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Assessing the sustainability of solvometallurgy for black mass processing – the LEACH (Low-impact Extraction and Assessment of CHemical solvometallurgy) tool

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The sustainable recovery of critical raw materials such as cobalt from spent lithium-ion batteries (LIBs) is a pressing challenge, particularly as the demand for electrification accelerates. Solvometallurgy, and in particular the use of deep eutectic solvents (DESs), has emerged as a promising alternative to conventional hydrometallurgical and pyrometallurgical approaches due to its potential for enhanced selectivity, reduced environmental impact, and process modularity. However, the scalability of DES-based leaching remains limited due to economic, technical, and safety concerns often overlooked during early-stage research. To address this gap, we present LEACH (Low-impact Extraction and Assessment of CHemical solvometallurgy), a modular, penalty-based tool designed to evaluate the sustainability of emerging solvometallurgical processes. Inspired by the EcoScale framework, LEACH incorporates economic, technical, and occupational safety criteria, assigning penalty points that reflect deviations from an ideal process. The tool is structured into three modules—solvent formulation, black mass leaching, and overall process evaluation—allowing for detailed diagnostics and early identification of sustainability bottlenecks. LEACH was applied to two case studies targeting cobalt extraction from black mass using DESs based on choline chloride combined, respectively, with citric acid or ethylene glycol. While process 1 (citric acid-based, mild conditions) achieved a higher final score (43.5/100) than process 2 (ethylene glycol-based, high temperature), both processes were classified as non-ideal (score < 50), underscoring significant limitations in terms of recyclability, toxicity, and regulatory compliance. Notably, safety-related penalties emerged as critical barriers to scale-up, highlighting the importance of integrating occupational hazard assessments from the outset. Overall, LEACH offers a practical, flexible, and safety-conscious approach to guide the design and optimization of sustainable solvometallurgical processes, aligning with Safe-and-Sustainable-by-Design principles and supporting more responsible LIB recycling technologies.

Green foundation

1. This work presents LEACH, a modular, penalty-based assessment tool designed to evaluate the sustainability of emerging solvometallurgical processes for critical metal recovery. It addresses a current gap by integrating economic, technical, and safety considerations within a single framework, supporting early-stage green chemistry decision-making. Uniquely, it incorporates occupational safety and hazard assessment at the laboratory scale, aligning with the European Commission's Safe-and-Sustainable-by-Design (SSbD) approach.
2. The tool enables qualitative and quantitative diagnosis of sustainability trade-offs in solvent design and leaching procedures, highlighting issues such as toxicity, recyclability, energy intensity, and regulatory compliance. By assessing safety aspects typically ignored in early research, LEACH helps flag scale-up risks from the outset and promotes inherently safer chemical process development.
3. LEACH could be further improved by incorporating more comprehensive and standardized data on black mass, including its composition, cost, environmental behaviour, and safety profile. The current lack of industrial standardization in BM characteristics limits accurate benchmarking and sustainability forecasting. Nevertheless, LEACH is designed with flexibility in mind and can be readily adapted to integrate future innovations and new data as they become available.

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1. Introduction

The rapid growth of lithium-ion battery (LIB) production, driven by electrification and energy storage demands, has intensified the pressure on critical raw materials such as lithium, cobalt, and nickel.[1] Currently, the supply chain is heavily concentrated, with China holding a dominant position across both production and recycling stages.[2] This geopolitical imbalance, alongside rising environmental concerns, has prompted the search for alternative sources and more sustainable processing technologies. One promising avenue is the recovery of valuable metals from spent LIBs, a strategy often referred to as urban mining.[3] When spent LIBs cannot be directly regenerated, they are discharged and ground to obtain a black powder (black mass, BM), whose composition depends on the pristine cathodes.[4] As the most commonly used cathodic configurations in the automotive sector and electronic devices are $LiCoO_2$ (LCO) and $LiNi_xMn_yCo_{1-x-y}O_2$ (NMC), most of the produced BM contains a mixture of Li, Co, Ni, and Mn, along with graphite recovered from the anode, and other elements to a minor extent, such as P, Fe, Cu, Al, and others.[5] In this context, exploitation of BM through solvometallurgy is emerging as a possible cleaner alternative to conventional hydrometallurgical and pyrometallurgical processes.[6] Solvometallurgy is characterized using non-aqueous solvents to extract metals and potentially reduce waste generation and improve selectivity. Among the most effective systems, deep eutectic solvents (DESs) stand out for their tunability, relatively low toxicity, and ease of preparation.[4] Despite these advantages, the practical industrial adoption of DES-based solvometallurgy is still far from being implemented, being currently limited to the laboratory scale. Several challenges hinder its scale-up from TRL 4 to 5–6, including the high cost of key components such as choline chloride and the lack of optimized solvent recycling strategies. Laboratory studies often fail to account for process efficiency, safety, and economic feasibility, factors that are crucial for practical implementation. There is a clear need to integrate these dimensions from the earliest research stages to support the development of scalable and responsible technologies. The DES-based solvometallurgical treatment of BM can be rationalised into two key steps: (I) the preparation of the eutectic solvent and (II) the leaching of the BM. Each of these steps introduces specific economic, technical, and safety concerns. Proper evaluation of these factors requires assessment tools capable of capturing the unique features of emerging processes. Some simplified tools have been proposed for early-stage environmental screening. For instance, frameworks that estimate embodied energy and carbon footprint, such as ESCAPE (*Evaluation of Sustainability of material substitution using CArbon footPrint by a simplifiEd approach*), have been used to compare leaching agents or assess process alternatives.[7] While such methods provide useful preliminary insights, they are not equipped to handle the full complexity of solvometallurgical systems. In particular, they tend to overlook critical aspects such as solvent degradation, toxicity, corrosiveness, and occupational safety. Recent studies have shown that common DESs, like ethaline, may release hazardous compounds under ambient conditions due to thermal or chemical instability.[8] These degradation pathways, along with process-specific issues such as high viscosity and limited metal loading capacity, influence both the safety and energy efficiency of the process.[9] Comprehensive evaluations are further constrained by the limited availability of life cycle inventory data for DESs, which complicates the use of more detailed tools such as Life Cycle Assessment (LCA). For example, Rinne *et al.*[10] used simulation-based LCA to study BM leaching *via* conventional hydrometallurgical routes and emphasized the need for optimized washing and acid usage to reduce impacts. Pražanová *et al.*[11] examined gate-to-gate impacts of pre-treatment stages for LIBs, while Klejnowska *et al.*[12] assessed pyrometallurgical BM processing conducted in a Waelz kiln. However, these strategies typically do not capture solvent formulation, reuse dynamics, or intermediate hazard mechanisms such as thermal instability or incompatibility with specific metals. These limitations reveal a broader gap in sustainability assessment frameworks. Existing tools often lack the resolution and flexibility needed to assess emerging technologies that do not yet have established industrial benchmarks. In parallel, broader policy and research agendas have called for more proactive and integrated frameworks to ensure that new chemical processes meet both functional and sustainability goals. One such initiative is the European Commission's *Safe-and-Sustainable-by-Design (SSbD)* framework, which promotes early integration of hazard minimization, environmental compatibility, and long-term viability in materials innovation.[13] In the case of the emerging solvometallurgy, a robust and affordable assessment tool should consider the solvent choice, the scalability, and the process safety, which should be balanced with extraction performances. Despite the conceptual alignment, however, there remains a lack of operational tools capable of implementing SSbD principles at the laboratory scale. Over the last three years, several complementary evaluation frameworks have been proposed for hydrometallurgical battery recycling. AI-assisted readiness/sustainability scoring has emerged to rank emerging hydrometallurgical options (DESs, ILs, membranes, supercritical fluids, and adsorbents) across complexity, energy, emissions, and economic potential. This approach converts qualitative evidence into quantitative readiness scores and highlights upscale prospects but offers limited process-specific diagnostics for solvent formulation and OSH risks.[14] Also, LCA-for-process-development workflows now use hotspot analyses and scenario modeling specifically to guide hydrometallurgical route design (*e.g.*, reagent sourcing, washing, and energy mixes) and to compare regional implementations. These are powerful tools when inventories exist but remain data-intensive at TRLs 3–5.[15] On the other side, integrated techno-economic analysis and life cycle assessment (TEA/LCA) reviews and modelling studies have expanded comparative evidence for hydro *vs.* pyro and direct regeneration, mapping cost/impact trade-offs and the need for harmonized assumptions, again emphasizing late-stage data rather than early-stage screening.[16,17] Alternatively, multi-criteria decision analysis (MCDA) has been applied to prioritize recycling technologies and even to choose leaching test methods. MCDA structures expert judgment well, but usually does not embed hazard/regulatory penalties or solvent stability diagnostics.[18,19] Finally, broad state-of-the-art reviews synthesize hydrometallurgical progress and performance benchmarks but stop short of actionable scoring tools for lab-scale iteration.[20]

