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ORIGINAL PAPER

Scenario-based inventory modelling for prospective life cycle assessment of mineral raw materials supply (SIMPL-Minerals)

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Abstract

Purpose The demand for mineral raw materials for the energy transition is expected to increase greatly in the coming years, raising concerns about the environmental impacts associated with their value chains. Prospective Life Cycle Assessment (pLCA) can be applied to explore such impacts under alternative future scenarios. However, pLCA studies in the mineral value chain often lack consistency, as they use different modelling approaches and a heterogeneous set of evolving parameters. This study develops a systematic approach to guide prospective life cycle inventory (LCI) modelling and the consistent use of parameters in the mineral value chain.

Methods The approach builds on the SIMPL approach for scenario-based inventory modelling for pLCA by adding extensions specific to mineral value chains, resulting in the SIMPL-Minerals (SIMPL-M) approach. These extensions include defining stages and processes of mineral value chains, identifying parameters that connect to these stages, and linking parameters to macro-level factors that influence their future development. The identified parameters were validated through semi-structured interviews with experts. Furthermore, the SIMPL-M approach is demonstrated through a case study on future global nickel sulfate supply for battery production.

Results and discussion The SIMPL-M identifies 19 relevant parameters that should be considered in pLCA studies of mineral value chain. These parameters depend on deposit characteristic, technology, and geography, and cover both primary and secondary value chains, from ore extraction or waste collection to final raw material product. The parameters are connected to a generic inventory model blueprint that shows to which stage they apply. The parameters are also linked to macro-level factors, enabling consistent scenario generation and coherent assumptions about future development of parameters. Applying the SIMPL-M approach in the nickel sulfate case study shows that including parameters beyond standard LCI background data significantly affects impact assessment results, as those result in a 35–38% decrease in the case of climate change impacts.

Conclusion The proposed approach adapts the SIMPL framework to the mineral value chain, resulting in the SIMPL-M approach. SIMPL-M enables practitioners to consistently apply parameters in inventory modelling and to build scenarios based on macro-level factors and their influence on parameter development. This ensures that practitioners consider relevant parameters, thus enhancing comparability between pLCA studies and can reduce modelling efforts for practitioners.

Keywords Life cycle inventory · LCA · Metals · Mineral commodities · Scenario analysis · Critical raw materials · Battery materials · Decarbonization

1 Introduction

The demand for clean energy technologies, including battery electric vehicles (BEVs), wind turbines, solar photovoltaic (PV) panels, and fuel cells, is expected to grow substantially in the coming years (Calderon et al. 2024). Combined with the increase in material requirements of digitalization (UNCTAD 2024), this trend raises concerns about the environmental impacts of expanding the mining and processing

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of mineral raw materials essential for these technologies. These impacts extend beyond commonly assessed pressures such as greenhouse gas (GHG) emissions to include water and land use, ecotoxicity, and biodiversity loss (Giljum et al. 2025).

Life cycle assessment (LCA) is a widely applied method for assessing the environmental impacts of mineral raw material value chains (Segura-Salazar et al. 2019). Prospective LCA (pLCA) extends these capabilities to explore environmental impacts over time (Thonemann et al. 2020) by considering future changes in resource characteristics, production methods, technology performance, and market conditions (Harpprecht et al. 2024). At its core, pLCA relies on scenario analysis to explore alternative futures based on consistent assumptions (Bisinella et al. 2021). The insights gained can guide technology development, support impact mitigation strategies, and inform policy and strategic planning on more sustainable mineral raw materials supply.

Despite its promise, the application of pLCA in this field remains nascent, with outcomes subject to substantial variability due to heterogeneity in approaches. A review of 40 scientific studies applying pLCA to metals revealed such variability in methodological assumptions, modelling approaches, and parameters considered (Harpprecht et al. 2024). For instance, while more than 20 studies accounted for future changes in ore grade or recycling rates, only 10 addressed shifts in processing methods (e.g., shift from evaporative ponds to direct lithium extraction technologies in lithium carbonate production), despite their critical influence on environmental performance (Roy et al. 2025; Schenker and Pfister 2025). Other important factors, such as the electrification of haul truck fleets (Balboa-Espinoza et al. 2023) or the decarbonization of the production of chemical reagents extensively used in mineral processing (Istrate et al. 2024), were largely neglected. This variability has led, in some cases, to inconsistent outcomes, with studies reporting either increasing or decreasing impact intensity over time for the same commodity (Harpprecht et al. 2024). Such divergences are particularly important, as they may lead to contradictory conclusions about future environmental hotspots, the prioritization of value chain stages or commodities for mitigation, and ultimately the future environmental performance of clean energy and digital technologies. Moreover, mineral raw materials can be substitutes for each other (De Volder 2025) or are used in competing technologies, e.g., nickel manganese cobalt (NMC) and lithium iron phosphate (LFP) batteries (IEA 2025b), making consistency in pLCA approaches across mineral raw materials essential.

The inherently unpredictable nature of the future, combined with the variability of practices across pLCA studies, highlights the need for structured modelling approaches that can better capture future dynamics and improve transparency. Notably, the development of scenarios based on a consistent set of relevant parameters has been identified as a critical step to advance pLCA for minerals and metals (Harpprecht et al. 2024).

To systematically integrate future scenario development and assumptions in the inventory modelling for pLCA, the SIMPL approach was introduced (Langkau et al. 2023). This stepwise approach aims to aid in the process of organizing possible potential technological, social, and economic developments through the identification of relevant inventory parameters (e.g., energy sources and efficiency increases) and the key factors influencing their evolution over time (e.g., decarbonization policies). The approach has been tested in academic case studies of renewable energies (Benitez et al. 2024), buildings (Alaux et al. 2025), rare earths (Langkau and Erdmann 2021), and biorefineries (Saavedra del Oso et al. 2023). However, its implementation requires practitioners to make tailored assumptions about, for example, relevant parameters and key factors. For an enhanced consistency, SIMPL can be tailored to particular sectors, such as minerals and metals, by introducing consistent set of parameters and factors to be considered.

In this study, we develop the SIMPL-Minerals (SIMPL-M) approach to conduct pLCA of mineral raw materials supply. It extends the SIMPL approach by specifying a generic inventory blueprint linked to a list of relevant parameters for the primary and secondary supply of mineral raw materials. Moreover, it identifies key macro factors used for scenario analysis and connects them to specific inventory parameters. We showcase the application of the approach through the example of global battery-grade nickel sulfate hexahydrate supply and discuss its potential for improved assessment across commodities.

2 Methods

Section 2.1 presents an overview of the SIMPL approach developed by Langkau et al. (2023). For a more detailed description, the reader is referred to the original publication. Section 2.2 describes how SIMPL-M was developed as an extension of the SIMPL approach, and Sect. 2.3 explains how SIMPL-M is applied in an exemplary case study. Figure 1 summarizes the steps of the SIMPL approach, shows how they are extended in SIMPL-M, and illustrates the use of SIMPL-M through the example of nickel sulfate production.

2.1 Overview of the SIMPL approach

SIMPL integrates future scenario development into the goal and scope definition and inventory analysis phases of

