significant factor, with e-waste and coal fly ash showing the highest recoveries. Posterior model probabilities (Bayes factors) strongly supported the inclusion of pH and pulp density as moderators (BF > 10), with other moderators showing anecdotal to moderate evidence.

2.2.4. Sensitivity and validation

Leave-one-out sensitivity analysis indicated that no single study exerted undue influence on the pooled recovery estimate. Potential for small-study effects and publication bias was assessed using funnel plots and Egger's regression tests, which revealed limited asymmetry and no strong evidence of bias (Supplementary Figures S4 and S5).

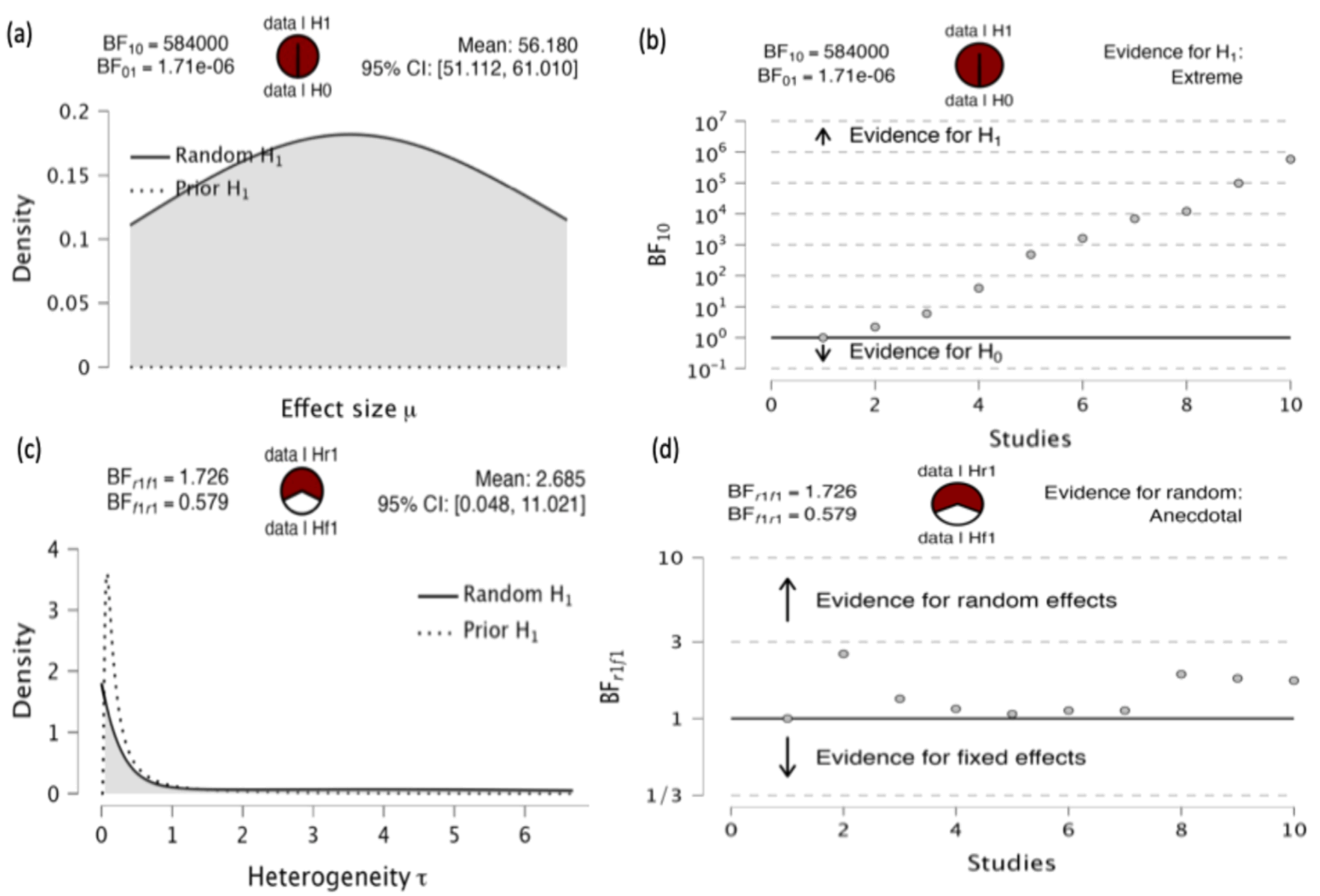

Fig. 3. Bayesian meta-analysis of REE recovery from bioleaching studies across multiple waste types. (a) Posterior distribution of the group-level effect size (μ) indicating an average REE recovery of 56.18 % with a 95 % credible interval [51.11 %, 61.01 %], providing decisive evidence in favor of a non-zero effect (BF_{10} = 584,000). (b) Cumulative Bayes Factor (BF_{10}) across studies shows extreme and increasing evidence for a positive effect of bioleaching on REE recovery. (c) Posterior distribution of between-study heterogeneity (τ), with a mean value of 2.685 (95 % CI: [0.048, 11.021]), suggesting moderate heterogeneity across studies. (d) Cumulative Bayes Factor comparison between random- and fixed-effects models (BF_{r/r1} = 1.726) provides anecdotal evidence in favor of random-effects assumptions. Collectively, these results confirm the overall effectiveness of bioleaching while highlighting variability based on waste type and study-specific conditions.

2.2.5. Synthesis with SEM and ML findings

The meta-regression results show remarkable alignment with our other analytical methods. The dominance of process parameters (pH, pulp density) as key moderators in the meta-analysis directly corroborates the structural equation modeling (SEM) results, where process variables had the strongest direct effect ($\beta = 0.895$). Furthermore, the superior performance of fungi in the meta-analysis is consistent with their high feature importance in the support vector machine model. This multi-method convergence underscores that while microbial choice is important, the control of abiotic process conditions is the most critical factor for optimizing REE bioleaching efficiency.

3. Experimental systems, process optimizations

Laboratory-scale bioleaching systems are fundamental for optimizing the bio-hydrometallurgical parameters before scaling-up to industrial operations. These systems are designed to closely replicate the chemical, physical, and biological conditions necessary for microbial leaching, providing a controlled environment to investigate variables such as pH, temperature, aeration, pulp density, and microbial strains [15,17–19] A typical lab-scale bioleaching setup includes a bioreactor or leaching vessel constructed from inert materials such as borosilicate glass or plastic to prevent chemical interference with leaching reactions [14,15,20]. The system comprised a stirred tank reactor equipped with an overhead motor-driven impeller to ensure homogeneity and promote microbial contact with ore particles. The reactor is also integrated with temperature sensors and a heating coil or water jacket to maintain thermophilic or mesophilic conditions, depending on the microorganisms used.

Temperature is a critical parameter; for mesophilic species such as *Acidithiobacillus ferrooxidans,* optimal activity occurs at 28–35 °C, while for thermophiles such as *Sulphobacilius thermosulfidooxidans*, the range may reach 50–70 °C [7,20,21]. In addition to temperature control, the pH of the system is maintained via acid feed pumps that inject sulfuric acid into the reactor. Bioleaching microbes typically thrive in highly acidic conditions (pH 1.5–3.0), where metal solubilization is more effective and competition from non-acidophilic organisms is minimized [22,23]. The air supply, introduced via spargers or diffusers, ensures adequate oxygenation, which is essential for iron- and sulfur-oxidizing bacteria dependent on aerobic respiration. Some systems also inject carbon dioxide to enhance the autotrophic growth of microorganisms [24,25]. The ore sample is usually crushed to fine particles (typically <75 μm) to increase surface area and maximize contact with the microbial community. The reactor is inoculated with a microbial consortium or pure culture known for its leaching capabilities. Commonly used microorganisms include *A. ferrooxidans, Leptospirillum ferrooxidans, Sulfobacillus spp*., and *Ferroplasma acidarmanus* [15] These microbes catalyze the oxidation of ferrous iron (Fe^{2+}) to ferric iron (Fe^{3+}), which acts as an oxidant to dissolve metal sulfides such as chalcopyrite, sphalerite, and pyrite [13,18,26]. Process variables such as the pulp density (weight of solid ore per volume of solution) significantly influence the efficiency of bioleaching. Typically, lab-scale studies use pulp densities between 1 and 10 % (w/v), although higher concentrations may lead to substrate inhibition or reduced microbial activity due to oxygen or nutrient limitations [1,17]. Continuous or batch-mode operations are employed depending on the experimental design. Batch systems are simple and useful for kinetic studies, whereas continuous systems better simulate industrial-scale operations and allow for steady-state conditions [18]. Effluent samples are collected at regular intervals through an outlet port and analyzed for pH, redox potential (Eh), microbial population density, and concentrations of dissolved metals such as copper, zinc, iron, and arsenic [26–28]. The results are presented in Table 1. Reactor configurations were categorized as batch, column, or continuous systems. Analytical methods for metal quantification (ICP-MS, AAS, ICP-OES) were recorded, but because method-specific biases were rarely benchmarked within studies, they were treated as equivalent for effect-size estimation. Analytical techniques such as atomic absorption spectroscopy (AAS), inductively coupled plasma mass spectrometry (ICP-MS), and ion chromatography are commonly employed for this purpose [29,30]. The use of bioleaching in lab-scale experiments has extended beyond base metals to include the recovery of rare earth elements (REEs), gold, uranium, and even electronic waste (e-waste) [7,17]. In these studies, pretreatment methods such as roasting, grinding, or bio-oxidation are often used to increase the accessibility of target metals [21].