In this context, this paper addresses the current lack of integrated sustainability tools tailored for DES-based solvometallurgy by introducing LEACH (Low-impact Extraction and Assessment of CHemical solvometallurgy). LEACH is a modular assessment framework designed to evaluate emerging processes by integrating economic, technical, and safety criteria into a unified scoring system. By enabling early-stage diagnostics, it supports researchers and developers in making informed, holistic design decisions. A key innovation of LEACH is its explicit incorporation of occupational safety and health (OSH) parameters, an often-neglected dimension in existing sustainability assessments. While many tools focus predominantly on environmental metrics, LEACH highlights the crucial need to evaluate risks to workers involved in solvent handling, leaching, and metal recovery operations. This focus aligns with the European Commission's SSbD initiative, which advocates for hazard reduction and safety considerations from the earliest stages of R&D.[21,22] By embedding OSH-related penalties and criteria, LEACH facilitates the identification of potential hazards, the implementation of appropriate control measures, and the promotion of inherently safer process designs. This integration helps ensure that green chemistry principles are pursued in parallel with regulatory compliance and ethical responsibility. The LEACH framework thus offers a comprehensive platform for advancing responsible solvometallurgical recycling, particularly in the context of lithium-ion battery (LIB) black mass recovery.[23,24] In this context, the LEACH framework offers a valuable resource for advancing the sustainability of solvometallurgical recycling.

2. Methodology

2.1. Field of application

LEACH is designed to evaluate solvometallurgical processes as they are reported in the literature or demonstrated experimentally. The tool scores a process based on solvent formulation, operational conditions, safety considerations, and regulatory aspects, without modelling the properties of the feedstock. For this reason, LEACH does not take black mass (BM) composition as an input parameter and does not incorporate composition–performance relationships. In hydrometallurgical studies, key performance indicators such as yield and selectivity are already normalised to the metal content of the specific BM used, typically determined by ICP analysis, and PMI reflects the mass of reagents and solvents required by the process rather than the impurity fraction of the BM. Consequently, small differences in BM composition across different sources (*e.g.*, variations in the Li/Co/Ni ratio or impurity levels such as C, Cu, or Al) do not influence any of the parameters used by LEACH. The tool therefore remains applicable to published processes involving BMs of a similar type but different origin, provided that the original performance data are reported. When comparing processes that rely on BMs with different impurity profiles, LEACH can be applied consistently, but interpretation should be accompanied by the authors' reported BM characterisation, as feed composition lies outside the scope of the tool.

Although cobalt is used in the case studies presented in this work, this choice reflects the information available in the source publications, which report complete analytical data only for Co. LEACH itself is metal-agnostic, and the scoring criteria can be applied to any metal (*e.g.*, Li, Ni, or Mn) if yield, selectivity, and related performance indicators are reported for that element.

To demonstrate versatility beyond DES-based systems, two additional solvometallurgical processes (one ionic-liquid system and one organic acid system) were evaluated using LEACH. The simplified assessments are reported in the SI.

To ensure methodological transparency and avoid arbitrary scoring, the penalty structure of LEACH was derived from established evaluation tools, including EcoScale, Analytical Eco-Scale, PGS, BSAT, and ECOLIBRA. The ranges and weightings used in LEACH follow the logic adopted in these frameworks and were adapted to the specificities of solvometallurgical processes. Each subcategory included in LEACH reflects a well-defined operational, safety, or environmental indicator described in the literature and discussed in detail in section 2.2. This structured derivation ensures that penalty values do not originate from subjective criteria but from the consensus methodology already validated in green process assessment.

2.2. Background for category definition

The starting point for building the assessment tool LEACH is the structure of the EcoScale. In particular, Van Aken and coworkers developed in 2006 a scoring model based on penalty points to evaluate the ecological feasibility of chemical reactions.[25] Their method assigned penalties across various categories that reflect not only synthetic and operational parameters, such as yield, technical simplicity, waste generation, atom economy, and solvent use, but also economic aspects (including reagent cost and energy consumption) and factors impacting human operators and the environment, such as toxicity and safety. The EcoScale is designed to assess laboratory-scale organic syntheses by assigning a total score from 0 to 100, with 100 representing an ideal green synthesis. Points are deducted based on deviations from best practices in sustainability, safety, and practicality. The assessment encompasses six key dimensions:

(I) Yield – penalizes inefficient reactions by deducting points proportional to the loss of product; (II) cost – evaluates the affordability of reagents on a small-scale basis (typically 10 mmol); (III) safety – assigns penalties based on the presence of hazardous or toxic chemicals, following standard safety classifications; (IV) technical setup – reflects the complexity and accessibility of the reaction conditions and equipment; (V) energy conditions – considers penalties for long reaction times and the need for extreme temperatures; and (VI) workup and purification – deduces points for methods requir-

Table 1 Summary of main penalty-based assessment tools

Entry	Tool	Focus area	Scoring method
1	EcoScale	Green chemistry (synthetic organic reactions)	Starts from 100; subtracts penalty points for non-green aspects (*e.g.*, low yield, toxic solvents, and high energy use)
2	Analytical Eco-Scale	Analytical chemistry	Penalty points for hazardous solvents, waste, and energy usage
4	Process Greenness Score (PGS)	Green chemical manufacturing	Composite metric with sub-penalties
5	Basic Sustainability Assessment Tool (BSAT)	Business/organizational sustainability	Multiple-choice format with point-based interpretation
6	ECOLIBRA	Product development sustainability	Screening tool using weighted scoring and penalties
7	Green Motion Tool (GSK)	Chemical process safety and sustainability	Color-coded matrix with penalty scoring for safety and environmental impact

ing extensive solvent use or complex separation techniques (*e.g.*, chromatography).

The scoring is transparent and cumulative: each parameter is individually assessed, and the total sum of penalties is subtracted from 100 to yield the final EcoScale score. This numerical output is then interpreted on a qualitative scale: excellent (>75), acceptable (51–75), or inadequate (<50). The EcoScale's logic offers a balance between usability and analytical depth, providing a rapid but structured approach to assess and improve green chemistry practices. Its semi-quantitative nature makes it especially well-suited to early-stage method development, where full life-cycle data may not yet be available. Moreover, the framework is intentionally flexible, allowing chemists to adapt criteria or weightings to reflect specific priorities or local contexts. Since its introduction in 2006, the penalty points approach pioneered by the EcoScale has influenced the development of several other sustainability assessment frameworks across diverse fields. For example, the Analytical Eco-Scale adapted the original concept to the context of analytical chemistry, penalizing procedures based on hazardous reagents, waste generation, and energy usage to assess the greenness of analytical methods.[26] Similarly, the Process Greenness Score (PGS) applies penalty-based logic to evaluate industrial chemical processes, incorporating a wider set of technical and environmental parameters.[27] Beyond the laboratory, tools like the Basic Sustainability Assessment Tool (BSAT) have extended the model to organizational and business contexts, using multiple-choice criteria to assign scores that reflect sustainability practices.[28] In the field of product development, ECOLIBRA employs a comparable scoring system to screen and guide sustainable innovation early in the research and development (R&D) phase.[29] The GSK tool emphasizes safety and environmental impact using a visual matrix, which can be valuable for immediately highlighting critical sustainability risks in an extraction process.[30] These evolutions demonstrate the versatility and enduring relevance of the penalty-based framework initiated by the EcoScale, reinforcing its role as a conceptual foundation for assessing sustainability in both scientific and applied settings. Table 1 provides a summary of some relevant penalty-based sustainability assessment tools. This table highlights each tool's focus area, scoring method, and overall approach. This initial comparison helps in understanding the range of methods available, their fundamental logic, and the potential for adaptation.