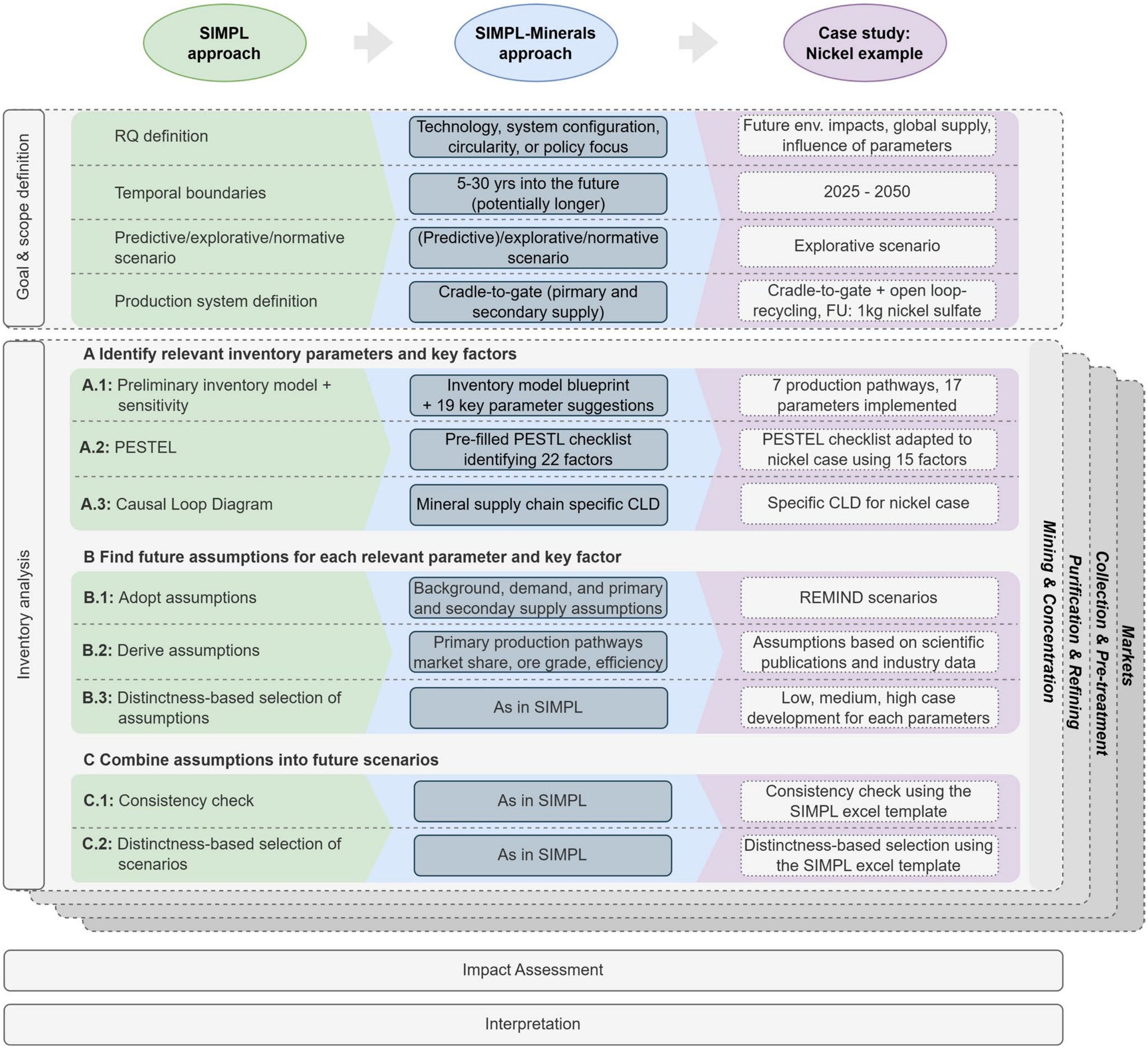


Fig. 1 Overview of the SIMPL-Minerals (SIMPL-M) approach. The SIMPL approach (green) is adapted to mineral raw materials supply (blue). This SIMPL-M approach aims to guide case studies (purple) conducting a pLCA of mineral value chains. Political, economic, socio-cultural, technological, environmental, and legal factors = PESTEL, causal loop diagram = CLD

LCA (green column in Fig. 1). In the goal and scope phase, scenario field identification is incorporated through the definition of the prospective research question (RQ), the time horizon, the scenario type, and the prospective definition of scope items, including the functional unit and system boundaries in line with the defined RQ. Furthermore, SIMPL integrates scenario field development into inventory modelling through three steps:

Step A: Identify relevant inventory parameters and key factors This step requires a preliminary inventory model and a sensitivity analysis (Step A1) to identify the inventory parameters that most strongly influence pLCA results. A PESTEL checklist (Issa et al. 2010) is used to identify political, economic, socio-cultural, technological, environmental, and legal factors that may influence the future development of the product system (step A2). The interrelations between these factors and their connection to the inventory parameters are represented in a causal loop diagram (CLD). The CLD facilitates the identification of key factors with the strongest influence on the inventory model, indicating reinforcing or balancing effects on factors and inventory parameters.

Step B: Find future assumptions for each relevant parameter and key factor Each parameter and key factor requires assumptions about its future development, which can either be adopted (step B1), e.g., from published scenarios, or derived (step B2), which can include expert elicitation or the use of upscaling techniques in the case of emerging technologies. When many plausible assumptions about a parameter exist, a distinctness-based selection is conducted (step B3) to choose those options that differ the most from each other while still remaining plausible.

Step C: Combine assumptions into future scenarios By performing a cross-consistency assessment (CCA), parameter assumptions are compared pairwise across all possible parameter combinations. Once a combination is identified as inconsistent, combinations including this pair can be excluded from further analysis (step C1). This reduces the number of possible parameter assumption combinations and leads to the final step of applying the distinctness-based selection of scenarios from the remaining possibilities (step C2), which ensures that the selected scenarios are sufficiently different.

2.2 Development of the SIMPL-M approach

Here, we explain how SIMPL-M was developed by building on top of the SIMPL approach (blue column in Fig. 1). We adapt the integration of future scenarios within the goal and scope definition and inventory analysis phases to the characteristics of mineral value chains. Within the inventory analysis phase, we specifically focus on steps A and B. SIMPL-M does not add further specifications to step C; therefore, for this step, we refer to the original SIMPL approach.

2.2.1 Integrating scenario field identification into the LCA goal and scope

pLCA can be applied to minerals and metals at different scales, from single sites (such as a mine) to company-wide operations or regional and global value chains, with different RQs and time horizons. The RQ, in turn, influences the choice of scenario type and other scope elements, such as the definition of the functional unit. Given these dependencies, it is not possible to provide prescriptive recommendations on defining the RQ. Instead, SIMPL-M offers guidance on best practices by analyzing the pLCA case studies compiled in the literature review by Harpprecht et al. (2024). This leads to the definition of RQ archetypes that pLCA can address, as well as considerations for the time horizon and the scenario type.

As mineral ores and waste feedstocks (e.g., spent batteries) usually contain multiple valuable metals, handling multifunctionality in prospective scenarios needs to be carefully assessed. The ISO 14,044 hierarchy defines that multifunctionality should be solved through subdivision, system expansion, or allocation (physical allocation preferred over economic allocation) (ISO 2022). Here, different ways of dealing with multifunctionality in mineral value chains are analyzed from the literature (Harpprecht et al. 2024; Lai et al. 2021; Santero and Hendry 2016), and the treatment of multifunctionality in the context of future scenarios is discussed.

2.2.2 Integrating scenario field development into inventory modelling

Step A: Identify relevant inventory parameters and key factors A main challenge in achieving more consistent inventory modelling practices is the wide variation in how mineral product systems are defined. For example, the mining stage may include only ore extraction in some cases, while in others it extends through concentration or even to refining processes (Segura-Salazar et al. 2019). Aggregating such diverse processes into a single stage is not recommended, as each stage is influenced by distinct parameters and dynamics (e.g., recovery efficiency improvement potential may be higher for concentration than already optimized refining processes) (Nassar et al. 2022). To address this challenge, SIMPL-M proposes an inventory model blueprint for a generic mineral value chain (step A1). This blueprint was developed based on an identification of processes and technologies from mineral and metal processing handbooks (Dunbar 2016; Dunne et al. 2019), metal recycling handbooks (Worrell and Reuter 2023), existing LCAs of mineral value chains (Lai et al. 2026), and the LCI database ecoinvent v3.11 (Wernet et al. 2016). It does not claim to be a complete overview, but it covers the most important technologies and stages (for further details on the processes and technologies identification, see Supplementary Information (SI) 1.4).

Relevant inventory parameters are identified (step A1) using a combination of literature review and expert elicitation. The literature review, covering existing pLCAs (Harpprecht et al. 2024), metallurgy literature, decarbonization roadmaps, and industry reports, resulted in an initial set of parameters (see SI 1.1 for the complete list and corresponding literature sources). This first list is refined to a subset of parameters considered temporally relevant, i.e., parameters expected to change over time and to influence the environmental performance of a value chain stage. From those, a further subset of parameters is flagged as relevant parameters, defined as those that can be linked to the inventory blueprint model and for which assumptions about their future development can be made based on available data and knowledge. The final list of parameters was checked with experts through semi-structured interviews (DiCocco-Bloom and Crabtree 2006). Sixteen experts were interviewed: eight from academia or research organizations, three from geological survey institutes, and five from industry. An anonymized list of interviewees can be found in SI 1.3. The expertise covers all stages of the mineral value chain. Depending on the interviewees' expertise, the focus of the interview differed. In the interviews, the list of parameters was presented, and interviewees were asked to give their opinion on the most relevant ones and identify any missing parameters.