The operational stability of the lab-scale bioleaching system depends on rigorous monitoring and control of bioprocess parameters. Advanced systems may include programmable logic controllers (PLCs) or software-based control systems to automate temperature, pH, and flow rate adjustments [20]. In addition, microbial community structure can be tracked using molecular biology tools (e.g., qPCR, 16S rRNA sequencing, and metagenomic analysis) to understand microbial dynamics and interactions [31]. Lab-scale bioleaching systems are vital tools for the development and optimization of biomining technologies. This approach enables researchers to study bioleaching mechanisms in detail, fine-tune operating conditions, and evaluate the efficacy of different microbial consortia under various physicochemical environments. The results obtained from such systems provide the foundational data required for scaling up to pilot and industrial-scale operations. Transitioning bioleaching from laboratory conditions to pilot and industrial scales requires careful attention to both biological performance and engineering design [7,17]. Key scale-up challenges include maintaining

Table 1
The relative abundance of different phyla in REE Leaching. Extraction efficiency of REE varies with microorganism type data extract from cited literature.

Waste Type	Microorganism	Time (h)	REEs Concentration (ppm)	Leaching Efficiency (%)	Key REEs	References
Base Metals	*Acidithiobacillus ferrooxidans, Aspergillus niger*	Varies	50–200	80–90	Different REEs	[29]
Alkaline Waste	*Penicillium simplicissimum, Leptospirillum ferrooxidans*	48–72	10–50	60–70	Neodymium (Nd) and Yttrium (Y)	[17,18]
E-Waste	*Aspergillus ficuum, Sulphobacilius thermosulfidooxidans*	12–48	100–500	85–95	Lanthanum (La) and Cerium (Ce)	[7,11,17]
Industrial Waste	*Ferroplasma acidarmanus, Acidithiobacillus thiooxidans*	24–48	30–150	70–80	Dysprosium (Dy) and Samarium (Sm)	[11,14, 17]
Red mud	*Aspergillus niger, Penicillium tricolor*	24–48	20–100	60–80	Cerium (Ce) and Lanthanum (La)	[11,17]
CFA	*Leptospirillum ferrooxidans, Sulphobacillus spp.*	12–72	50–200	75–85	Mixed REEs	[15,20, 26]
Industrial waste	*A. ferrooxidans, Aspergillus niger, Leptospirillum ferrooxidans*	48–72	40–150	80–90	Neodymium (Nd) and Yttrium (Y)	[11,13, 26]
Complex polymetallic compound	*Acidithiobacillus thiooxidans, Penicillium simplicissimum*	12–48	30–200	70–80	Lanthanum (La) and Dysprosium (Dy)	[15,17]
Ores	*Sulphobacillus thermosulfidooxidans, Ferroplasma acidarmanus*	12–48	50–200	85–90	Cerium (Ce) and Neodymium (Nd)	[17,21, 30]

adequate oxygen transfer (characterized by kLa), ensuring CO_2 dosing for autotrophic microbial groups, and managing shear forces that influence biofilm stability [32] . Foam formation and solids handling are additional bottlenecks that can reduce process efficiency if not properly controlled [33]. Modern stirred-tank and airlift reactor designs increasingly incorporate on-line sensing platforms to monitor critical parameters such as pH, oxidation–reduction potential (ORP), and optical density (OD) [34]. These sensors enable real-time feedback control, while recent advances in soft sensors and machine learning frameworks allow for predictive optimization of setpoints, enhancing stability under fluctuating feed conditions [35]. Based on compiled dataset, a practical design envelope emerges the from pH: 1.5 to 3.0 ensures proton activity sufficient for mineral dissolution while maintaining microbial viability [36] Temperature from 30 to 40 °C to supports mesophilic leachants with strong enzymatic activity [37,38] Pulp density: typically, 5–15 % (w/v) to balances kinetics and leachate selectivity against potential microbial inhibition by suspended solids and toxic intermediates [39–41].

These ranges highlight trade-offs to lower pH and higher pulp density accelerate dissolution kinetics but risk microbial stress and reduced selectivity, while milder conditions preserve community stability but slow recovery. To optimize across such trade-offs, advanced optimization algorithms have been proposed in recent engineering literature provide efficient means to fine-tune multivariable systems, while hybrid frameworks integrating mechanistic knowledge with metaheuristics hold promise for future bioleaching reactor control. Incorporating these methods could support multi-objective optimization of operating windows, ensuring efficient recovery while safeguarding microbial health [37].

Bioleaching efficiency depends heavily on the compatibility between microbial species and specific waste or ore types, as illustrated in Fig. 4. Each microbe has evolved distinct metabolic capacities and environmental tolerances that make it better suited to solubilize particular metals or mineral matrices [42,43]. Optimizing bioleaching parameters such as pH, temperature, pulp density, and oxidation–reduction potential (ORP) for each microbe–waste pair is critical for maximizing metal recovery while maintaining microbial viability [14,15,20]. Table 2 summarizes commonly studied microbes, the types of waste or ore they are most effective at leaching, and their corresponding optimal conditions based on experimental and industrial reports. Microbes such as *Acidithiobacillus ferrooxidans* and *Leptospirillum ferrooxidans* dominate low-temperature, acidophilic leaching systems, especially for base metals, like copper and zinc from sulfide ores [7,15] Their oxidative metabolism targets ferrous iron and reduced sulfur compounds,