The assessment tools reported in Table 1 cover the application of the EcoScale logic in different application fields, providing a solid set of validated procedures to use as a starting point for the development of new tools able to assess the sustainability (in a broad sense) of any solvometallurgical recovery of metals from black mass. Thus, the choice of the categories and the attribution of specific penalty points are pivotal steps. In this context, to develop a tool able to assess the sustainability of solvometallurgical BM exploitation, the principles and scoring methodologies of the already validated sustainability tools reported in Table 1 were considered as guidelines. At first, it is important to highlight that each of these tools, while developed for diverse fields ranging from green chemistry to process safety, shares a common approach of evaluating environmental, economic, and safety aspects of processes using a penalty point system or weighted scoring. To adapt these principles to the context of solvometallurgy, a careful analysis of the key factors influencing the sustainability of solvometallurgical processes was conducted. According to Binnemans and coworkers,[31] solvometallurgical processes are influenced by several key parameters, including the choice of solvent, which must be environmentally benign, chemically suitable, and capable of dissolving target metal species. The type and concentration of the lixiviant (*e.g.*, mineral acids, organic acids, or chelating agents) play a critical role in determining leaching efficiency and selectivity. Feed material characteristics, such as metal content, mineralogy, and impurity levels, also impact process performance. Additionally, process conditions like temperature, solvent-to-solid ratio, and mixing intensity affect metal recovery. Finally, environmental and operational factors, such as water usage, energy consumption, and solvent recyclability, are essential for ensuring process sustainability and feasibility.

2.3. Category definition

LEACH was organized into three macro-categories: economic, technical, and safety analyses. Considering that no solvometallurgical BM processing has reached TRL 5 to date, the economic analysis was considered important but less critical.

The subcategories were defined to ensure a comprehensive evaluation of the sustainability of solvometallurgy, considering the preparation of the solvent (often a DES but not necessarily limited to) and the BM leaching, as follows:

(I) Economic category: this category covers key aspects such as materials cost, use of renewable feedstocks, and use of critical raw materials (CRMs). These parameters were inspired by the economic focus of ECOLIBRA and the Process Greenness Score (PGS), which both emphasize cost efficiency, resource utilization, and the reduction of critical materials in sustainable processes.

(II) Technical category: this category encompasses yield, temperature × time, workup, process/product stability, biodegradability, process mass intensity, recyclability, and selectivity. These parameters align with the technical performance criteria of the Analytical Eco-Scale and EcoScale, where process efficiency, product quality, and material recycling are fundamental to assessing sustainability.

(III) Safety category: this category includes intrinsic hazards, handling and control, emergency measures, environmental fate, and regulatory impact. These parameters reflect the safety-focused evaluation approach of the Green Motion Tool (GSK), which is designed to assess chemical safety and regulatory compliance, ensuring that processes do not pose risks to human health or the environment.

By systematically adapting these established assessment criteria to the specific challenges and requirements of solvometallurgy, the tool ensures a comprehensive evaluation of sustainability. This approach not only validates the relevance of each category but also enhances the tool's applicability to real-world metal recovery processes from black mass.

2.4. Penalty point attribution

Once the list of categories was assessed, the fair distribution of the penalty points was addressed. To reduce the arbitrariness of LEACH, a deep analysis of the logic behind the categories and the relative attribution of penalty points in the tools reported in Table 1 was conducted (Table 2). This analysis is crucial for identifying how different tools structure their penalty mechanisms, including their base score, granularity of penalties, safety considerations, environmental focus, economic criteria, and output interpretation.

The tools compared in Table 2 share a common foundation in the penalty point methodology, yet they diverge significantly in how penalties are structured and applied across domains. The EcoScale and Analytical Eco-Scale follow a deductive model starting from a perfect score (100), subtracting fixed penalty points for inefficiencies, safety risks, and environmental impacts. These tools offer clear, quantitative deductions based on lab-scale parameters such as yield, solvent use, and toxicity. In contrast, the Process Greenness Score (PGS) employs a more complex, weighted penalty system, assigning scores based on process-level indicators and integrating technical, economic, and environmental variables. This structure allows greater granularity and customization for industrial applications. The BSAT (Basic Sustainability Assessment Tool) differs by relying on a qualitative or categorical approach: it penalizes based on the presence of less sustainable practices,

Table 2 Comparison of penalty logic structures of tools reported in Table 1

Tool	Base score/benchmark	Penalty point structure	Granularity	Safety factor	Environmental focus	Economic cost criteria	Output interpretation	Feature
EcoScale	100[a]	Deductive, penalties for each subcategory	Moderate (6 categories)	Explicitly considered (hazard symbols)	Core emphasis (*e.g.*, solvents and waste)	Cost of reagents (per 10 mmol)	>75 = excellent, 51–75 = acceptable, <50 = inadequate	Laboratory-scale reaction assessment
Analytical Eco-Scale	100	Similar to EcoScale; penalties for reagents, waste, and energy use	Moderate (specific to analytical methods)	Considers toxicity, flammability, and explosiveness	Strong (especially waste and reagent impact)	Reagent cost considered	Same as EcoScale	Analytical method evaluation
Process Greenness Score (PGS)	Process-specific benchmarks	Penalty weights for technical, economic, and environmental factors	High (process-level indicators)	Included as specific safety parameters	Comprehensive (life-cycle view)	Includes process economics	Composite score (greenness rating)	Industrial process scoring
Basic Sustainability Assessment Tool (BSAT)	Category-based scoring (no fixed base)	Points deducted per unsustainable response	Low to moderate (qualitative answers)	Partially considered	Moderate (within broader sustainability)	General cost-awareness	Categorical sustainability level	Organizational self-assessment
ECOLIBRA	Custom baseline (R&D-oriented)	Penalty-based scoring per indicator set	Medium-high (designed for R&D screening)	Included in early design phase assessments	Strong (aligned with green innovation)	Screening for cost feasibility in design	Sustainability index or qualitative profile	Tool for the R&D stage of product design
Green Motion Tool (GSK)	Color-coded matrix	Penalty scoring with color indicators	High (process-level safety)	Explicitly safety-focused	Strong (toxicity and waste focused)	Not primarily economic	Color-coded performance rating	Safety-focused chemical assessment

[a] Ideal process.

using multiple-choice assessments rather than numerical inputs. Its simplicity favours broader organizational evaluations rather than chemical-specific analysis. Lastly, ECOLIBRA applies a flexible indicator-based structure, tailored for early-stage R&D. Penalties are linked to sustainability indicators relevant to innovation screening, including safety, cost feasibility, and environmental impact, but allow adaptability depending on the context. The safety category is strongly considered in the GSK tool which emphasizes hazard identification, control, and regulatory compliance. Looking at how the considered tools handle category weighting, it is possible to extrapolate some rationale or trend to be implemented in our assessment tool. Table 3 focuses on the main categories and weighting strategies used by the studied tools. It provides insight into how sustainability dimensions are prioritized in each model. This analysis is vital for designing a balanced scoring model for the extraction process tool, ensuring that the most critical aspects (such as economic, technical, and safety) are appropriately weighted.