The PESTEL method is applied (step A2) to create a list of most relevant macro factors influencing future development of mineral value chains. Information from mineral raw material specific scenarios from INTRAW (Correia et al. 2024), market outlooks from the IEA (2022, 2024) and USGS (Alonso et al. 2025), and policy announcements (European Commission 2021, 2023, 2024) were used to identify these factors. From those factors, several key factors are identified (see SI 3.1 for the complete list and selection of key factors). These key factors are defined as those exerting a high impact on future developments of other factors and parameters (Langkau et al. 2023). The connection between the factors, selected key factors and parameters is visualized in a CLD (step A3).

Step B: Find future assumptions for each relevant parameter and key factor The specific values to be assigned to each key parameter and factor are case study-dependent; therefore, rather than collecting data (e.g., ore grade trends for a specific mineral), we focused on reviewing the existing literature to identify relevant parameters and factors for which assumptions can be adopted (step B1) and those for which they should be derived (step B2). For each key parameter and factor, we mapped potential scenario data sources and documented the modelling approaches applied in the literature to derive them. SIMPL-M does not introduce additional specifications for the distinctness-based selection of parameter assumptions (step B3).

2.3 Showcasing the SIMPL-M approach

The application of SIMPL-M is shown for an exemplary case study on global nickel sulfate supply for battery production (purple column in Fig. 1). The case study is implemented using the specific guidance of SIMPL-M for the goal and scope definition and inventory analysis (step A and step B1-B2), as well as the generic guidance provided by the SIMPL approach for step C of the inventory analysis phase. To calculate impact results, the impact family Environmental Footprint (EF) v3.1 (European Commission 2022) is chosen. The modelling including the parametrization of inventories was performed in the Activity Browsers (AB) (Steubing et al. 2020). Further methodological choices are explained in Sect. 4, as these decisions follow the guidance provided by SIMPL-M, which is introduced in the next section.

3 SIMPL-minerals approach

3.1 Integrating scenario field identification into the LCA goal and scope definition

3.1.1 Definition of the prospective research question

pLCA is a valuable tool for addressing a wide range of RQs related to future mineral value chains across different topics and scopes. At the single site scope, pLCAs often address the mitigation potential of new technologies and the comparison of technological alternatives in prospective product systems (Khakmardan et al. 2025). These RQs are equally relevant at the company scope, further including considerations of supply diversification with respect to primary and secondary supply. At regional and global scopes, RQs can focus on sectoral or value chain performance, identifying future hotspots to support the prioritization of mitigation measures, and assessing both relative and absolute emissions trends. Furthermore, pLCA can be used to examine how supply diversification, such as reliance on lower-quality ores or increased recycling shares, influences environmental impacts and whether these trends align with or diverge from international policy targets like climate neutrality (Harpprecht et al. 2024). Since mineral value chains are highly dynamic and shaped by geopolitical, socio-economic, and environmental factors, RQs that emphasize relative comparisons and the identification of trends across a wide range of future conditions are particularly valuable. The choice of RQ also influences the choice of temporal boundaries and scenario type as explained in the following two section. Table 2 in SI 3 provides exemplary RQs for analyses ranging from site-level to global-scale assessments.

3.1.2 Choice of temporal boundaries/time horizon

The SIMPL approach emphasizes that an appropriate time horizon should allow the emerging technology under study to reach maturity (Langkau et al. 2023). Most pLCA studies in the mineral value chain consider a time horizon extending to 2050 (Harpprecht et al. 2024). This is justified because most national emission pledges are aiming for net zero emissions until 2050 (UNFCCC 2023), which also applies to pledges by mining companies (GlobalData 2024). The choice of the time horizon should account for long lead times from resource discovery to production, which can take up to 16 years on average (IEA 2021). At the same time, a rapid expansion of mining and refining capacity is expected in the short- to medium-term (by 2030–2035) to meet increasing demand (IEA 2025a), while recycling and secondary raw material sources for some minerals are projected to play a significant role only after 2040 (Calderon et al. 2024). Consequently, depending on the RQ, longer timeframes (beyond 2050) may be necessary to capture the full dynamics of the system, such as the full development of expected mines and an established recycling industry. However, prospective studies with a time horizon longer than 20–30 years must recognize the increasing uncertainties related to future policies and technological developments within and beyond the mineral value chain. For example, although integrated assessment model (IAM) scenarios provide projections for the energy system up to 2100, Sacchi et al. (2022) note that it is difficult to reliably extend the coupling between IAM and LCA beyond 2050–2060, as disruptive technologies that may emerge in the long term are not adequately represented.

3.1.3 Choice of scenario type

Three scenario types are typically considered in prospective modelling: predictive (what *will* happen), normative (what *should* happen) and explorative (what *could* happen) (Börjeson et al. 2006). Most pLCA studies in the mineral value chain rely on explorative approaches, with relatively few using predictive or normative ones (Harpprecht et al. 2024). The choice of scenario type should consider the unique features of the mineral and metal markets: (1) high volatility and geopolitical sensitivity of markets (e.g., due to trade disputes, technological disruptions, or resource nationalism) (IRENA 2023); (2) long lead times and capital intensity in the mining sector, which mean that supply is relatively inelastic in the short term, making price and demand projections particularly uncertain (Bhuwalka et al. 2023); and (3) system shocks, which are common in mineral markets (e.g., sudden export bans or price crashes) (Sprecher et al. 2015). These features make predictive scenarios highly uncertain, thus rendering explorative and normative scenarios more suitable. Different RQs relate to different scenario types: normative scenarios are better suited to explore policy-related RQs, whereas technology-related, system configuration, and circularity RQs are more appropriately addressed with explorative scenarios.

3.1.4 Prospective definition of the production system and related scope items

The SIMPL-M approach by default adopts a cradle-to-gate perspective for both primary and secondary supply. Primary supply covers the full mineral raw material value chain from ore extraction to refining. Secondary supply starts at available end-of-life (EoL) waste and its collection and ends at refining. The gate is chosen as the system boundary because minerals are used in a variety of products with different manufacturing steps and applications, which makes providing generic guidance difficult and beyond the scope of mineral raw materials supply.

As mineral value chains usually produce co- or by-products, handling multifunctionality in scenarios is an important aspect. Since subdivision is not applicable to processes handling products containing multiple valuable materials, such as the concentration of ores, practitioners should use system expansion, substitution, or allocation (Lai et al. 2021). SIMPL-M adapts the preferred allocation choices for the metal and mining industry: mass allocation for base metals (when the economic value between co-products is similar), economic allocation when there is disproportionately high market price differences between co-products, and substitution for non-metal co-products (Santero and Hendry 2016). While prospective mass allocation factors could in theory be estimated based on changes in recovery efficiency and ore mineralogy, changes in economic allocation factors over time are highly uncertain due to dependence on future market prices and their volatility. To minimize the effect of price volatility, 10-year price averages could also be used in prospective scenarios. Yet, future research is needed to determine how alternative trajectories in mineral commodities prices could influence the estimated allocation factors. Moreover, since the recommendations refer to preferred choices, testing the influence of alternative approaches on results and reporting them transparently is important. Secondary supply processes are inherently multifunctional, as they both treat waste and produce valuable products. To address multifunctionality in recycling processes, we recommend a simple cut-off approach (Ekvall et al. 2020), where waste enters the system without environmental burdens, and environmental impacts for products from such processes are associated only with the impacts of the waste treatment itself. For the treatment of multifunctionality due to multiple valuable products from recycling processes, the same recommendations as for primary supply apply.

Ultimately, the choice of allocation method rests with the practitioner and may be bound by standards that are used (Husmann et al. 2025a, b). Each approach has distinct advantages and limitations and should be selected based on the specific context and characteristics of the case under study, while also considering the influence of alternatives on results through sensitivity analysis (Guinée et al. 2021).

3.2 Integrating scenario development into inventory modelling

3.2.1 Step A: Identify relevant inventory parameters and key factors

Step A1: Inventory model blueprint and parameters Inventory model blueprint We propose a generic inventory model blueprint for mineral value chains, which includes stages (e.g., mining or concentration), processes (e.g., crushing or leaching), intermediate and final products (e.g., concentrate or alloy), co-/by-products, and waste flows (Fig. 2). This blueprint provides guidance when creating commodity-specific value chains and facilitates a structured identification of inventory parameters relevant to each component of the inventory model. The blueprint is adaptable to geographical, geological, and technological specificities across the diverse existing metal and mineral value chains.