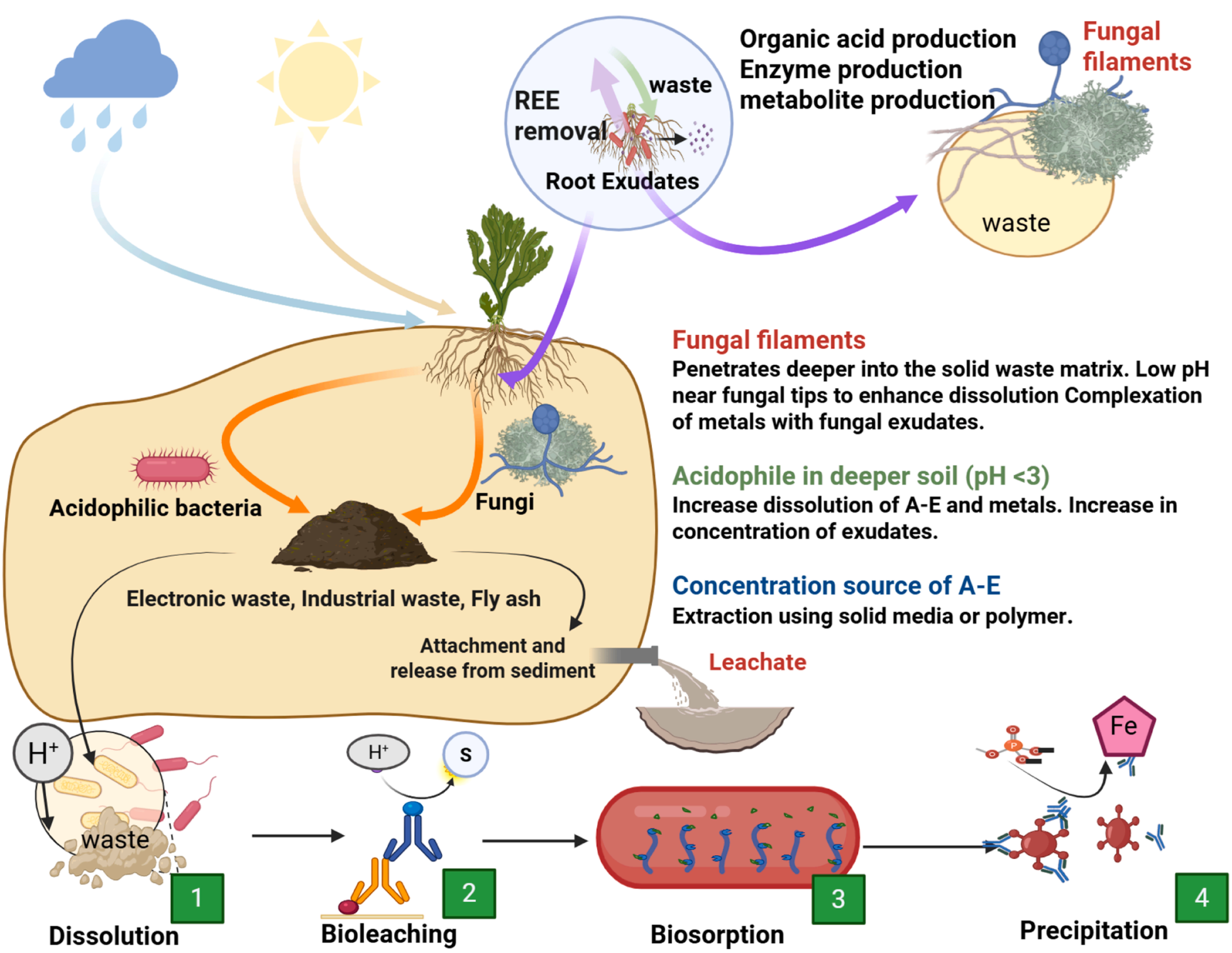

Fig. 4. Schematic representation of biologically enhanced leaching of REE from landfill or waste ditch environments. Mechanisms for the bioleaching of rare earth elements (REEs): **(a)** Interaction between fungal filaments and waste particles, showing the role of organic acids and enzymes in releasing REEs. The inset illustrates conditions affecting fungal growth and REE mobilization. Schematic of REE bioleaching involving acidophilic microorganisms. The process includes: (1) Dissolution of REE-containing minerals, (2) Bioleaching through acid production, (3) Biosorption of REEs by microbial cells, and (4) Precipitation of REEs as phosphate compounds.

Table 2
Studied microbial extraction efficiency of REEs from different waste sources.

Microorganism(s)	Waste/Ore Type	Target Metal(s)	Extraction Rate	References
A. ferrooxidans and *L. ferrooxidans*	Sulfide ores	Cu, Zn, Sc, Y, Ce	High – NQ[1]	[7,15]
S. thermosulfidooxidans and *A. caldus*	Arsenopyrite, polymetallic ores	Multiple base/trace metals	High - NQ	[17,26,45]
P. putida and *A. niger*	Waste PCBs	Precious metals	NQ	[30,46]
C. violaceum	Gold ores (biocyanidation)	Au	NQ	[47]
G. oxydans (DSMZ 46616)	Red mud	*Sc*	94 %	[48]
Aspergillus spp., *P. aeruginosa*, and *Penicillium* spp.	Carbonaceous shales	Mixed REEs	33–86 %	[49,50]
G. oxydans	Synthetic phosphogypsum	Y, Ce, Nd, Sm, Eu, Yb	36.7–91.2 %	[51]
G. oxydans	Bauxite residue	Y, Al, Ca, Ti, Sc, La, Ce, Nd	10.7–80.1	[39]
A. thiooxidans + oxalic acid	Gold mine tailings	Pr, Ce, Eu	Enhanced – NQ	[27]
A. ferrooxidans and *L. ferrooxidans*	Various ores/wastes	La, Ce, Nd, Pr, Dy, Lu	22–100 %	[27]
Bacillus sp. and *Aspergillus* sp.	Ion-adsorption clay, bauxite	La, Ce, Dy, Lu	Variable	[39,40, 55].
Acidophilic microorganisms Gluconobacter oxydans	Electronic waste	Pr, Nd, La, Ce, Dy, Lu	24–100 %	[36,37]
S. fungicides	Fluorescent powders, spent catalysts	Y	40–90 %	[56]
C. bombicola	Coal fly ash	Dy, Y, Sc, Er, Yb, Gd, Eu, Sm, La, Ce, Pr, Nd	Moderate–high - NQ	[49]
A. thiooxidans	Ground e-waste	Nd, Cu	98 %	[35]
L. casei and *Komagataeibacter*	Fluorescent phosphors	Y, La, Ce, Eu, Gd, Tb	6.1–12.6 %	[16,57]
A. niger	Spent auto catalysts	Ce, La	25.9–100 %	[29,49,50]
A. ferrooxidans + sulfur-oxidizing bacteria	Ores, quartz-pebble conglomerates	U, Th, Y, Ce, Pr, Nd, La, Dy, Sm	6–76 %	[52,59]
Sulfur-/iron-oxidizing bacteria	Ores	U, Th	6–60 %	[60]
G. oxydans	Spent NiMH batteries	Total REEs	7.8–56.1 %	[52]
A. thiooxidans + other microbes	Gold tailings, various ores	Pr, Nd, Ce, La, Sm	Up to 100 %	[49]

[1] NQ = not quantifiec.

generating ferric iron and sulfuric acid that chemically leach the ore matrix.

Thermophilic species like *Sulfobacillus thermosulfidooxidans* and *Acidithiobacillus caldus* are employed in high-temperature systems where enhanced solubilization kinetics are needed [26]. These microbes can withstand extreme conditions and are particularly useful for leaching arsenopyrite and complex polymetallic ores [17,44]. For urban mining applications, such as processing waste printed circuit boards (PCBs), microbes like *Pseudomonas putida* and *Aspergillus niger* are used. These organisms employ biosurfactant production and organic acid secretion, respectively, to mobilize precious metals from complex waste matrices [45,46]. Unlike acidophilic autotrophs, these heterotrophs thrive in near-neutral environments and are sensitive to heavy metal toxicity, necessitating lower pulp densities. Biocyanidation, the microbial production of cyanide to solubilize gold, is enabled by species such as *Chromobacterium violaceum*, offering a less toxic alternative to chemical cyanide leaching [47]. Although this method remains underutilized, its selectivity and potential for environmentally benign gold recovery continue to attract attention [27]. The choice of microorganism must therefore be tailored not only to the waste matrix but also to downstream requirements such as metal specificity, recovery rate, process stability, and environmental safety [45].

Successful bioleaching operations depend on fine-tuning each of these parameters through rigorous experimentation, often starting at the lab-scale before pilot testing the bioleaching of REEs from various sources. *Gluconobacter oxydans* (DSMZ 46,616) achieved a high extraction rate of 94 % for scandium (Sc) from red mud, as reported by [48]. Other microorganisms, including *Aspergillus species* (*niger, flavus, terreus, ficuum*), *Pseudomonas aeruginosa*, and *Penicillium* species have been investigated for use in the bioleaching of REEs from carbonaceous shales, with extraction rates ranging from 33 % to 86 % for mixed REEs [49,50]. *Gluconobacter oxydans* was also applied to synthetic phosphogypsum, resulting in a 36.7 % to 91.2 % extraction for a variety of REEs, including yttrium (Y), cerium (Ce), neodymium (Nd), samarium (Sm), europium (Eu), and ytterbium (Yb) [51]. Another study demonstrated that *Gluconobacter oxydans* enhanced the dissolution of bauxite residue, achieving metal recovery rates of 41.18 % for yttrium, 67.79 % for aluminum, 80.16 % for calcium, and 59.41 % for titanium, while only achieving marginal dissolution rates of 13.40 % for scandium, 14.74 % for lanthanum, 24.41 % for cerium, and 10.67 % for neodymium, with a further decrease over time [38].