Based on the comparative analysis of existing penalty-based sustainability tools, several key insights can guide the development of the proposed extraction process assessment tool. Looking at the simplicity and transparency, the EcoScale's straightforward penalty-based model is suitable for a wide range of users. Adapting its structure can maintain usability while ensuring clear sustainability assessments. Regarding the safety and environmental emphasis, the GSK tool's visual emphasis on safety and environmental impact is valuable. This can be integrated into the extraction tool to highlight critical risks. A certain adaptability for early-stage design is addressed by ECOLIBRA, which focuses on early-stage R&D, highlighting the importance of a flexible model. LEACH can incorporate an adaptive scoring system for different process stages, such as the solvent formulation (module 1) and the BM leaching (module 2). Focusing on a categorical and qualitative evaluation, BSAT's qualitative, category-based evaluation can be useful for broad sustainability assessments, allowing categorical scoring for extraction methods. Also, granularity and customization are two important aspects. The PGS tool's granular, multi-factor structure provides a model for creating a highly customizable tool, capable of assessing technical, economic, and environmental aspects based on user-defined criteria. Considering these characteristics, the LEACH tool was designed to be comprehensive and user-friendly. In particular, the concept of starting from an ideal score and deducting points based on unsustainable practices is directly derived from EcoScale's penalty-point approach. Categories like yield, cost, and use of renewable feedstocks were considered as consistent with EcoScale's focus on efficiency and sustainability. The inclusion of multiple subcategories within the Technical and Environmental criteria was also implemented as it reflects PGS's multi-dimensional approach. The granularity in penalty points (*e.g.*, >90% yield = 0, 60–90% yield = 5, <60% yield = 10) was aligned with PGS's method of differentiating the severity of sustainability impacts. Also, qualitative ranges (*e.g.*, fully renewable, partially renewable, and non-renewable) inspired by BSAT's categorical approach were considered. The scoring method of LEACH avoids excessive complexity, maintaining simplicity and user-friendliness, similar to BSAT. The use of renewable feedstocks and critical raw materials (CRMs) was considered in analogy with ECOLIBRA's focus on sustainable material selection and innovation. Finally, the subcategories were grouped into two families, each one associated with a different treatment module. This approach recalls ECOLIBRA's multi-context application. The emphasis on safety and environmental impact through CRMs and renewable feedstocks is consistent with GSK's focus on critical risk factors. In the end, LEACH demonstrates a strong foundation in existing, literature-backed frameworks, reducing the arbitrary subjectivity often encountered when new assessment tools are proposed.[32]

2.5. Structure of the sustainability tool

Based on a penalty-point framework, LEACH aims to highlight less sustainable aspects of a process by assigning scores that reflect economic, technical, and safety-related shortcomings. Unlike reward-based systems, the LEACH tool penalizes features that detract from sustainability, thereby guiding users toward more responsible process design. Its structure is flexible and can be applied at two different stages of development or operation: the formulation of the solvent (typically a low-melting mixture or eutectic solvent) and the leaching procedure of the black mass. The user can also decide to evaluate the entire process, which includes all the categories in the score calculation. In Table 4, the structure of LEACH is reported.

The LEACH evaluation framework is structured around three main macro-categories: economic, technical, and safety, which contribute 30%, 35%, and 35% to the total sustainability penalty score. Each macro-category is further broken down

Table 3 Technical and logical structure of the considered assessment tools

Tool	Main categories	Weighting strategy	Observations/rationale
EcoScale	Yield, cost, safety, technical effort	Implicit weighting *via* penalty size	Prioritizes safety and yield
Process Greenness Score (PGS)	Atom economy, PMI, energy, safety, solvent score	Often equal-weighted, or adjusted based on context	Customizable for process types
BSAT	GHG emissions, materials, HR, energy	Equal weights	Simplified for organizational use
ECOLIBRA	Solvent, energy, yield	Traffic light weighting (implicit)	Focused on green innovation
Green Motion Tool (GSK)	Efficiency, safety, environmental impact	Visual weighting (color-coded)	Focused on safety and environmental harm

Table 4 LEACH categories and penalty point system

	Subcategories	Ranges	Penalties	Max penalties	Module 1[a]	Module 2[b]	Module 3[c]
Economic	Materials cost	<10 € per kg	0			n.a.[d]	
		10–100 € per kg	7				
		>100 € per kg	13	13			
	Use of renewable feedstocks	Fully renewable	0			n.a.	
		Partially	5				
		Non-renewable	9	9			
	Use of critical raw materials (CRMs)	Not present	0			n.a.	
		Partially	5				
		Fully CRMs	8	8			
Technical	Yield	>90%	0		n.a.		
		60–90%	2.5				
		<60%	5	5			
	Temperature × time	≤25 °C for ≤1 hour	0				
		25–50 °C for ≤4 hours	2				
		>50 °C or >4 hours	4	4			
	Workup	Simple filtration	0				
		Aqueous workup	2				
		Multiple steps	4	4			
	Process/product stability	No degradation reported	0			n.a.	
		Degradation reported for HBD or HBA	2				
		Degradation reported for the mixture	4	4			
	Biodegradability	Biodegradable DES	0			n.a.	
		HBD and/or HBA biodegradable	2				
		No biodegradable components	4	4			
	Process mass intensity (PMI)	<10	0				
		10–50	2.5				
		>50	5	5			
	Recyclability	Reagents fully reusable	0				
		Partially	2.5				
		Not reusable	5	5			
	Selectivity	>90%	0		n.a.		
		70–90%	2				
		<70%	4	4			
Safety	Intrinsic hazards	Based on GHS classification (H-statements)					
		No hazard	0				
		Irritant	1				
		Flammable	2				
		Carcinogen/explosive/acute toxicity	6	9			
	Handling and control	Based on the PPE required and special handling precautions					
		PPE of category 1	0				
		PPE categories 1–2	4				
		PPE category 3	7	7			
	Emergency measures	Severity of first-aid, spill/fire risk					
		Basic first aid – risk 1 exposition	0				
		Fire hazard	3				
		Spill response needed	5	5			
	Environmental fate	Persistence, bioaccumulation, and ecotoxicity					
		Biodegradable/inert	0				
		Moderate risk	4				
		PBT/vPvB[e]	7	7			
	Regulatory impact	Based on REACH/CLP listing or transport classification					
		Not listed	0				
		ADR/RID[f] required	5				
		ICAO/IMDG/ADN[g] forbidden	7	7			
	Total		100	100			

[a] Solvent formulation. [b] BM leaching. [c] Overall. [d] n.a. stands for not applicable. [e] PBT/vPvB: persistent, bioaccumulative and toxic/very persistent, bioaccumulative and toxic. [f] ADR/RID stands for European Agreement concerning the International Carriage of Dangerous Goods by Road/ Regulations concerning the International Carriage of Dangerous Goods by Rail. [g] ICAO/IMDG/AND stand for International Civil Aviation Organization/International Maritime Dangerous Goods Code/European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.

Table 5 Distribution of PP across the macro-categories in reference tools

Tool	Economic (%)	Technical (%)	Safety (%)
EcoScale	17	67	17
Analytical Eco-Scale	0	67	33
Process Greenness Score	15–25	40–50	30–40
BSAT	~15	~10	~60
ECOLIBRA	~20	~35	~45
Green Motion Tool (GSK)	~33	~50	~17
LEACH	30	35	35

into specific subcategories, enabling a detailed and multifaceted assessment of process sustainability. The attribution of specific weights to the LEACH macro-categories was based on a detailed cross-analysis of the distributions in the reference tools (Table 1) and the specific scope of each tool. In Table 5, the distribution of the penalty points across the economic, technical, and safety categories for the reference tools is reported.