In the proposed blueprint, primary feed, i.e., ore and waste rock, is extracted from the lithosphere during the mining stage. It is then further processed in the concentration stage to reduce the size of the feed and increase the concentration of valuable material. Sludge generated during this processing is treated in the tailings management stage, which may not only dispose of waste but also potentially recover valuable products through tailings reprocessing. Secondary feed comes from collected waste products that are further processed in the pre-treatment stage. Both primary and secondary feed (i.e., concentrate and treated scrap) can enter the

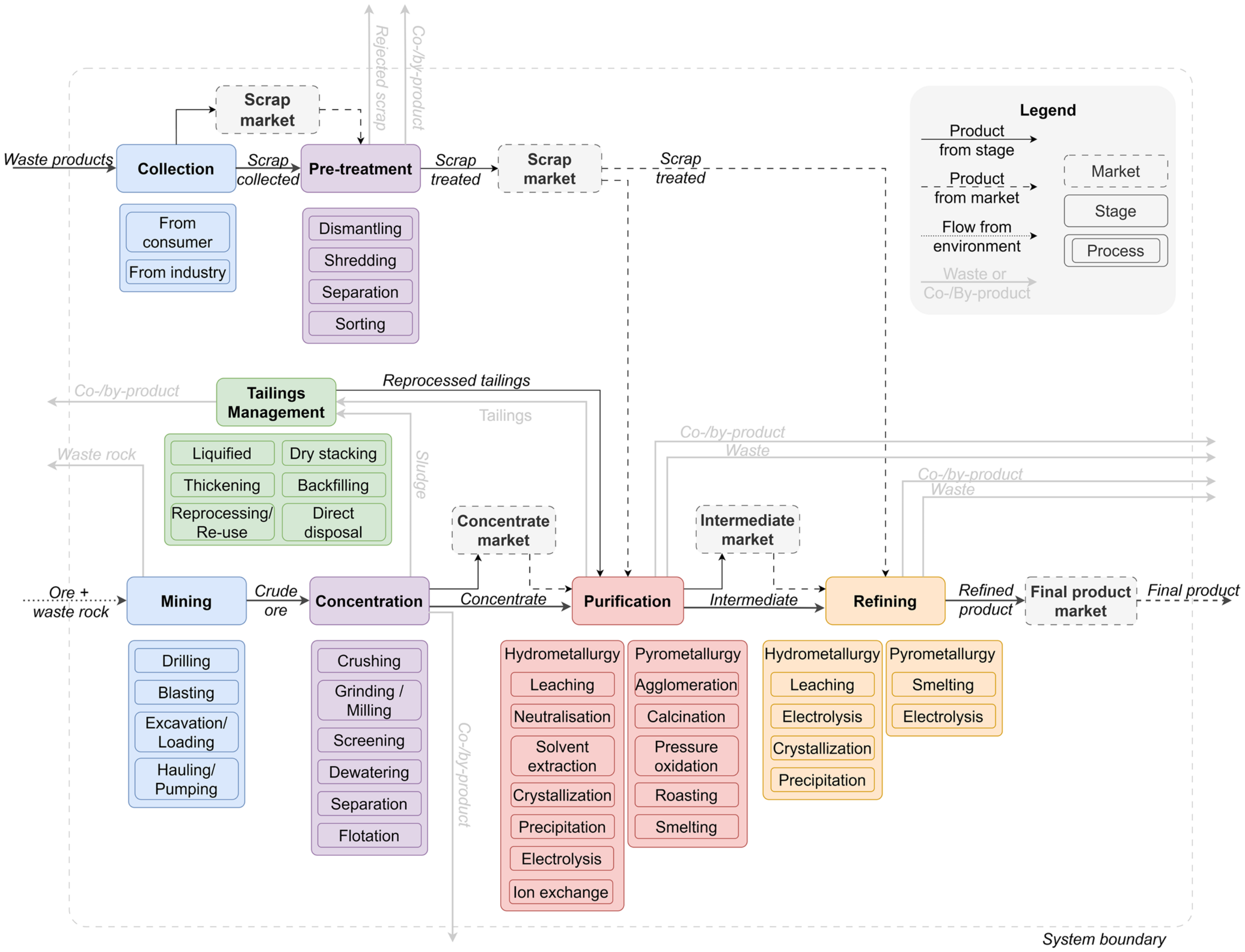


Fig. 2 Inventory model blueprint specifying life cycle stages, processes, and markets in the mineral value chain. Displayed in bold font are the life cycle stages, under them are their respective processes that can be used in the stage. Mining refers to the extraction of ore (e.g., nickel sulfide ore) and waste rock, concentration reduces ore size and increases the concentration of valuable material in the ore (e.g., milling and flotation of the sulfide ore), purification use hydro- or pyrometallurgical processes to further increase valuable material concentration (e.g., flash smelting to nickel matte), and refining produces the final product for further use in other applications (e.g., nickel class I production via Sherritt-Gordon process and further processing to nickel sulfate)

purification stage, where they are treated either separately (e.g., nickel sulfate from battery recycling and nickel sulfate from ore) or together (e.g., steel scrap added in the basic oxygen furnace in steel refining). In this stage, the concentrate or scrap is processed to extract the valuable material using hydro- or pyrometallurgical processes, or a combination of both. Finally, in the refining stage, the concentration of the valuable material is further increased by removing residual impurities to produce products that are nearly pure, again using hydro- or pyrometallurgical methods. In subsequent refining stages, the material may be further processed or alloyed with other materials to achieve the desired properties and characteristics.

Different stages can be geographically separated (ICMM 2025). For primary supply, the mining and concentration stages are commonly located at one site, while purification and refining are located at another. For example, lithium-containing spodumene pegmatites can be mined and concentrated in Australia, and purified and refined in China (IEA 2025a). Another configuration is the vertical integration of mining, concentration, and purification at a single site. Integration of all stages at one site is also possible, as is sometimes the case for copper production. For secondary supply, collection and pre-treatment are usually geographically separated from purification and refining; however, pre-treatment can also occur at the same location as purification and refining. This geographic separation affects inventory modeling in terms of transportation processes, energy sources, technology choices, and potentially the evolution of relevant parameters over time.

The stages represented in the inventory model blueprint can be modelled at different granularity levels, ranging from site-specific to global averages. We propose a defined hierarchy of granularity approaches depending on data availability (further details can be found in SI 3.1). The first approach is to use site-specific data, which can be applicable for single-site (e.g., Khakmardan et al. 2025) or global assessments (e.g., Eckelman 2010; Northey et al. 2013; Schenker and Pfister 2025; Weng et al. 2016) analysis. If this is not possible, the second approach uses average production pathways, characterized by combinations of distinctly different deposit types, ore grades, technologies, and countries or regions. For example, Ambrose & Kendall (2020) performed a pLCA for lithium using the combination of deposit types (brine/pegmatite) and a categorization of ore grades (low/medium/high), whereas van der Meide et al. (2022) conducted a pLCA on cobalt, disaggregating the global value chain by cobalt from copper, nickel laterite and nickel sulfate production, as well as hydro and pyrometallurgical treatment of spent lithium-ion batteries (LIB).

Parameter list Figure 3 shows the initial set of 40 parameters and the 19 identified as relevant. Parameters are categorized along the horizontal axis according to stage, as previously defined in the inventory model blueprint (Fig. 2). The vertical axis indicates whether the parameters are influenced by or dependent on deposit characteristics, technology, or geography. Further sub-categories are represented using color-coding. Relevant parameters are highlighted with a black outline. A list with a more detailed description of the parameters, including a synthesis of interviewee opinions, can be found in SI 1.1.

Among the deposit characteristic-dependent parameters, ore grade was identified as a relevant parameter (see Sect. 2.2.2 for the definition of relevant parameters). The high significance of ore grade, and its anticipated decline in the future for certain commodities, is reflected in its frequent occurrence in pLCA studies (Harpprecht et al. 2024). This finding was corroborated by interviewees with expertise on mining and concentration stages. Opinions on other deposit characteristic-dependent parameters were less aligned; while some experts foresee trends in increasing mine depths, strip ratios, and a growing share of underground mining (i.e., mine type), others stressed that these parameters depend strongly on new deposit discoveries, which remain highly uncertain. We note that while approaches for projecting ore grades into the future have been widely explored in the literature (Calvo et al. 2016), modeling future trends of other deposit-related parameters (e.g., mine depth, strip ratio, or ore density) remains largely underexplored, with limited empirical evidence available (see SI 1.1).