In the case of gold mine tailings, the combination of *Acidithiobacillus thiooxidans* with oxalic acid pretreatment enhanced REE recovery, particularly for praseodymium (Pr), cerium (Ce), and europium (Eu). Additionally, *Acidithiobacillus ferrooxidans* and *Leptospirillum ferrooxidans* have demonstrated significant REE extraction (22–100 %) from various ores and waste materials, with a focus on lanthanum (La), cerium (Ce), neodymium (Nd), praseodymium (Pr), dysprosium (Dy), and lutetium (Lu) [27,52]. Studies involving *Bacillus sp.* and *Aspergillus sp.* in ion-adsorption clay and bauxite yielded variable REE recovery rates for lanthanum (La), cerium (Ce), dysprosium (Dy), and lutetium (Lu) [37,38,48,53]. Microbial bioleaching of electronic waste, using acidophilic microorganisms, has shown extraction rates ranging from 24 % to 100 % for REEs such as praseodymium (Pr), neodymium (Nd), lanthanum (La), cerium (Ce), dysprosium (Dy), and lutetium (Lu) [17,39,54]. *Streptomyces fungicides*, when applied to fluorescent powders and spent catalysts, resulted in an extraction rate of 40 % to 90 % for yttrium (Y) [55].

Candida bombicola has demonstrated moderate to high extraction rates from coal fly ash, covering a broad range of REEs, including dysprosium (Dy), yttrium (Y), scandium (Sc), erbium (Er), ytterbium (Yb), gadolinium (Gd), europium (Eu), samarium (Sm), lanthanum (La), cerium (Ce), praseodymium (Pr), and neodymium (Nd) [35]. In ground electronic waste, *Acidithiobacillus thiooxidans* achieved an impressive 98 % extraction of neodymium (Nd) and copper (Cu) [36]. *Lactobacillus casei* and *Komagataeibacter* were used to leach REEs from fluorescent phosphors, but their extraction rates were lower, ranging from 6.1 % to 12.6 % for yttrium (Y), lanthanum (La), cerium (Ce), europium (Eu), gadolinium (Gd), and terbium (Tb) [34,56]. Similarly, *Aspergillus niger* was employed to extract cerium (Ce) and lanthanum (La) from spent automobile catalysts, with recovery rates ranging from 25.9 % to 100 % [16,49,50,57].

The combination of *Acidithiobacillus ferrooxidans* and sulfur-oxidizing bacteria was effective in extracting REEs from ores and quartz-pebble conglomerates, with recovery rates ranging from 6 % to 76 % for elements such as uranium (U), thorium (Th), yttrium (Y), cerium (Ce), praseodymium (Pr), neodymium (Nd), lanthanum (La), dysprosium (Dy), and samarium (Sm) [33,58]. Additionally, sulfur- and iron-oxidizing bacteria have been used to extract REEs from ores, with extraction rates ranging from 6 % to 60 % for uranium (U) and thorium (Th) [59]. Finally, *Gluconobacter oxydans* has been tested for bioleaching REEs from spent NiMH batteries, resulting in an extraction rate ranging from 7.8 % to 56.1 % for total REEs [33]. The combination of *Acidithiobacillus thiooxidans* and other microorganisms for the bioleaching of gold mine tailings and various ores demonstrated up to 100 % REE extraction, including praseodymium (Pr), neodymium (Nd), cerium (Ce), lanthanum (La), and samarium (Sm) [49].

3.1. Leaching of REEs from waste ditches, landfills and bioleaching mechanisms

Biologically enhanced leaching represents a sustainable and innovative approach for the extraction of valuable elements such as lithium (Li), cobalt (Co), ions, and REEs from municipal and industrial solid waste deposited in landfills or waste ditches. This method utilizes the synergistic interaction of fungi and acidophilic microorganisms to promote the solubilization, mobilization, and recovery of these elements while concurrently reducing their environmental risk profiles. Fungal filaments, particularly those from species like *Aspergillus niger* and *Penicillium simplicissimum*, can penetrate deeply into solid waste matrices [52]. These fungi acidify their immediate surroundings by secreting organic acids (e.g., citric and oxalic acids) creating localized microenvironments with pH values as low as 2.5–3.5 near the hyphal tips [60]. This acidic microenvironment significantly enhances the dissolution of alkaline and transition metals from complex waste matrices, thereby increasing their availability for extraction. Additionally, fungal exudates form complexes with metal ions, increasing the solubility and mobility of elements such as La, Ce, and Nd, which are key REEs with applications in electronics and clean energy technologies (Fig. 4). Studies have shown that fungal bioleaching can achieve recovery rates of up to 75 % for certain REEs from industrial waste [33]. These metal-organic complexes are relatively stable and mobile, facilitating their downward transport.

In deeper soil zones, where the pH can naturally drop below 3 due to microbial respiration and organic acid accumulation, acidophilic bacteria such as Acidithiobacillus ferrooxidans become more active. These microorganisms further catalyze the dissolution of metal-bearing phases, especially under oxidizing conditions, leading to the increased release and transport of A-E into the leachate. Acidophiles are known to accelerate leaching by up to 40 % compared to abiotic conditions [16, 56,57,61]. The resulting leachate, which is rich in dissolved metals and exudates, accumulates at the base of landfills and ditches. This leachate becomes a concentrated source of REEs that can be subsequently extracted using solid-phase adsorbents or functionalized polymers. For example, polymeric resins functionalized with phosphonic or carboxylic groups have shown over 90 % selectivity and adsorption efficiency for REEs under optimized pH conditions [52]. By integrating biological processes into the waste management framework, this method not only enables efficient resource recovery but also contributes to environmental remediation. The reduction in metal persistence within landfills minimizes the risks to groundwater and surrounding ecosystems, aligning with circular economy principles and sustainable waste valorization [51,62].

The bioleaching of REEs involves the microbially mediated mobilization of REEs from solid matrices into the aqueous phase. The underlying mechanisms differ based on the type of microorganism involved and can be broadly classified into three categories: redoxolysis, acidolysis, and complexolysis. These mechanisms are summarized in Fig. 4. In redoxolysis, REE dissolution is driven by redox reactions wherein microorganisms (e.g., *Acidithiobacillus ferrooxidans* and *Leptospirillum ferrooxidans)* oxidize Fe^{2+} to Fe^{3+}. The resulting Fe^{3+} then facilitates the oxidative dissolution of REE-bearing minerals. This process may occur via two modes: contact and non-contact. In contact mode, microbes attach to mineral surfaces through extracellular polymeric substances (EPSs), forming localized zones for Fe^{2+} oxidation and subsequent sulfuric acid generation, which promotes mineral breakdown [20,52,60].

In the non-contact mode, similar redox reactions occur, but the microbes do not physically attach to the mineral surfaces. Acidolysis involves REE solubilization through microbial acid production. Autotrophic sulfur-oxidizing bacteria, such as *A. ferrooxidans* and *A. thiooxidans*, oxidize sulfides to produce sulfuric acid, which facilitates the release of REEs into the solution. Alternatively, heterotrophic microbes such as *Lactobacillus casei, Yarrowia lipolytica*, and various *Aspergillus* species metabolize organic substrates to generate organic acids (e.g., acetic, citric, gluconic, and oxalic acids), lowering the pH and enhancing REE dissolution [34,56,61]. Beyond acidolysis, organic acids also promote complexolysis, where REEs form soluble complexes via chelation. The dominance of complexolysis over acidolysis depends on the pH. At low pH (below the pKa of the acids), protonation reduces complex stability, favoring acidolysis. Conversely, at near-neutral pH, complexation becomes more dominant [33]. In addition to organic acids, microbes may also release siderophores, which are small, high-affinity iron-chelating compounds that can bind to $REEs^{3+}$, facilitating their mobilization [52].