(I) Economic dimension (LEACH: 30%): LEACH's 30% allocation to economic factors is notably higher than that of all tools surveyed except for GSK (33%). Most tools, such as EcoScale (17%) and PGS (15–25%), allocate relatively limited weight to economic aspects, while some like the Analytical Eco-Scale assign no explicit economic weighting at all. This elevated economic consideration reflects LEACH's inclusion of material cost, CRM dependency, and feedstock renewability, elements often overlooked or oversimplified in traditional lab-based or policy-driven tools. Importantly, as shown in Table 3, LEACH aligns well with both GSK and ECOLIBRA in terms of cost-effectiveness and economic resilience. These dimensions are increasingly recognized as critical at TRLs 4–5, where economic viability often determines whether a technology can progress beyond the pilot scale. Thus, LEACH offers a more holistic economic lens that aligns with real-world deployment and industrial uptake. (II) Technical dimension (LEACH: 35%): with 35% allocated to technical criteria, LEACH positions itself at the lower-middle range compared to established tools such as EcoScale and Analytical Eco-Scale, both of which assign a dominant 67% weight to technical aspects. By contrast, Process Greenness Score (PGS) ranges between 40–50%, ECOLIBRA sits at ~35%, and the Green Motion Tool (GSK) assigns 50%. LEACH's positioning is deliberate: rather than replicating the lab-centric emphasis of tools like EcoScale, it aligns more closely with process-oriented tools such as PGS and ECOLIBRA. These tools, like LEACH, are designed with scale-up and translational development in mind, especially critical at TRLs 3–5, where practicality and technical robustness must be balanced against other sustainability pressures. LEACH's moderated technical weighting also reflects a strategic departure from overemphasizing laboratory feasibility. While technical metrics remain essential, LEACH recognizes that scalability, system integration, and downstream constraints are equally important. By avoiding disproportionate emphasis on technical perfection, LEACH supports realistic innovation pathways for early-stage sustainable technologies. (III) Safety dimension (LEACH: 35%): safety is another area where LEACH makes a significant and deliberate impact, assigning it a full 35%, a figure that places it in line with several modern tools. While BSAT places an especially high weight on safety (60%), others such as the Analytical Eco-Scale (33%), PGS (30–40%), and ECOLIBRA (~45%) also treat safety as a substantial factor. GSK's quantitative weighting appears lower (17%), but it compensates with a strong qualitative emphasis on safety-related indicators. LEACH goes beyond basic hazard classification by incorporating a broad range of risk indicators, including GHS classifications, personal protective equipment (PPE) requirements, emergency and process risks, as well as environmental persistence and regulatory restrictions (*e.g.*, PBT/vPvB). As demonstrated in Tables 2 and 3, safety considerations are often underrepresented in technically focused tools. LEACH addresses this gap directly, aligning itself with emerging SSbD principles promoted by the European Union. This focus is particularly pertinent in contexts such as BM solvometallurgy, where toxicity, thermal instability, and reactivity present serious risks during scale-up. By embedding safety deeply into its framework, LEACH ensures these hazards are neither underestimated nor deferred to later development stages, supporting a more robust and responsible innovation trajectory.

Looking at the subcategories listed in Table 4, in the economic category, two core aspects are considered. The first concerns the cost of raw materials, with penalties increasing in accordance with market price: no penalty is applied for materials priced below €10 per kg, moderate penalties are assigned to those between €10–100 per kg, and high penalties are incurred for materials exceeding €100 per kg due to their financial burden. The second subcategory evaluates the use of renewable feedstocks. Processes based on fully renewable inputs receive no penalty, while those relying on partially renewable or non-renewable resources are penalized progressively, in line with the goal of promoting long-term resource sustainability. The economic component of LEACH is intentionally restricted to material-level indicators because the tool is designed for early-stage (TRLs 3–5) screening, where the detailed process inventories required for full techno-economic assessment (TEA) or life-cycle costing (LCC) are typically unavailable. As a result, LEACH does not include capital costs, equipment requirements, energy consumption, utility demand, or downstream recovery infrastructure. These cost categories become meaningful only once a process reaches a higher maturity level and reliable mass and energy balances can be established. For comprehensive evaluation beyond early-stage design, LEACH should therefore be used in combination with TEA-, LCA-, or process-simulation-based costing tools that incorporate energy usage, equipment sizing, and long-term operational expenditure. The technical category encompasses six subcategories that collectively assess the operational performance and environmental compatibility of the leaching system. Yield and the combined impact of process temperature and duration were considered at first. These operational parameters are directly linked to energy efficiency, and their evaluation draws on methodologies established in existing assessment tools. The EcoScale assigns penalty points for deviations from ideal conditions, including elevated temperatures and extended reaction times. Reactions conducted at room temperature (approximately 25 °C) with short durations (≤1 hour) are considered optimal, incurring minimal or no penalty points. Thus, ≤25 °C for ≤1 hour was considered as the ideal condition. Also, looking at the 12 principles of green chemistry, principle 6 emphasizes designing energy-efficient processes, advocating for ambient temperature operation to minimize energy consumption.[33] In the LEACH tool, the combination of 25–50 °C for ≤4 hours was considered a moderate condition. Finally, the high-risk condition was determined to be >50 °C or >4 hours. In addition, the workup complexity is considered, which can be discriminant in the scale-up phase. Processes involving multiple and complex steps are penalised. Then, the robustness of the solvent systems is considered. Sometimes, harsh conditions are required to promote the leaching of the metals from the BM, and many components used to formulate eutectic systems are known to decompose under specific conditions. The nature of the solvent is also addressed through the biodegradability of its components. To complete the technical assessment, process mass intensity (PMI) was considered as an indicator of mass balance, while the selectivity was introduced to reward leaching with high selectivity. Finally, solvent recyclability is assessed, with higher scores awarded to systems that allow for efficient solvent recovery or reuse. The safety category, contributing 35% to the final score, includes six subcategories designed to capture the potential hazards to both operators and the environment. The first of these is the toxicity of the chemicals used, measured *via* GHS health hazard classifications. Less toxic systems are rewarded with lower penalty scores, while the use of substances with known severe health impacts increases the penalty burden. Flammability is similarly considered, along with other hazard properties such as irritant and carcinogen/explosive. The need for specific ventilation equipment is included to account for operational complexity; processes requiring specialized air-handling systems are penalized more than those that can be operated under ambient conditions. The presence of explosive components or reactivity under common conditions is also penalized, as is the need for specialized personal protective equipment (PPE); the more intensive the safety requirements, the higher the penalty. In the view of a safety by design approach, pivotal aspects (handling and control, emergency measures, environmental fate, and regulatory impact) which can be easily measured by using the information contained in the safety sheet of any commercialised chemical are considered. All the conditions that determine an increase in the complexity of industrial management of a chemical, including its storage, transport and disposal, are associated with penalty points.

Beyond identifying non-ideal performance, the LEACH results provide direct guidance on how each process can be improved. Because the tool assigns penalties at the subcategory level, the highest-impact penalties indicate the most effective optimisation routes. For both case studies, three dominant penalty sources were identified.

(I) Safety and regulatory burden.

High penalties associated with intrinsic hazards, environmental fate, and ADR/RID classification suggest that optimisation should prioritise replacing hazardous solvent components or additives with alternatives exhibiting lower toxicity, reduced persistence, and benign degradation behaviour. Reducing the need for specialised PPE or containment also lowers safety-related penalties. Solvent reformulation (*e.g.*, substituting ethylene glycol with less hazardous polyols or organic acids or avoiding persistent metal-based reductants) represents a primary pathway for improvement.

(II) Energy and operational intensity.

Temperature–time penalties reveal that milder conditions significantly improve sustainability. Optimisation pathways include increasing DES reactivity through adjusted HBD/HBA ratios, incorporating catalytic or redox-active components with benign profiles, or enhancing mass transfer *via* mixing or particle-size optimisation to avoid prolonged high-temperature leaching. These strategies reduce both technical penalties and indirect economic burdens.

(III) Recyclability, selectivity, and PMI.

The recyclability and PMI penalties indicate that solvent recovery and metal separation strategies must be strengthened. Potential improvements include introducing regeneration steps for DES components, reducing water usage in washing sequences, and improving selectivity through ligand tuning or controlled speciation of target metals. Enhanced selectivity also reduces downstream purification burdens and associated waste streams.