At the technology-dependent level, energy consumption- and sourcing-related parameters are frequently assessed in the pLCA literature. Nearly all experts emphasized energy input parameters as the most important, given the expected decarbonization of future energy supply. This includes low-carbon electricity from decarbonized grids or on-site renewable generation, renewable fuels, and electrified process heating. Experts generally expect improvements in process efficiency through optimization and process integration for existing technologies. A major trend identified for new technology parameters is the electrification of mines, particularly hauling trucks. Other technology switches are expected to play only a minor role, as most sites are tailored to specific ores and processes, making changes to the entire process chain difficult to implement. Instead, novel technologies, such as bioleaching, are more likely to be added in additional processing steps to enhance material recovery. Furthermore, direct emissions from smelters using reductants are a major concern for most experts from mining and processing companies, making the substitution of reductants with bio-based or hydrogen-based alternatives an important parameter. Applying carbon capture and utilization and/or storage (CCUS) to direct emissions was not considered a relevant parameter due to limited technological

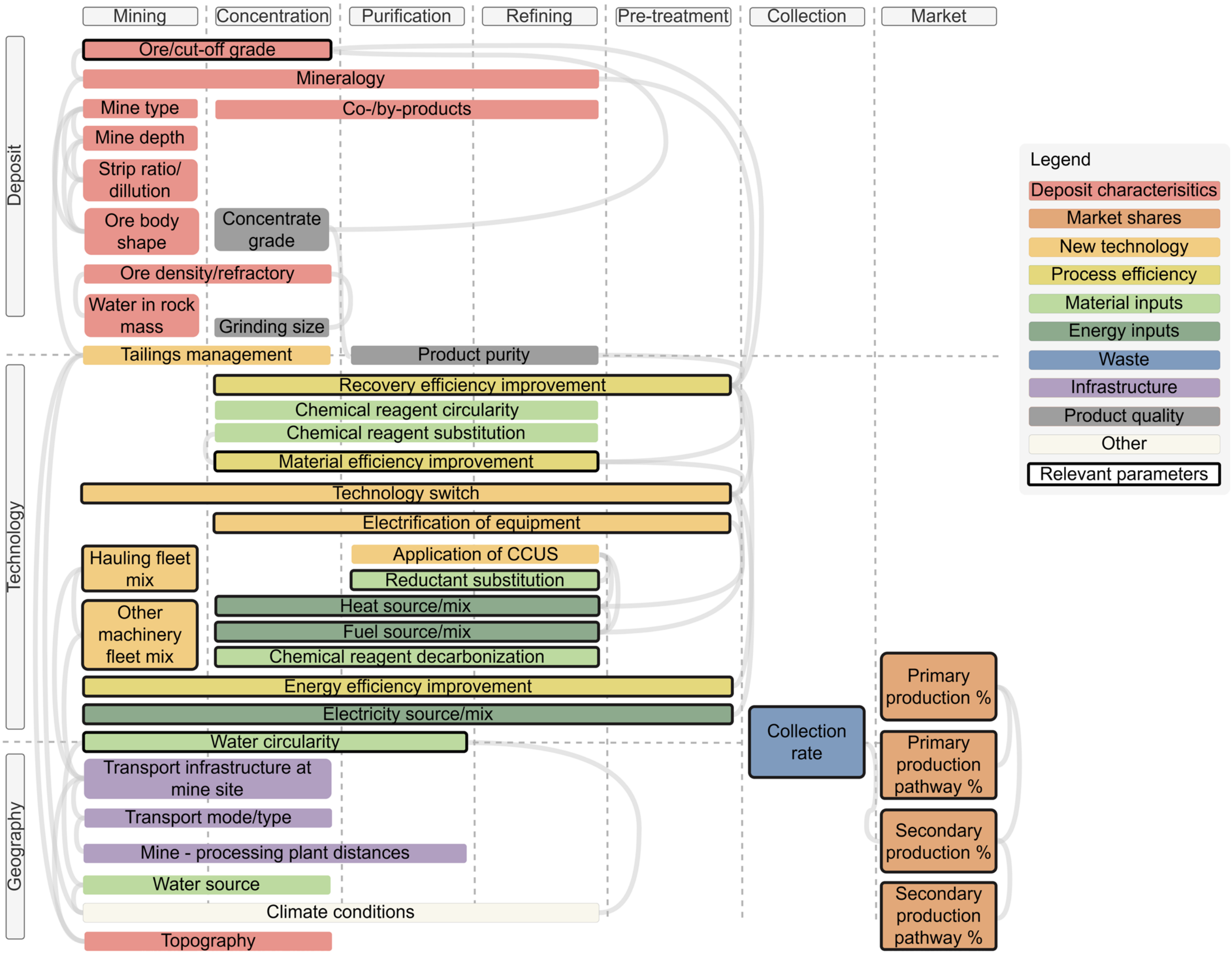


Fig. 3 List of analyzed parameters categorized by deposit characteristics, technology and geography dependent, and by the respective value chain stage. The selection of relevant parameters in this study is marked in with a black outline. Parameter connections are shown in grey

and economic feasibility, aligning with previous findings from Wyns and Khandekar (2019). Other material input-related parameters, such as chemical reagent substitution, were not identified as relevant, as these would require entirely new process designs. Instead, future impacts linked to reagents are expected to be primarily driven by changes in their production, reflecting the chemical industry's decarbonization goals (Istrate et al. 2024). Tailings management is a key parameter dependent on both deposit characteristics and technology. Tailings disposal is often identified as a large contributor to the toxicity and land use impacts of mining (Beylot et al. 2022). However, this parameter was not classified as a key parameter, as experts emphasized that projecting future adoption trends for emerging management practices is inherently uncertain. Such uptake is highly site-specific (depending on topography and climate conditions) and ore mineralogy. Moreover, water circularity is a key parameter dependent on both technology and geography, which is of high concern for mining companies, with improvements being forced due to regional water scarcity.

Finally, at the market level, both secondary supply market shares and shares of primary production pathways were identified as relevant parameters both in the pLCA literature and by the experts.

Implementing these parameters in the inventory model can have varying implications. Some parameters can be summarized and represented by a single variable to simplify modelling. This is the case, for example, with hauling fleet mix and other machinery fleet mix, which can be summarized as mine electrification. Pre- and post-consumer collection rates and recovery efficiencies can be modelled as overall recycling efficiencies. Some parameters, such as changes in efficiencies or market shares, can be integrated relatively easily, as they only require adjustments to existing inventory flows (e.g., increasing or decreasing the market share of a given production route). In contrast, the integration of new technologies often requires supplementary LCI modelling to adequately capture their impacts. Parameters related to the background system (i.e., activities outside the mineral value chain that interact with it), such as the decarbonization of the electricity grid mix, can be incorporated using prospective LCI databases generated via the open-source tool *premise* (Sacchi et al. 2022). However, for parameters related to sectors not explicitly modeled in prospective LCI databases, such as specific chemical reagent production, additional modeling of future background scenarios may be necessary. More details on the implications of parameter modeling in inventories, including the affected stages and processes, are provided in SI 1.1. Moreover, an exemplary collection of the implementation of selected parameters in existing studies is available in SI 1.2.

Step A2, A3: PESTEL and Causal Loop Diagram The PESTEL checklist is used to identify 22 external parameters, also called factors, that may influence the future development of the mineral value chain represented in the inventory model blueprint (the complete PESTEL checklist is provided in SI 3.1 Table 1). The CLD shows the connections between these factors and the key inventory parameters (Fig. 4a). We identify three key factors, outlined in purple, namely raw material demand, secondary supply capacity, and primary supply capacity, which have a major influence on other factors and the future development of the entire system. Increasing demand for mineral commodities, which is itself influenced by multiple factors, positively affects the financing of research and development (R&D). Moreover, demand indirectly influences deposit qualities, as higher raw material demand leads to greater primary raw material supply (indirectly via higher prices) in the context of limited secondary supply in the short term due to relatively long product lifetimes. Figure 4a also shows which parameters are influenced by which factors. R&D influences all technological parameters, while global decarbonization efforts impact background parameters. The factor deposit qualities influences ore grade. Furthermore, primary and secondary supply factors influence all market share parameters. Figure 4b shows the connection of the parameters to the inventory stages, with some parameters applying only to specific stages, such as ore grade for mining and concentration, and others applying to all stages, such as efficiency improvement parameters.