3.2. Element-specific selectivity

Element-wise recovery patterns revealed consistent differences between light and heavy rare earths (LREE vs HREE). Across waste types, La and Ce exhibited broader recovery distributions, typically ranging 30–75 %, while Nd clustered around higher recoveries (50–80 %). In contrast, HREEs such as Dy and Y showed lower and more variable recoveries (20–60 %). Sc was the least efficiently mobilized, rarely exceeding 30 %. Microbial strategies influenced selectivity: fungal pathways (e.g., *Aspergillus, Penicillium*) generally favored LREE mobilization via organic acid production, while acidophilic bacteria (e.g., *Acidithiobacillus*) enhanced HREE solubilization under low pH, oxidative conditions. When pretreatments were combined with microbial action, both LREE and HREE recoveries improved, though trade-offs emerged in the co-dissolution of base metals (Cu, Zn, Fe). Organic acids tended to solubilize LREEs alongside Al and Fe, whereas sulfuric acid-driven systems favored HREE release but increased base metal contamination. These patterns highlight mechanistic trade-offs in targeting specific REE groups depending on waste type and microbial pathway (Supplementary Fig. S16). These element-specific patterns emphasize that microbial strategies are not uniformly effective across the REE spectrum. Organic acid producers provide relatively selective mobilization of LREEs, but often at the expense of higher Al/Fe co-dissolution [33]. By contrast, sulfur-oxidizing bacteria create oxidative, low-pH environments that favor HREE solubilization but increase transition-metal contamination. These trade-offs underscore the need for process optimization tailored to the desired REE subgroup, particularly when designing downstream separation flowsheets [20,52,60].

4. Structural equation modeling (SEM) & total effects analysis

In present work structural equation modeling (SEM) was used to evaluate relationships between process conditions, microbial communities, and REE recovery outcomes. Two latent constructs were defined: process variables (pH, pulp density, temperature, leaching time) and microbial communities (fungi, bacteria, consortia). Recovery of LREEs, HREEs, and transition metals were modeled as observed outcomes, with waste characteristics (particle size, REE content) as exogenous predictors. The model was identified using a fixed marker-variable approach and estimated via maximum likelihood with robust standard errors in JASP (0.95.2). Fit indices indicated excellent model performance (χ^2/df = 0.20, p = 0.688; GFI = 1.00; RMSEA = 0.004), meeting stringent thresholds for model acceptability [1,52]. Standardized path coefficients with 95 % CIs are reported in Supplementary Tables S3–S10. The results shows that Waste characteristics: REE content had a strong positive direct effect on recovery (β = 0.566*, $p < 0.05$), and particle size also contributed significantly (β = 0.51**, $p < 0.01$).Process variables has strongest direct influence on recovery (β = 0.895**, $p < 0.01$). Fungal activity showed a stronger direct effect (β = 0.636*, $p < 0.05$)

compared to bacteria (β = 0.375**, $p < 0.01$). *Acidithiobacillus* spp. were positively associated with HREE recovery (β = 0.615, 95 % CI [0.42–1.98]), whereas chemolithoautotrophs exerted a negative effect (β = –1.22, 95 % CI [–2.10, –0.34]) [52]. Several indirect pathways highlighted microbial mediation of process conditions, consistent with known bioleaching mechanisms are provided in supplementary table S8 [1]. The SEM explained 88 % of variance in LREE recovery (R^2 = 0.875) and 80 % in HREE recovery (R^2 = 0.799). Total REE recovery (Rc %) was most influenced by HREE recovery (β = 0.895**), followed by transition metals (β = 0.615*) and LREEs (β = 0.578**). These results confirm that microbial community composition mediates the effects of process parameters on REE mobilization. Fungi favored LREE recovery through complexolysis and organic acids, while Acidithiobacillus-driven redoxolysis was central to HREE and transition-metal mobilization [1,52]. The path diagram is shown in Fig. 5.

5. Machine learning models in bioleaching optimization

Predictive modeling was implemented using JASP's regression module with support vector regression (SVR), k-nearest neighbors regression (KNN), and random forest regression. To avoid data leakage, JASP's internal train/validation/test split design (70/15/15) was used, with preprocessing (scaling and imputation) performed separately within folds.

5.1. Data preprocessing for machine learning analysis

The target variable was the **total REE recovery (%)**, calculated as the arithmetic mean of all individual REE recoveries reported in a given observation. Subgroups for LREEs: La, Ce, Pr, Nd, Sm; and HREEs: Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Y were similarly aggregated by their mean recovery. Predictor variables were harmonized into three categories: (1) Process parameters (pH, temperature, pulp density, leaching time); (2) Waste composition, including the concentrations of major elements (e.g., Al, Fe, Zn, Cu) and total REE content; and (3) Biological factors, represented as binary indicators for the presence of key microbial types (e.g., fungi, acidophilic bacteria). All continuous features were standardized to z-scores to neutralize the influence of differing units and scales. This balanced feature engineering strategy allowed the models to equitably learn from the complex interplay between biological activity and physicochemical conditions.

Given the modest dataset size ($n \approx 50$), predictive modeling was conducted using an exploratory framework. Support Vector Regression (SVR), k-Nearest Neighbors Regression (KNN), and Random Forest Regression within JASP, were applied. To ensure robustness and avoid data leakage, the analysis used JASP's internal 70/15/15 train/validation/test split, with all preprocessing (scaling and imputation) performed separately within each fold. Model performance was evaluated exclusively on the held-out test set. Feature importance was assessed using a model-agnostic, permutation-based method, quantified by the increase in Root Mean Squared Error (RMSE) after permuting a predictor. To evaluate the stability of these importance rankings across 100 bootstrap resamples, the median rank, rank variability (SD), and Spearman correlation with the baseline ranking, were recorded. The results, detailed in Supplementary Tables S8-S14, show high correlations ($\rho > 0.75$) for most features, indicating robust importance attributions despite the small sample size. The analysis revealed that pretreatments like roasting and acid pre-leaching were associated with a significant uplift in REE recovery. A mean uplift of +12–15 percentage points compared to organism-only systems (posterior mean: +13.4, 95 % CrI: [6.2, 20.1]). The strongest benefits were observed for e-waste, where acid pre-leaching significantly improved the mobilization of La, Ce, and Nd. Coal fly ash showed smaller, though positive, effects (generally < 10 % uplift). A weak negative interaction with pulp density was detected, suggesting the benefit of pretreatment may diminish at higher solid loadings (>15 % w/v). However, the credible intervals for this effect overlapped zero, indicating uncertainty. Overall, pretreatments explain a meaningful fraction of the heterogeneity in REE recovery outcomes across studies. These findings are reported in Supplementary Table S14-S16.