In combination, these optimisation pathways illustrate how LEACH can serve as a design tool: high-penalty categories signal actionable targets for reformulation or operational adjustment, enabling researchers to rapidly converge toward safer, more energy-efficient, and more scalable solvometallurgical configurations before committing to TEA/LCA-level analysis.

By consolidating these detailed assessments across economic, technical, and safety dimensions, the LEACH tool provides a structured and quantitative means of evaluating sustainability in solvometallurgical leaching processes. Its modular application at the solvent, procedure, or full-process level ensures adaptability across research, development, and implementation phases. Ultimately, the tool encourages a holistic and precautionary approach for process design, supporting the transition toward more responsible, efficient, and safe chemical operations in the recycling and recovery of valuable materials. The present version of LEACH is focused exclusively on the solvometallurgical stages of black-mass processing, namely solvent formulation and leaching. Therefore, it does not include a module for upstream pretreatment operations such as discharge, crushing, milling, sieving, magnetic separation, or density-based sorting. These steps can have a substantial influence on overall sustainability, particularly through energy demand, equipment requirements, dust and particulate management, and the generation of intermediate waste streams. However, pretreatment parameters are highly process- and equipment-specific and often lie outside the control of laboratory-scale solvometallurgical development. For this reason, LEACH evaluates only the chemical and operational aspects directly associated with leaching. In future extensions, pretreatment metrics (*e.g.*, specific energy consumption, particle-size distribution effects, dust hazard classification, and waste factors) could be incorporated as an optional upstream module to provide a more comprehensive cradle-to-gate assessment when reliable data become available.

An important feature of LEACH is its modular structure which can be applied to the solvent formulation, to the BM leaching or to the overall process. When modules 1 and 2 are used, the result of the assessment is expressed in penalty points and thus a lower score corresponds to a more sustainable system or process. When module 3 is employed, the EcoScale logic is applied (100-PP). In the next section, the potential of LEACH is reported through the analysis of two case studies.

To ensure full reproducibility, the complete decision rules used for assigning penalty points to each subcategory are provided in the SI, together with a step-by-step scoring guide and fully populated scoring sheets for all evaluated processes. These materials specify the intrinsic indicators and quantitative thresholds governing each penalty assignment, enabling any user to reproduce the LEACH scoring independently. Furthermore, by highlighting the subcategories that contribute the most to the overall penalty, LEACH provides direct diagnostic guidance for improving process sustainability rather than merely quantifying it.

3. Case studies

3.1. Selection of case studies

To demonstrate the applicability and diagnostic capabilities of the LEACH tool, a selection of two literature case studies was compiled. These studies focus on the use of DESs in the leaching of BM derived from spent LIB and, in particular, on Co recovery. The selection aimed to show the potential of LEACH in comparing different processes and in isolating specific issues related to further scale-up. A detailed step-by-step scoring guide and the full reproducibility flowchart for LEACH are provided in the SI.

3.2. Application of LEACH scoring

Each system was independently assessed using the LEACH tool across the three defined modules:

Module 1 (solvent formulation): evaluated the sustainability attributes of the leaching system itself, including raw material cost, use of renewable feedstocks, critical raw material content, biodegradability, recyclability, and hazard profile.

Module 2 (BM leaching): assessed the operational phase of the process (leaching), including leaching efficiency (selectivity), temperature–time footprint, workup complexity, process stability, selectivity, and safety/environmental aspects related to processing.

Penalty points were assigned according to the criteria defined in Table 4, with final scores calculated by summing penalties within each category. The overall sustainability performance of each process was then interpreted based on module 3.

3.3 Results and discussion (application of LEACH – case studies)

The LEACH tool is able not only to assess the sustainability of a solvometallurgical process, but also to provide insight into possible technical, economic, and safety improvements. To show the power of this tool, two recently reported processes, respectively based on choline chloride : citric acid (ChCl : CA)[34] and choline chloride : ethylene glycol (ChCl : EG),[35] were considered. In both cases, the aim was to extract Co from BM samples. The best conditions reported by each study are highlighted in Table 6. Despite the similarity between the two DESs (both based on choline chloride), the operating conditions are sensibly different, as is the use of additives (Table 6). Regarding DES preparation, in both papers, classic thermal mixing (50 °C) is reported.

In Table 7, the analysis of module 1 (solvent formulation) for both processes is reported.

The results from module 1 analysis illustrate how differences in solvent formulation, even when based on a common component such as choline chloride, can lead to divergent sustainability profiles due to the distinct characteristics of the hydrogen bond donor (HBD) and the presence or absence of additives. In process 1, citric acid is employed as a HBD, offering partial renewability and a relatively low intrinsic hazard classification (H319 and H335), which contributes to a modest safety penalty. However, the inclusion of copper as a stoichiometric reductant introduces significant sustainability concerns. Copper is neither biodegradable nor easily recoverable within the system, and its persistence and potential for environmental accumulation are reflected in higher penalties under the environmental fate and recyclability categories. This highlights a critical trade-off: while citric acid contributes to a safer and moderately green solvent matrix, the co-use of

Table 6 Case studies and reported optimized conditions

ID	Solvent	Temperature/time	Substrate/solvent	Leaching efficiency
Process 1	ChCl : CA (2 : 1), 35 wt% of H_2O, 35 wt% of Cu	40 °C/1 h	20 g of BM per L of DES	Co 98%
Process 2	H_2O/NaOH then ChCl : EG (1 : 2)	180 °C/20 h	50 wt_{eq} of DES	Co 90%

ChCl stands for choline chloride; CA stands for citric acid; EG stands for ethylene glycol.

Table 7 Assessment of the solvent formulation through the LEACH – Module 1

Criterion	Process 1	Penalty	Process 2	Penalty
Materials cost	10–100 € per kg	7	10–100 € per kg	7
Renewable feedstocks	Partially	5	Non-renewable	9
Use of CRMs	Not present	0	Not present	0
Temperature × time	25–50 °C for ≤4 h	2	25–50 °C for ≤4 h	2
Workup	None	0	None	0
Process/product stability	No degradation reported	0	No degradation reported	0
Biodegradability	Cu not biodegradable	2	Biodegradable DES	0
Process mass intensity	<10		<10	0
Recyclability	Not reusable	5	Reagents fully reusable	0
Intrinsic hazards	Irritant[a]	1	Acute toxicity (oral) – specific target organ toxicity – repeated exposure[b]	6
Handling and control	1–2-PPE of category 1	0	1–2-PPE of category 1	0
Emergency measures	Basic first aid – risk 1 exposition	0	Basic first aid – risk 1 exposition	0
Persistence, bioaccumulation, and ecotoxicity	PBT/vPvB[36]	7	Biodegradable/inert	0
Regulatory impact	Not listed	0	Not listed	0
Score Module 1		29		24

[a] H319 and H335 for citric acid. [b] H302 and H373 for ethylene glycol.

copper compromises the overall solvent sustainability by introducing a non-renewable and non-benign component. Conversely, process 2 utilizes ethylene glycol as the HBD, which allows the formulation to be fully biodegradable and recyclable under the reported conditions, thus earning zero penalty in these subcategories. However, this benefit is offset by the significant health risks associated with ethylene glycol, which is classified under multiple hazard statements (H302 and H373) due to its acute toxicity and organ-specific effects upon prolonged exposure. The contrast between these two systems exemplifies the tension between functional solvent performance and occupational safety and demonstrates how improvements in one area may come at the cost of others. From a regulatory and practical standpoint, neither formulation currently falls under transportation restrictions, and both can be handled with standard PPE protocols at the laboratory scale. Nonetheless, the identification of PBT/vPvB behaviour in process 1 and the toxicological profile of process 2 suggest that scale-up will inevitably amplify the relevance of these penalties, particularly as exposure potential increases and waste volumes grow. These findings emphasize the importance of early integration of toxicological and environmental data in solvent design and selection, particularly when aiming for processes that are not only effective in metal extraction but also compliant with Safe-and-Sustainable-by-Design principles. In sum, the module 1 assessment demonstrates that although both processes achieve similar penalty totals, the origin and nature of these penalties differ markedly. Process 1 is penalized for the inclusion of a persistent additive (Cu), while process 2 is penalized for the intrinsic toxicity of the solvent itself. These divergent profiles offer a clear indication that sustainability in solvent formulation is not reducible to a single parameter such as biodegradability or cost but must be assessed holistically through the combined lens of technical feasibility, environmental compatibility, and human safety. In Table 8, the LEACH analysis related to module 2 (BM leaching) is reported.