3.2.2 Step B: Find future assumptions for each relevant parameter and key factor

Scenarios used in pLCA background databases (Sacchi et al. 2022) that rely on Shared Socioeconomic Pathways (SSPs) (Riahi et al. 2017) and their implementation into IAMS do not include mineral-specific considerations but can be used to inform assumptions for factors such as decarbonization (see Table 1). Whenever adopting assumptions from IAM scenarios, the practitioner should be aware of their respective assumptions and disclose them as outlined by de Bortoli et al. (2025). For adopting assumptions (step B1), other already existing scenarios (Calderon et al. 2024) can provide consistent assumptions of economy-wide developments (background parameters) and resulting mineral demand, with some also providing primary and secondary supply shares. Table 1 provides an overview of sources that can be used to adopt and derive assumptions.

As most of the identified parameters are likely not part of existing scenarios, deriving assumptions (step B2) for them is of high importance. Most derived assumptions in literature include historic projections of ore grade, efficiency increases, and market shares of production pathways (Harpprecht et al. 2024). Deriving assumptions for some parameters may require the use of models, such as stock and flow models for secondary supply shares (e.g., Takimoto et al. 2024) or mining scheduling models (e.g., Ambrose and Kendall 2020a; Northey et al. 2023). Additionally, upscaling techniques like described in Langkau et al. (2023) can be applied. Decarbonization pathways outlined by companies also represent a valuable source for deriving assumptions (Antonini et al. 2025).

4 Showcasing SIMPL-M

In this section, the SIMPL-M approach is illustrated using the example of global battery-grade nickel sulfate hexahydrate supply. Nickel sulfate demand is projected to increase significantly in the near term due to its critical role in cathodes for BEVs (IEA 2025a). The purpose of this case study is not to provide a thorough assessment but to demonstrate the application of the SIMPL-M approach. Accordingly, several simplifications were made (see SI 3.2), and the impact assessment results should be interpreted while taking these limitations into account.

4.1 Goal and scope definition

Definition of the prospective research question The RQ addressed in this case study is: What are the potential future environmental impacts of global battery-grade nickel sulfate supply by 2050, and how may changes in relevant parameters influence these impacts?

Choice of temporal boundaries The temporal boundary is from the current situation (2025) until the year 2050, which

Table 1 Examples of parameter assumptions that can be derived and adopted

		Step B1: Adopt assumptions	Step B2: Derive assumptions
Key factors (or external parameters)			
Environmental policy and legislation		SSP2 narratives in IAM scenarios (IPCC 2023) and regulations like the EU's Battery Regulation (European Commission, 2023) or Critical Raw Materials Act (CRMA) (European Commission 2024)	To be avoided
Primary supply capacity		Industry report and outlooks (e.g., Alonso et al. 2025; IEA 2025a)	Announced production capacity (e.g., from S&P Capital IQ Pro database)
Secondary supply capacity		Announced recycling targets like in the CRMA	Announced recycling capacity based on recycling roadmaps
Commodity demand		Demand scenarios from literature (Calderon et al. 2024)	Derived from population or service demand (e.g., transport, energy) from IAMs
Parameter category	**Inventory parameters**		
Deposit characteristics	Ore grade	Ore grade projections from existing literature (e.g., Calvo et al. 2016; Northey et al. 2014)	Regression models based on historical ore grade trends (as done by: Harpprecht et al. 2021; van der Meide et al. 2022; Van der Voet et al. 2019). Endogenously estimated by mine scheduling (e.g., Bradley et al. 2025; Northey et al. 2023) or cost optimization (e.g., Busch et al. 2025) models
Market shares	Primary (production pathway) market shares	Industry report and outlooks (e.g., Alonso et al. 2025; Fraser et al. 2021; IEA 2025a)	Mine scheduling models (e.g., Bradley et al. 2025; Northey et al. 2023) Cost optimization models (e.g., Busch et al. 2025)
	Secondary (production pathway) market shares	Industry report and outlooks (e.g., Alonso et al. 2025; IEA 2025a)	Stock and flows models based on technology capacity deployment, lifetimes, and EoL recycling rates (e.g., Husmann et al. 2025a, b)
New technology	Electrification of equipment Technology switch	Not available	Mining and refining industry roadmaps (Antonini et al. 2025)
	Hauling/other machinery fleet mix	Heavy-duty vehicle electrification of IAM scenarios	Company targets of mine electrification (Antonini et al. 2025)
Process efficiency	Recovery/Material/Energy efficiency improvement	Efficiency improvement projections from existing literature or IAMs	Regression models based on historical improvement rates Achievement of best available techniques (BAT) performance or current technologies with low TRL
Material inputs	Reductant substitution	Not available	Refining industry decarbonization roadmaps (Antonini et al. 2025) or supplier industry roadmaps like hydrogen
	Chemical reagent decarbonization	Partially considered through energy decarbonization in premise (Sacchi et al. 2022), but without specific modelling of chemical reagents	Chemical industry decarbonization roadmaps, e.g., for lime (EuLA 2023) Achievement of best available techniques (BAT) performance
Energy inputs	Electricity source/mix	Electricity grid mixes from existing scenarios (e.g., IAMs or IEA scenarios) or national policy targets	Use company targets for on-site renewable power generation (Antonini et al. 2025)
	Heat source/mix Fuel source/mix	Use existing broader industrial heat supply and transportation scenarios (e.g., from IAMs) as proxy	Company decarbonization strategies (Antonini et al. 2025)

is chosen as the time horizon because secondary supply is expected to make significant contributions to global supply (IEA 2025a).

Choice of scenario type The use of explorative scenarios allows for assessing environmental impacts and the evolution of relevant parameters, considering their influence under different configurations of a potential future nickel sulfate value chain, in alignment with the RQ.

Prospective definition of the production system and related scope items The case study uses attributional LCA, with mass allocation preferred over system expansion. Cradle-to-gate