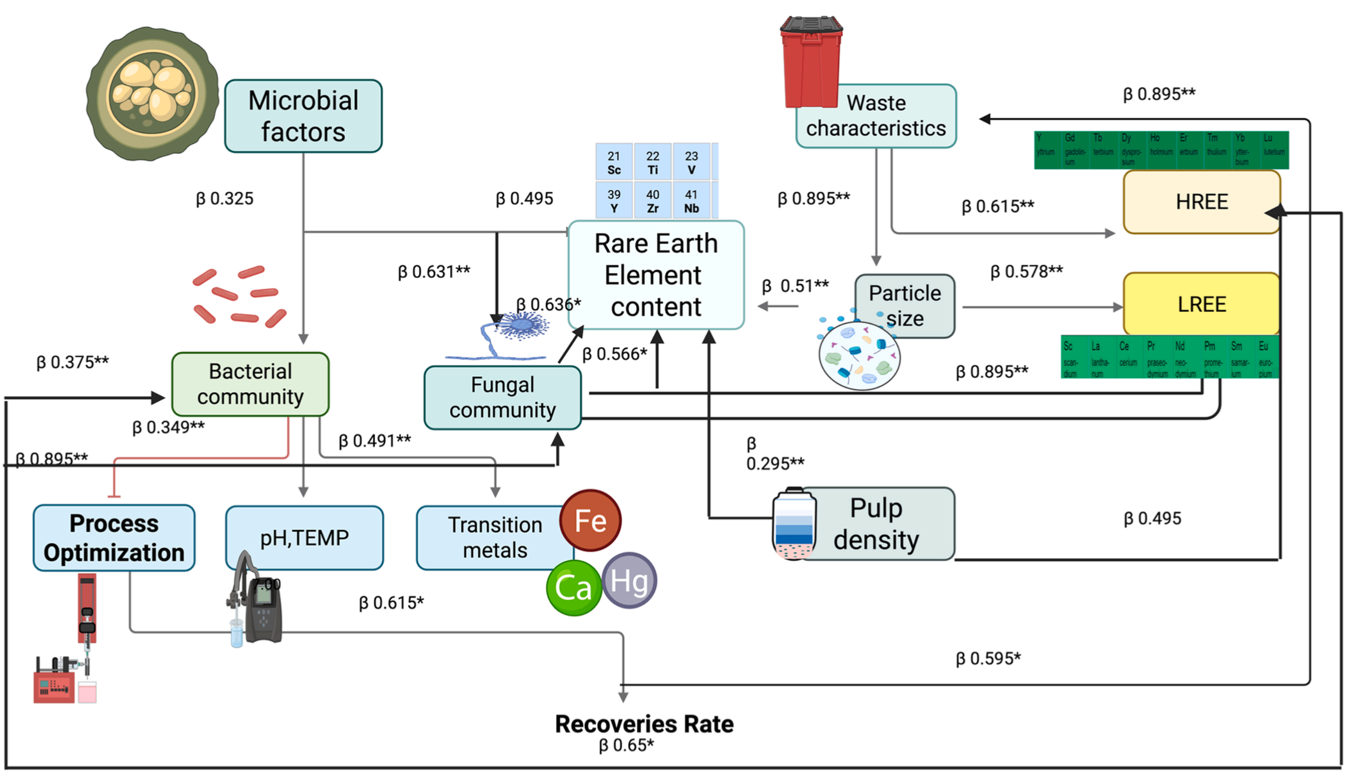

Fig. 5. SEM path diagram with regression weights. Where W/dfd = 0.200 (P = 0.688), GFI = 1.000 and RMSEA = 0.004.

5.2. Support vector regression (SVR)

An RBF kernel was employed with hyperparameters tuned over C ∈ {0.1, 1, 10, 100}, ε ∈ {0.001, 0.01, 0.1, 1}, and γ ∈ {0.001, 0.01, 0.1, 1}. The optimal configuration was $C = 10$, $\varepsilon = 0.01$, $\gamma = 0.1$. SVR achieved $R^2 = 0.87$, explaining 87 % of variance in REE recovery, with MSE = 82.50, RMSE = 9.08, MAE = 6.09, and MAPE = 10.59 %. The scaled MSE was 0.121, confirming effective normalization [63]. Permutation dropout loss identified Al (5.727) and transition metals (5.538) as top predictors, followed by Zn (5.101) and fungal presence (4.703). Among microbes, both fungi and bacteria (e.g., *Aspergillus, Acidithiobacillus*) contributed significantly, consistent with their mechanistic roles [39, 63]. Other relevant predictors included Cu, La, and Y, along with process variables such as temperature and leaching time [64]. Despite collinearity among elemental features, importance rankings remained stable across bootstraps (median Spearman $\rho = 0.84$; Supplementary Table S14).

5.3. K-Nearest Neighbors regression (KNNR)

The best configuration was $k = 1$ with Euclidean distance and rectangular weights. KNNR achieved $R^2 = 0.787$, MSE = 28.21, RMSE = 5.31, MAE = 3.16, and MAPE = 6.02 %. The scaled MSE was 0.203, indicating moderate generalization [65]. Feature importance analysis highlighted temperature (0.739), aggregate REE groups such as "Others" (0.601) and HREE (0.601), and individual REEs including Gd, Nd, Ce, and LREEs (0.377–0.387). Microbial features (fungi, bacteria, acidophiles) contributed minimally, showing negligible dropout loss [66]. Bootstrap stability tests confirmed high consistency of predictor rankings ($\rho > 0.75$; Supplementary Table S11).

5.4. Divergence between models

Notably, several key REEs such as La, Y, Tb, Ho, Tm, Yb, and Lu, also demonstrated minimal importance in this context. These findings suggest that under the given data structure and modeling approach, physicochemical features, particularly temperature and elemental concentrations, play a dominant role in driving REE recovery predictions [43]. However, microbial factors were less influential in the non-parametric KNN model compared to more complex models like SVM. The KNN model performance is presented in Fig. 6c and d. The predicted versus observed test values (Fig. 6c) demonstrated moderate predictive ability, with some deviation from the regression line. The model achieved a coefficient of determination (R^2) of 0.787, indicating that it could capture approximately 79 % of the variance in REE recovery outcomes. The RMSE was 5.31, and the mean absolute error (MAE) was 3.16. Model tuning based on the number of nearest neighbors (Fig. 6d) revealed that the prediction error increased with higher values of k. The lowest MSE occurred at $k = 1$, suggesting that the simplest model yielded the most accurate predictions [65]. However, the model showed high sensitivity to small changes in the number of neighbors, reflecting its vulnerability to local variations and potential overfitting [52]. The divergence in feature importance between SVR and KNN likely reflects algorithmic sensitivities rather than contradictory findings. SVR, which leverages nonlinear kernels, can capture interaction effects between microbial community features (e.g., fungal presence) and elemental composition, thereby attributing substantial weight to fungal predictors. In contrast, KNN relies on Euclidean distance, where binary microbial indicators contribute minimally relative to continuous geochemical variables, leading to near-zero fungal importance. This highlights the dependence of feature attribution on model

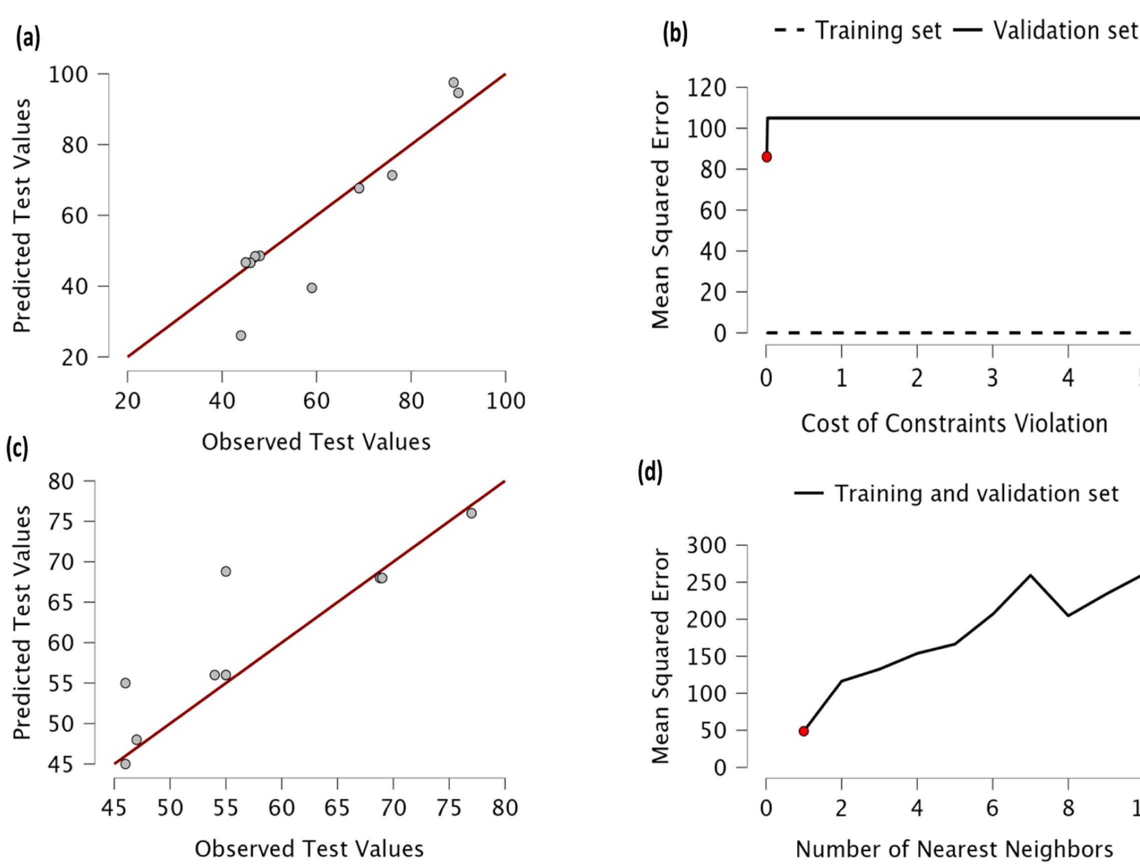

Fig. 6. Machine Learning Regression Models pipeline for REE prediction (a) Predication test value vs observed test value based on SVMR, (b) Mean squared error of training and validation test (c) Predication test value vs observed test value based on KNNR model. (d) Mean squared error of training and validation test vs Number of nearest Neighbors.