Table 8 Assessment of BM leaching through the LEACH – Module 2

Criterion	Process 1	Penalty	Process 2	Penalty
Yield	>90%	0	60–90%	2.5
Temperature × time	25–50 °C for ≤4 h	2	>50 °C for >4 h	4
Workup	Multiple steps	4	Aqueous workup	2
Process mass intensity	>50	5	>50	5
Recyclability	Partially	2.5	Not reusable	5
Selectivity	<70%	4	>90%	0
Intrinsic hazards	Carcinogen/explosive	9	Carcinogen/explosive	9
Handling and control	Multiple PPE categories 1–2	4	Multiple PPE categories 1–2	4
Emergency measures	Basic first aid – risk 1 exposition	0	Basic first aid – risk 1 exposition	0
Persistence, bioaccumulation, and ecotoxicity	PBT/vPvB	7	PBT/vPvB	7
Regulatory impact	ADR/RID[a] required	5	ADR/RID required	5
Score Module 2		42.5		43.5

[a] ADR (European Agreement concerning the International Carriage of Dangerous Goods by Road) and RID (Regulations concerning the International Carriage of Dangerous Goods by Rail).

The Module 2 evaluation underscores how operational parameters and leaching performance directly influence the overall sustainability of the process, particularly in terms of energy demand, efficiency, and safety-related considerations. Both processes target cobalt recovery from black mass, but they do so under markedly different conditions that manifest in distinct penalty distributions. Process 1 demonstrates favourable sustainability indicators due to its high leaching efficiency (>90%) achieved under relatively mild conditions (40 °C for 1 hour). This contributes to minimal penalties in the yield and temperature–time categories. However, the process suffers from a more complex post-leaching workup, including multiple separation steps, and only partial recyclability of the leaching medium. Additionally, the lower selectivity towards cobalt (below 70%) results in further penalties, as the system co-leaches undesired elements, which complicate downstream purification and increase reagent consumption. Safety-related penalties also accumulate due to the intrinsic hazard classification of copper used in the leaching mixture and the hazardous nature of the resulting leachate. The environmental fate of the BM, which is classified under European regulation as hazardous waste (CER 19 14 02), further contributes to the total sustainability burden and highlights an area of concern for future regulatory compliance.[37]

In contrast, process 2 operates under significantly harsher conditions, requiring prolonged reaction times (20 hours) at elevated temperatures (180 °C). These energy-intensive parameters are reflected in the highest penalty value attributed to the temperature–time category. Despite this, process 2 benefits from a streamlined workup and a high degree of selectivity for cobalt (>90%), which helps mitigate penalties in those areas. However, the process exhibits poorer performance in terms of recyclability (the DES is not reusable under the tested conditions) and only moderate leaching efficiency, leading to further deductions. Importantly, both processes incur the maximum penalties in categories related to intrinsic hazard, environmental fate, and regulatory impact, primarily due to the classification of BM and the carcinogenic potential of metal-rich leachates. The need for multiple PPE elements during handling and the requirement for ADR/RID compliance also highlight the latent safety risks associated with black mass processing.

What emerges clearly from module 2 comparison is that neither process offers a fully optimized solution when evaluated against all technical and safety criteria. While process 1 benefits from mild operating conditions and high efficiency, its selectivity and workup complexity remain barriers to scalability. Process 2, though selective and operationally simpler post-leaching, demands significantly more energy and involves toxic reagents that would necessitate enhanced containment and control strategies at a larger scale.

Overall, the results emphasize that safety and regulatory compliance are not peripheral aspects of leaching strategy development, but central parameters that heavily influence the practical feasibility of scale-up. Even when extraction efficiencies appear satisfactory at the laboratory scale, the burden of operational hazards, energy consumption, and waste classification can undermine the sustainability of the process. The LEACH tool, through its modular scoring approach, brings visibility to these hidden trade-offs and provides a structured means to prioritize improvements in future process optimization efforts.

The overall scores reported in Table 9, when interpreted through the logic of the EcoScale (on which the LEACH framework is based), offer a clear and structured indication of the sustainability of the overall process. As with EcoScale, the maximum theoretical score is 100, representing an ideal, penalty-free process. Any deviation from this benchmark results in cumulative deductions that reflect economic, technical, or safety-related shortcomings. In this case, process 1 reaches a final score of 43.5, while process 2 falls slightly lower at 36.5. According to the EcoScale interpretation, where scores below 50 indicate inadequate sustainability, both processes fall into the non-ideal category, highlighting substantial room for improvement before any consideration of scale-up. Crucially, the aggregated scores are not simply the sum of isolated inefficiencies, but the outcome of interacting factors across modules. LEACH captures these interdependencies by quantifying how technical performance, solvent formulation, and hazard potential influence one another. For example, high selectivity or solvent recyclability cannot fully compensate for significant penalties linked to toxicity, non-renewable inputs, or energy-intensive operation. This systemic approach prevents misleading conclusions that might arise from evaluating individual parameters in isolation. Rather than identifying a clearly superior process, the overall analysis reveals that each route embodies a different set of compromises. Process 1 demonstrates better performance under mild conditions but is penalized for additive use and lower selectivity, while process 2 scores well on selectivity and recyclability but suffers from toxic solvent choice and elevated thermal demands. These outcomes reinforce the notion that early-stage processes must be optimized across multiple dimensions simultaneously, a task for which LEACH is particularly well suited. Ultimately, neither of the investigated processes can be considered sustainably robust in their current form. Their placement well below the ideal threshold confirms that further refinement is necessary, especially in addressing recurring high-penalty categories such as environmental persistence, regulatory impact, and safety. In this context, LEACH proves valuable not only for comparing alternatives but also for mapping critical sustainability bottlenecks and guiding the design of next-generation solvometallurgical systems with a more balanced and integrated performance profile.

3.4. Comparison with EcoScale

To complement the LEACH assessment, the two case studies (process 1 and process 2) were re-evaluated using the classical EcoScale methodology, originally developed for green organic synthesis. Although EcoScale was not specifically designed for solvometallurgical processes, its penalty-based structure provides a useful benchmark for comparing perceived sustainability under more traditional green chemistry criteria, primarily focused on technical feasibility, yield, cost, and basic safety considerations. As a result, process 1 is rated as excellent (score > 75), while process 2 is evaluated as acceptable (score > 50) (Table 10). Even if the EcoScale and LEACH agree in attributing a higher score to process 1, the analysis of the solvometallurgical parameters as well as the detailed assessment of the differences between the two processes is very basic, not allowing an accurate analysis of the weak aspects. The more adequate results obtained with LEACH are related to the incorporation of additional dimensions such as occupational safety, environmental persistence, regulatory impact, and process recyclability, which are not fully captured by EcoScale. For instance, while EcoScale does account for toxic reagents and reaction conditions, it does not penalize persistent or bioaccumulative species like copper (used in process 1), nor does it account for regulatory classifications (*e.g.*, ADR/RID requirements). Similarly, process 2's high energy demand and chronic toxicity profile are treated more leniently by EcoScale. The comparison shows the highest feasibility of LEACH for flagging critical scale-up risks and sustainability trade-offs in early-stage metallurgical process development.