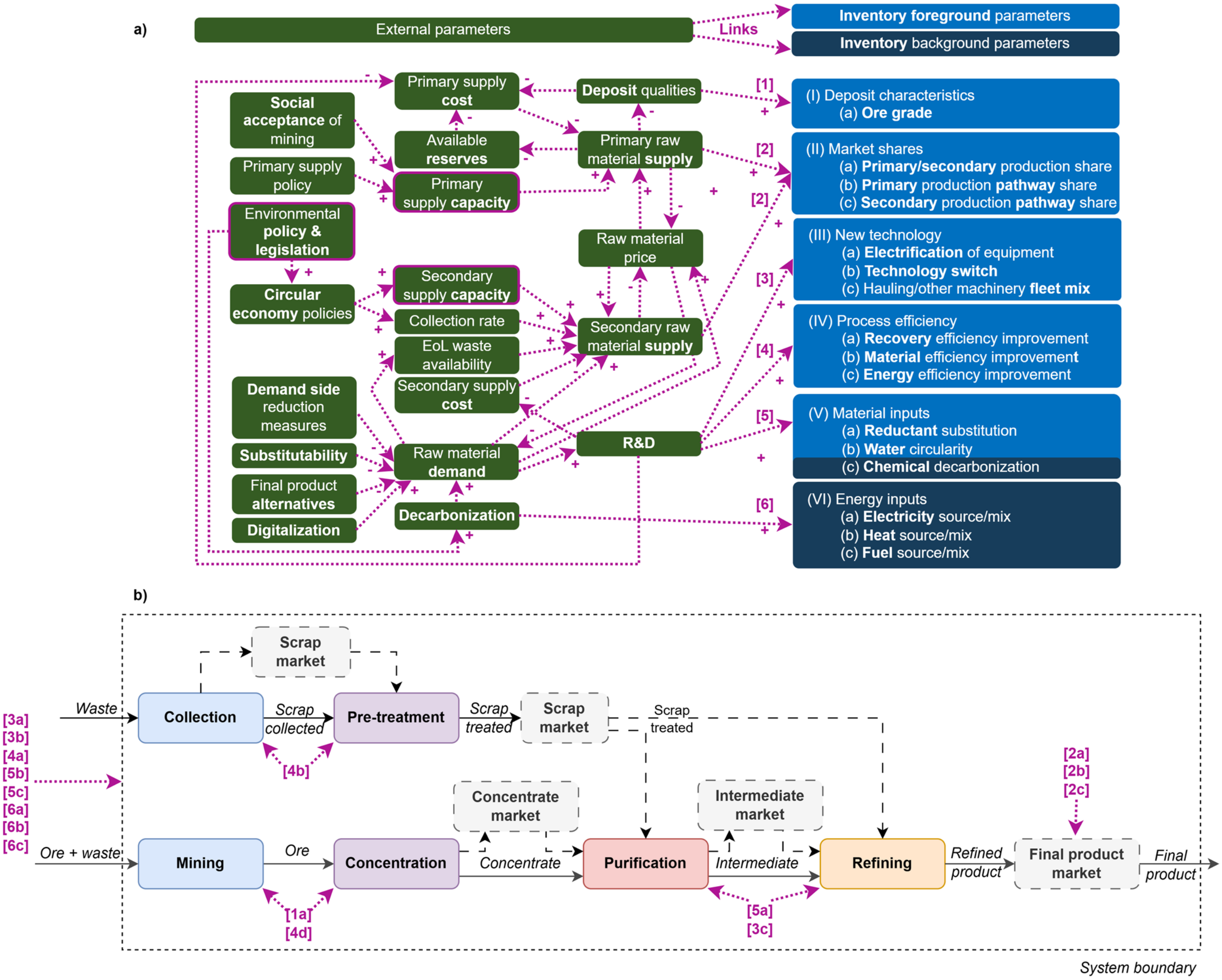


Fig. 4 Diagram of (**a**) the CLD of factors (here external parameters), key factors (marked with a purple outline) and their connection to inventory foreground/background relevant parameters, and (**b**) the parameters connection to the inventory model blueprint. Research and development = R&D

and EoL-to-gate system boundaries are chosen for primary and secondary supply, respectively. The functional unit is defined as 1 kg of battery-grade nickel sulfate hexahydrate, with a nickel metal content of 22%, supplied to the current and 2050 global market.

4.2 Inventory analysis

4.2.1 Step A: Identify relevant inventory parameters and key factors

Figure 5a shows the adapted CLD of factors linked to relevant parameters, while Fig. 5b shows the inventory flow diagram, indicating where the parameters connect to the respective stages and flows. In the following, steps A1-A3 are explained.

Step A1: Inventory model and parameters The SIMPL-M's generic inventory model blueprint is adapted to represent the simplified global supply of battery-grade nickel sulfate (Fig. 5b). Deposit types, technologies and regions were used to characterize different production pathways, corresponding to the second preferred approach to modelling granularity, since site-specific modelling is limited by data availability. Deposit types for primary production are either nickel-bearing laterites or sulfides ores, while spent LIBs are considered the feedstock for secondary production. Main technologies used for the processing are high pressure acid leaching (HPAL) and rotary kiln electric furnace (RKEF) for laterite ores and flash smelting (FS) for sulfide ores, as well as pyro- (RePyro) and hydrometallurgical (ReHydro) recycling processes. Regions for modelling primary supply are other Asia (OAS) including Indonesia, Philippines and

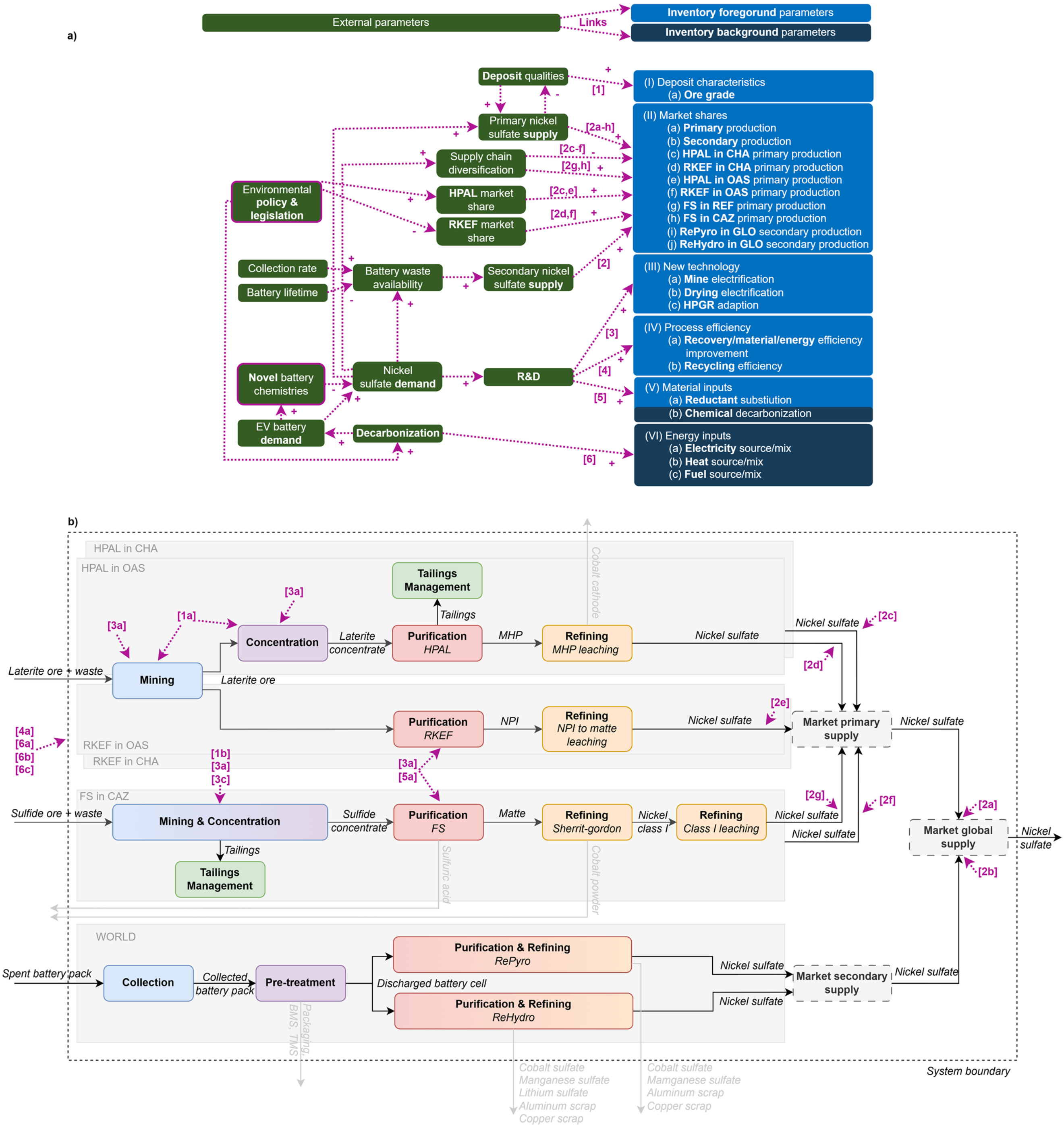


Fig. 5 (**a**) CLD of key factors' connection to selected main parameters. (**b**) Process flow chart for the supply of 1 kg nickel sulfate for the global market and the connection of relevant parameters to the inventory. Only product in- or outflows from the foreground are illustrated. Waste outflows are not displayed. Abbreviations: High Pressure Grinding Roll = HPGR, High Pressure Acid Leaching = HPAL, Rotary Kiln Electric Furnace = RKEF, Flash Smelting = FS, Pyrometallurgical Recycling = RePyro, Hydrometallurgical Recycling = ReHydro. Geographic regions: China = CHA, Other Asia = OAS, Countries from the Reforming Economies of the Former Soviet Union = REF, Canada, New Zealand, and Australia = CAZ, Global = WORLD

New Caledonia; China (CHA) with ore coming from OAS; and Canada, New Zealand, Australia (CAZ). This regionalization is applied for consistency with the IAM REMIND (Aboumahboub et al. 2020), which is used to project future changes in the background system. For the secondary supply, the two production pathways are only modelled on a global level. Foreground inventories are taken from the literature (Eckelman 2010; Kallitsis et al. 2022; Roy et al. 2025), with further details in SI 3.2 and the inventories provided in Brightway format in SI 4. Background inventories are taken from ecoinvent v3.10 (cut-off system model), using the open-source tool *premise* v2.2.9 (Sacchi et al. 2022) to generate prospective background databases aligned with projections from REMIND scenarios.