structure and metric choice. We therefore interpret machine learning outputs as complementary and exploratory, providing qualitative insight into feature relevance rather than definitive causal rankings. Despite strong performance on the test set, the models' robustness to domain shift such as application to new waste types or pilot-scale conditions requires careful assessment. A leave-one-waste-out validation revealed a performance drop (R^2: 0.45–0.60) when predicting for waste categories absent from training, highlighting this challenge. Addressing such generalization issues is an active focus in computational ecosystem [6]. For future deployment, strategies like transfer learning, where a model pre-trained on a large, diverse lab-scale dataset is fine-tuned with limited pilot-scale data, or the use of advanced metaheuristic frameworks for model calibration could be essential to improve generalizability and ensure reliable performance in real-world, heterogeneous industrial settings [67].

5.5. Mechanistic insights tied to SEM and ML outcomes

The SEM results demonstrated that process variables (pH, pulp density, temperature) exerted the strongest direct influence on REE recovery ($\beta = 0.895$, $p < 0.01$). This finding is mechanistically consistent with acidolysis and complexolysis, where low pH and fungal secretion of citric and oxalic acids accelerate the dissolution of LREEs such as La, Ce, and Nd. The strong positive path from fungal activity to LREE recovery ($\beta = 0.578$) supports this interpretation, highlighting the centrality of organic acid proxies in mobilizing light REEs. In contrast, *Acidithiobacillus* and related acidophilic bacteria showed stronger associations with redoxolysis pathways, reflected in higher mobilization of HREEs (Dy, Y, Lu) and transition metals. SEM coefficients ($\beta = 0.615$ for *Acidithiobacillus* to HREE recovery) align with the bacterial oxidation of Fe^{2+} to Fe^{3+}, which drives mineral breakdown and enhances the solubility of heavy REEs. ML models further reinforced these mechanistic patterns. The SVR model ranked fungal presence (importance = 4.703) and organic acid–linked metals (e.g., Al, Zn) as top predictors of REE recovery, whereas the KNNR model highlighted temperature and HREE concentrations as dominant features, consistent with bacterial redox activity under acidic conditions . These findings align with the broader evolution of optimization research, where emphasis is shifting from purely metaphor-driven heuristics toward more rigorous, mathematically grounded algorithms the framework proposed in "Optimization Algorithms Surpassing Metaphor" [68]. highlights the limitations of relying solely on analogy-inspired heuristics and advocates for mechanism-driven designs that enhance reliability, transparency, and scalability. This perspective reinforces the importance of integrating advanced algorithmic strategies into bioleaching research, particularly for parameter optimization and predictive modeling. By adopting such approaches, future studies could improve not only recovery efficiency but also the generalizability of predictive models across different waste matrices. These quantitative associations map directly onto known biochemical mechanisms inculding fungal complexolysis favoring LREEs, and bacterial redoxolysis driving HREE and transition metal co-dissolution. Collectively, the integration of SEM, ML, and mechanistic pathways demonstrates that fungal-driven organic acid production is the primary route for LREE mobilization, whereas acidophilic bacterial oxidation is dominant for HREE recovery. This element-specific mechanistic mapping provides a robust explanatory framework that links microbial metabolism with quantitative recovery outcomes. In addition to traditional regression and SEM approaches, the integration of efficient metaheuristic optimizers offers promising opportunities for enhancing predictive accuracy in bioleaching research. For example, the INFO algorithm [6]. which leverages the weighted mean of vectors, has demonstrated high efficiency in handling nonlinear, high-dimensional problems. Applying such algorithms to optimize key process parameters (e.g., pH, pulp density, microbial ratios) could substantially improve recovery predictions and guide experimental design. This suggests that future work should consider hybrid frameworks that combine mechanistic SEM insights with INFO-based optimization to better capture the complexity of waste microbe and process interactions.

Our results highlight that optimizing multiple interdependent parameters such as pH, temperature, and pulp density requires approaches that can simultaneously account for nonlinearities and trade-offs. In this context, the application of predictive models such as random forest for fluid property estimation provides a useful analogy for predicting leachate behavior across different pulp densities and waste types [8]. Similarly, our SEM-based framework could be further enhanced by adopting gaussian process regression approaches as soft sensors to capture microbial activity and system fluctuations that are difficult to monitor directly [69]. Moreover, the challenge of balancing kinetics, selectivity, and microbial tolerance observed in our meta-analysis parallels multi-objective problems in water resources management, where hybrid metaheuristics such as bat algorithm combined with differential evolution have proven effective (Ahmadianfar et al., 2016). These approaches support our finding that scaling bioleaching systems will benefit from hybrid frameworks integrating mechanistic insights with advanced optimization algorithms.

6. Research gaps and innovation roadmap

Despite significant advances in bioleaching for REE recovery, several critical research gaps still remain. A deeper mechanistic understanding of microbial-mineral interactions is essential for optimizing bioleaching efficiency, yet genomic and metabolic studies to identify and engineer ideal microbial strains are still underdeveloped. Additionally, bioleaching processes often exhibit slower reaction kinetics than conventional chemical methods, posing a challenge to improving extraction rates while preserving environmental benefits [49]. Most research has been confined to laboratory or pilot scales, with a notable lack of robust, scalable bioreactor designs and operational protocols capable of maintaining optimal microbial growth conditions and pulp densities for industrial applications. Furthermore, the efficient recovery of REEs from complex, low-grade, and heterogeneous wastes such as e-waste, coal ash, and industrial residues remains difficult due to their intricate matrices and low metal concentrations [21]. The integration of bioleaching with downstream separation technologies also requires further development to achieve effective, sustainable, and selective purification of solubilized REEs. Finally, comprehensive environmental impact assessments and techno-economic evaluations are limited, impeding the broader industrial adoption and investment in bioleaching technologies. Addressing these gaps is crucial for advancing bioleaching from experimental stages to viable, large-scale solutions for sustainable REE recovery. Furthermore, incorporation of the technologies into life cycle assessment (LCA) tools is the key to trigger industrial investment and to help design regulatory policies towards making widespread implementation feasible. With incorporation of the progress in biotechnology into data-guided process control and enabling policies, bioleaching can emerge as a key technology for future sustainable rare earth element supply chains. As tecno-economic assessment (TEA)/LCA outcomes are highly sensitive to system boundaries (e.g., scale, reagent recycling, downstream separation method), producing reliable quantitative anchors (e.g., $/kg REE, GHG/kg REE) would require dedicated process flow-sheet development and sensitivity/uncertainty analysis. Therefore, it is recommended that future research integrates TEA and LCA with process modelling to bridge laboratory-scale findings with industrial feasibility assessments. Several recent studies illustrate the opportunities and challenges of integrated assessments. Alipanah et al. (2020) performed TEA and LCA for REE recovery from coal byproducts via biosorption and highlighted that reagent use and material recycling dominate costs and emissions. Sánchez Morán (2024) conducted a techno-economic and environmental analysis of an acid-free dissolution route for didymium from e-waste, showing that the choice of solvent system directly influences cost and GHG profiles. More recently, probabilistic TEA/LCA frameworks for waste streams such as phosphogypsum (Smerigan et al., 2025) have underscored how profitability and sustainability depend strongly on feed concentration, process scale, and design assumptions.