To quantify the origin of the score divergence between EcoScale and LEACH, we decomposed the LEACH penalty for

Table 9 Module 3, overall process

Criterion	Process 1	Penalty	Process 2	Penalty
Materials cost	10–100 € per kg	7	10–100 € per kg	7
Use of renewable feedstocks	Partially	5	Non-renewable	9
Use of critical raw materials (CRMs)	Not present	0	Not present	0
Yield	>90%	0	60–90%	2.5
Temperature × time	25–50 °C for ≤4 h	2	>50 °C for >4 h	4
Workup procedure	Multiple steps	4	Aqueous workup	2
Process/product stability	No degradation reported	0	Degradation reported for the mixture[32]	4
Biodegradability	Cu not biodegradable	2	Biodegradable DES	0
Recyclability	Partially	2.5	Not reusable	5
Selectivity	<70%	4	>90%	0
Process mass intensity	>50	5	>50	5
Intrinsic hazards	Carcinogen/explosive/acute toxicity	9	Carcinogen/explosive/acute toxicity	9
Handling and control	Multiple PPE categories 1–2	4	Multiple PPE categories 1–2	4
Emergency measures	Basic first aid – risk 1 exposition	0	Basic first aid – risk 1 exposition	0
Environmental fate	PBT/vPvB	7	PBT/vPvB	7
Regulatory impact	ADR/RID required	5	ADR/RID required	5
Score Module 3	100–56.5 = 43.5		100–63.5 = 36.5	

Table 10 EcoScale assessment of processes 1 and 2 (overall process)

Criterion	Process 1	Penalty	Process 2	Penalty
Yield	>90%	5	60–90%	12.5
Price of reaction components	ChCl + citric acid + Cu + BM	5	ChCl + ethylene glycol + BM	5
Safety	Irritant (citric acid, Cu PBT), toxic (BM)	5	Toxic (ethylene glycol, BM)	10
Technical setup	Common setup	0	Common setup	0
Temperature/time	Heating, >1 h	3	Heating, >1 h	3
Workup and purification	None of the penalty conditions match	0	None of the penalty conditions match	0
Total penalty points		18		30.5
EcoScale score		82		69.5

Table 11 Differences in EcoScale and LEACH analyses for process 1

Category	EcoScale penalty (process 1)	LEACH penalty (process 1)	Difference	Contribution to LEACH–EcoScale gap
Economic (materials cost, renewability, CRMs)	5	12	+7	12%
Technical (yield, temperature–time, workup, stability, PMI, selectivity, recyclability)	8	23	+15	27%
Safety & regulatory (intrinsic hazards, handling, emergency measures, environmental fate, ADR/RID)	5	21.5	+16.5	29%
BM-specific hazard categories (not included in EcoScale)		(Embedded across safety and technical)	+18	32%
Total	18	56.5	+38.5	100%

Process 1 (total PP = 56.5) into its economic, technical, and safety/regulatory components and compared these with the corresponding penalty contributions in EcoScale. Table 11 summarizes this comparison.

This breakdown shows that most of the penalty difference (about 60%) arises from the newly introduced safety, environmental fate, and regulatory subcategories, which EcoScale does not explicitly evaluate. A further 30% difference originates from technical criteria that are either absent from EcoScale (*e.g.*, PMI, recyclability, and stability) or treated more lightly. Only 10–15% of the gap is attributable to differences in economic scoring. This quantitative analysis demonstrates the added diagnostic value of LEACH: solvometallurgical systems that appear "excellent" under EcoScale receive substantially lower scores once occupational hazards, environmental persistence, and regulatory burdens are included. LEACH therefore provides a more realistic assessment of scale-up feasibility and aligns the evaluation with Safe-and-Sustainable-by-Design principles.

4. Conclusions

The development and application of the LEACH (Low-impact Extraction and Assessment of CHemical solvometallurgy) tool presented in this study respond to a growing need for an early-stage sustainability assessment method tailored to emerging processes such as solvometallurgical recycling of black mass (BM) from spent lithium-ion batteries. In contrast to many conventional tools focused primarily on environmental or technical performance, LEACH integrates economic, technical, and safety dimensions within a unified and penalty-based framework. This makes it particularly suited to evaluate processes that are still in the laboratory phase, where detailed life cycle inventories are often unavailable, but critical design decisions are being made. The application of LEACH to two representative solvometallurgical case studies, both targeting cobalt recovery through DES-based systems, illustrates its capacity to differentiate between process configurations in a meaningful and actionable way. The first process, based on a choline chloride : citric acid solvent system operated at 40 °C for one hour, achieved a cobalt leaching efficiency of 98% and exhibited lower overall sustainability penalties. The second process, employing a two-step method with choline chloride : ethylene glycol and operating at 180 °C for twenty hours, reached a slightly lower leaching efficiency of 90% and incurred higher penalties across several LEACH categories. The main differences between processes 1 and 2, as quantified by LEACH, arise from the higher toxicity of ethylene glycol (process 2) with respect to citric acid (process 1), and from the combination of temperature and time, which penalize process 2, despite no additives were used. When the total penalty scores are considered, process 1 achieved a final LEACH score of 43.5, compared to 36.5 for process 2, suggesting a moderately more sustainable profile overall. However, both processes exhibited significant shortcomings, the detection of which is facilitated through LEACH analysis.

In general, the severity of safety-related issues identified by LEACH highlights a fundamental barrier to scale-up. Although laboratory-scale experiments can often tolerate the use of moderately hazardous materials under controlled conditions, transitioning to pilot or industrial scale requires far stricter consideration of occupational hazards, environmental fate, and regulatory compliance. The presence of flammable or carcinogenic substances, high-temperature processing, or reagents that exhibit persistence and bioaccumulation not only increases the technical complexity of a process but may render it economically or legally unfeasible at larger scales. In this regard, LEACH provides more than a sustainability snapshot; it acts as an early warning system capable of revealing design weaknesses that could compromise future implementation. Moreover, the LEACH tool effectively captures the trade-offs that arise in process development. While process 2 benefited from a fully biodegradable solvent and excellent selectivity, these advantages were offset by higher toxicity and energy demand due to the long reaction time and elevated temperature. Conversely, process 1 used a partially renewable solvent and incurred some penalties for using copper as a reducing agent but operated under milder conditions with superior yield and reduced toxicological impact. Such trade-offs, often overlooked in unidimensional assessments, are made explicit through the modular structure of LEACH, which separates solvent formulation and leaching performance into distinct but interconnected modules.

Ultimately, the findings of this study reinforce the notion that sustainability must be treated as a multidimensional construct from the earliest stages of chemical process design. By incorporating occupational safety and health considerations alongside technical and economic factors, LEACH aligns with the principles of Safe-and-Sustainable-by-Design promoted by the European Commission. Its transparent scoring structure, grounded in literature-backed criteria and adapted from proven assessment models, offers researchers and technologists a practical tool to guide responsible innovation. In conclusion, the LEACH framework represents a valuable addition to the methodological toolkit for evaluating solvometallurgical processes. Its application not only facilitates objective benchmarking and informed material choices but also helps anticipate and mitigate scale-up challenges associated with safety and regulatory impact. As solvometallurgy continues to evolve as a viable strategy for LIB recycling, tools like LEACH will be essential in ensuring that laboratory successes can be translated into industrially relevant and socially responsible technologies.

Author contributions

Alberto Mannu: conceptualization, methodology, investigation, writing – original draft, and supervision. Maria Enrica Di Pietro: data curation, validation, and writing – review & editing. Marco Yuri Basilico: investigation and data analysis. Elza Bontempi: resources, data analysis, funding acquisition, and writing – review & editing. Andrea Mele: resources, funding acquisition, and writing – review & editing.

Conflicts of interest

There are no conflicts to declare.

Note added after first publication

This article replaces the version published on 06 January 2026, which did not include the final revisions. Section 2.1 has been added to the manuscript, and additional information has also been added to the Introduction, section 2.5 and section 3.4 (including Table 11). References 14–20 have also been added. The Royal Society of Chemistry apologises for any confusion.

Data availability

Data are available upon request from the corresponding author.

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