Bioleaching innovations for REE recovery have advanced through several key strategies. The development and engineering of specialized microbial strains, such as *Gluconobacter oxydans* which are capable of producing effective organic acids from low-cost and waste substrates, is central to enhancing bioleaching efficiency and reducing operational costs [38,48]. Process optimization leveraging machine learning and system analytics is being applied to fine-tune parameters like pH, temperature, pulp density, and nutrient supply to maximize metal extraction rates [43]. The design and scale-up of controlled bioreactor systems with real-time monitoring aim to maintain optimal microbial growth conditions for industrial applications. Integrating bioleaching with complementary downstream separation techniques, including biosorption and greener solvent extraction, has been pursued to improve selectivity and recovery yields. The valorization of agricultural and food waste as feedstocks for microbial lixiviant production supports circular economy goals and sustainability [57]

Comprehensive techno-economic analyses and life cycle assessments guide the economic viability and environmental impact reduction of bioleaching plants [57]. Ongoing research has focused on overcoming challenges posed by heterogeneous waste streams, such as e-waste, by combining bioleaching with bioaccumulation and material conditioning strategies to ensure reproducible and efficient REE recovery [15,21]. These innovations collectively aim to transition bioleaching from laboratory-scale experiments to profitable, scalable, and environmentally friendly industrial processes for critical raw material recovery.

Furthermore, a critical gap exists in the safety and environmental risk management framework for scaled-up bioleaching operations. The potential release of acidophilic or engineered microbes, the generation of acidic effluents rich in residual metals, and the management of bioleached residues pose significant biosafety and environmental challenges [28–30]. Future research must prioritize a "safety-by-design" approach, integrating robust containment strategies (e.g., closed-loop bioreactors), effective effluent polishing (e.g., neutralization, constructed wetlands), and thorough toxicological profiling of process streams. Quantifying the net environmental benefit, such as the reduction in contaminant load (e.g., heavy metals, radionuclides) in landfill leachates through the prior extraction of these elements, will be crucial for holistic life-cycle assessment and regulatory approval [41–43]. Making the process safer and more sustainable by design is a prerequisite for its industrial adoption.

7. Future directions and emerging technologies

The future outlook for the bioleaching of rare earth elements is promising, driven by increasing demand for sustainable and environmentally friendly recovery methods from both primary ores and secondary waste sources such as e-waste and printed circuit boards (PCBs). Emerging technologies focus on optimizing bioleaching processes through advanced microbial consortia, including fungi and bacteria capable of producing organic acids (e.g., citric, gluconic, and oxalic acids) and oxidizing agents that increase metal solubilization [50].

The integration of bioleaching with machine learning and process analytics is enabling precise control of key operating conditions, including pH, temperature, pulp density and aeration rate. This level of optimization will not only be improving efficiency, but also makes the process more reproducible and scalable [42] Additionally, novel biological strategies including integration of biosorption, bioflotation, and bioelectrochemical methods are being investigated to enhance the bioleaching process and further improve REEs selectivity and recovery efficiencies [27]. Synthetic biology is opening new opportunities for tailoring microbial capabilities to the specific requirement of REE recovery, whether that means tolerating high metal concentrations, producing high number of organic acids, or deploying specialized enzyme systems. Notably, engineered strains of *Aspergillus niger* and *Acidithiobacillus ferrooxidans* have demonstrated both improved leaching kinetics and broader pH tolerance, thus broadening their utility for the processing of diverse waste streams [50]. Despite current limitations, such as slow kinetics and scale-up challenges, ongoing research aims to overcome these barriers by developing robust bioreactor designs, as well as hybrid processes which combine bioelectrochemical systems, and nanotechnologies that combine biological, chemical, and physical or mechanical methods.

For future prospectus, incorporation of bioleaching with environmentally friendly downstream separation processes (e.g., solventless precipitation of REE, ionic liquid extraction, or membrane-based selective filtration) can enhance the recovery process, by ensuring both economical as well as environmental objectives.

Future studies should incorporate techno-economic and life-cycle assessment (TEA/LCA) alongside mechanistic and predictive modelling to ensure that bioleaching advances are both environmentally and economically sustainable. Building on the SEM and ML insights presented here, future work can construct standardized process boundaries and develop flow-sheet models for representative scenarios such as e-waste and coal fly ash. In addition, random forest and gaussian process regression models illustrate how predictive machine learning methods can function as soft sensors, enabling uncertainty quantification and scenario analysis within TEA/LCA frameworks . Collectively, these advances suggest that coupling mechanistic TEA/LCA approaches with modern optimization and ML tools offers a pathway toward more reliable and scalable assessments of REE recovery processes. This would allow for defensible estimates of key indicators, including cost per kilogram REE recovered, acid consumption, energy intensity, and greenhouse gas emissions, and provide a direct comparison with state-of-practice hydrometallurgical methods. Such integration will be critical to de-risk scale-up, attract industrial investment, and guide policy frameworks supporting circular economy transitions. Such integration would allow defensible estimates of key indicators, including cost per kilogram REE recovered, energy intensity, acid consumption, and greenhouse gas emissions, while providing a direct comparison with state-of-practice hydrometallurgical methods. For example, TEA/LCA work on coal byproducts [19] electronic waste [32] demonstrates the feasibility of such analyses and the importance of scale sensitivity. Leveraging these approaches for bioleaching will be critical to de-risk industrial scale-up, attract investment, and inform policy frameworks that support sustainable circular economy transitions.

8. Conclusion

Bioleaching presents a sustainable and environmentally friendly alternative to conventional physicochemical methods for recovering rare earth elements (REEs) from primary ores and diverse waste sources. Compared to traditional extraction methods, it offers significant advantages, including reduced energy consumption, minimal greenhouse gas emissions, and elimination of hazardous chemicals, thereby minimizing environmental impacts while supporting circular economy goals. Microorganisms like *Aspergillus niger* and acidophilic bacteria facilitate REE solubilization through both direct enzymatic action and the production of biodegradable metabolites, enabling efficient recovery without damaging mineral structures.

The integrative approach of this review, by combining Bayesian meta-analysis, structural equation modeling, and machine learning, introduces fresh quantitative evidence on the determinants of bioleaching efficiency, with a well-developed predictive process optimization framework. Despite challenges such as slow kinetics and scale-up limitations, emerging innovations in microbial strain engineering, adaptive process optimization, and integration with green downstream separation technologies are enhancing the feasibility, selectivity and scalability of bioleaching. Adaptability of this biotechnology at low-grade and complex waste matrices can further improve the potential of bioleaching to alleviate supply risks of critical raw materials, during any global supply chain disruption. Overall, bioleaching is not only a low-cost and low-footprint solution to sustainable REE mining but also a game-changing tool in the creation of sustainable, resource-efficient, and green supply chains of the future.

Despite the promising recovery efficiencies demonstrated at the laboratory scale, the industrial translation of bioleaching faces specific and non-trivial engineering bottlenecks. These include managing the acid balance and reagent consumption over long residence times, dealing with the challenging rheology and mass transfer limitations at industrially relevant pulp densities (>10 % w/v), and preventing microbial washout in continuous systems. As evidenced by our analysis (Fig. 2c), the vast majority of current research is confined to TRL 1–3 (basic research to proof-of-concept), with very few studies advancing to prototype-scale (TRL 4) or higher. Therefore, while the integrated data-driven framework presented here lays a strong foundational roadmap, overcoming these specific unit operation challenges is the critical next step to advance the technology readiness level and achieve viable industrial implementation.

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the authors used Gemini by Google to improve the readability and language used in some parts of the review. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

CRediT authorship contribution statement

Hamid Rehman: Writing – original draft, Resources, Methodology, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Eyup Debik:** Supervision, Project administration, Funding acquisition. **Kubra Ulucan-Altuntas:** Writing – review & editing, Formal analysis, Data curation. **Neslihan Manav-Demir:** Writing – review & editing, Methodology, Formal analysis. **Baris Canci:** Resources. **Mazhar Iqbal:** Validation, Formal analysis. **Rocío Barros:** Methodology, Formal analysis. **Wasif ur Rehman:** Software, Methodology, Data curation. **Sanjay K. Mohanty:** Writing – review & editing, Data curation, Conceptualization. **Aqib Hassan Ali Khan:** Writing – review & editing, Software, Methodology, Formal analysis, Data curation.

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.

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Supplementary materials

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Data availability

Data will be made available on request.

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