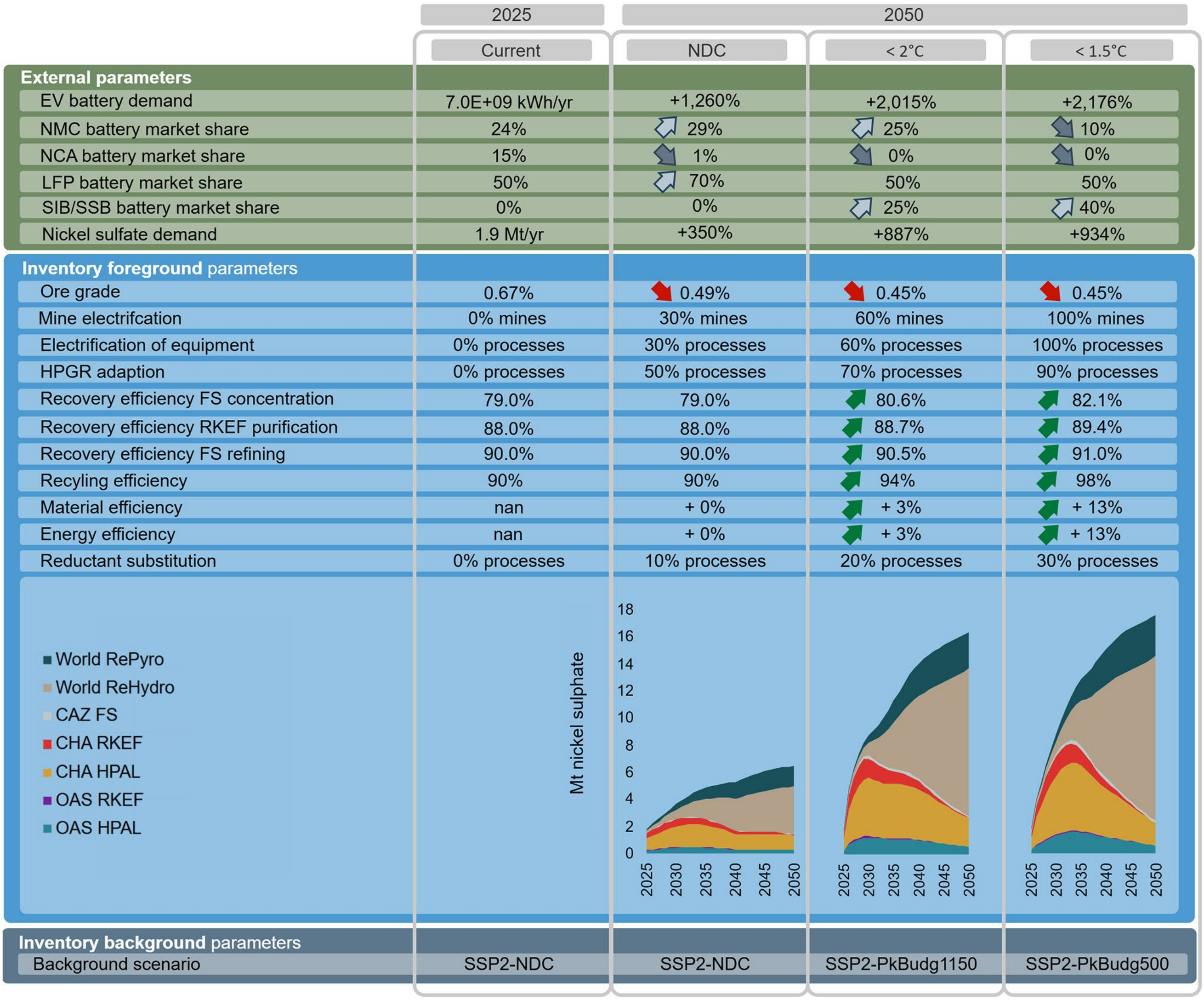
Relevant parameters are selected based on the parameter list provided by SIMPL-M and literature-derived inventories. Of the 19 high-importance parameters, all are implemented resulting in 17 parameters used for modelling (see Fig. 5a). The reduced number of parameters is due to parameters being combined because of low granular LCI data. Specifically, water circularity is included in the modeled parameter material efficiency and the mine electrification parameter combines the hauling fleet mix and other machinery fleet mix. Mine electrification is implemented by converting fuel energy inputs to electricity equivalent. This simplified approach is analogous to the reductant substitution parameter implementation method, where the energy equivalent of coal is calculated for hydrogen. Efficiency-related parameters are applied by adjusting energy or material inputs, while recycling efficiency is modeled directly as an assumption in a stock and flow model rather than within the inventory itself. The detailed application of parameters to the inventory can be found in SI 4.

Step A2 and A3: PESTEL and CLD Potential factors affecting the selected parameters were identified through the PESTEL checklist of the SIMPL-M approach. Figure 5a shows the 15 factors considered in this example, accounting for factors specific to the commodity value chain and model implementation. Key factors are environmental policy and legislation, and the penetration of novel battery chemistries into the market. Environmental policy and legislation drives decarbonization, which in turn determines demand for EV batteries. This demand, together with the market share of (novel) battery chemistries, determines the demand for nickel sulfate. Higher demand leads to increased R&D, resulting in more optimistic assumptions for technology performance-related parameters. At the same time, higher demand also results in greater primary supply, accelerating ore grade decline and increasing the political will to diversify value chains. Furthermore, stricter environmental policy and legislation focused on decarbonization encourages a stronger shift toward HPAL production over RKEF pathways. Our modelling does not include mining capacity or nickel reserve considerations, although some studies indicate the possibility of a supply shortage (IEA 2025a; Watari et al. 2018).

4.2.2 Step B: Find future assumptions for each key factor and relevant inventory parameter

Step B1: Adopt assumptions Assumptions for absolute transport service demand for BEVs, as well as projected changes in background parameters such as electricity, heat, and fuel mix, and chemical reagents production (partly modeled through the decarbonization of energy supply), are adopted from REMIND scenarios using *premise*. Three scenarios, based on the middle-of-the-road SSP (SSP2), are selected. First, NDC serves as a business-as-usual scenario, representing current climate policy plans. This scenario considers Nationally Determined Contributions (NDCs), with an estimated global mean surface temperature (GMST) increase of approximately 2.5 °C by 2100. Secondly, PkBudg1150 represents a more ambitious scenario that meets the Paris Agreement (PA) goal of staying below 2 °C, resulting in a GMST increase of 1.6–1.8 °C by 2100 (<2 °C scenario). Finally, PkBudg500 is the most ambitious scenario, meeting the PA goal of staying below 1.5 °C, resulting in a GMST increase of 1.2–1.4 °C by 2100 (< 1.5 °C scenario).

Step B2: Derive assumptions Based on the absolute transport service demand from REMIND scenarios, we derive assumptions for several parameters. Nickel sulfate demand is derived by combining battery chemistry market shares (see SI 2.6) from Degen et al. (2023) with absolute transport demand (see SI 2.5). A stock and flow model is applied to estimate secondary supply shares (see SI 2.7–SI 2.14), and primary production pathway shares are derived based on Fraser et al. (2021) (see SI 2.4). Ore grade decline is derived from van der Meide et al. (2022), aligning their stated policy scenario with the NDC scenario and their sustainable development scenario with the < 2 °C and < 1.5 °C scenarios. Electrification rates are based on reported company goals. Increases in recovery efficiency over time are estimated based on current efficiencies and a maximum efficiency of 95%, using Wright's Law to link future improvements to cumulative demand. SI 2.2 presents quantified assumptions for all parameters. A distinctness-based selection of assumptions (step B3) was not necessary, as assumptions were selected according to low, medium, and high development cases, corresponding to the scenarios chosen in step C.



	2025	2050		
	Current	NDC	< 2°C	< 1.5°C
External parameters				
EV battery demand	7.0E+09 kWh/yr	+1,260%	+2,015%	+2,176%
NMC battery market share	24%	↗ 29%	↗ 25%	↘ 10%
NCA battery market share	15%	↘ 1%	↘ 0%	↘ 0%
LFP battery market share	50%	↗ 70%	50%	50%
SIB/SSB battery market share	0%	0%	↗ 25%	↗ 40%
Nickel sulfate demand	1.9 Mt/yr	+350%	+887%	+934%
Inventory foreground parameters				
Ore grade	0.67%	↘ 0.49%	↘ 0.45%	↘ 0.45%
Mine electrifcation	0% mines	30% mines	60% mines	100% mines
Electrification of equipment	0% processes	30% processes	60% processes	100% processes
HPGR adaption	0% processes	50% processes	70% processes	90% processes
Recovery efficiency FS concentration	79.0%	79.0%	↗ 80.6%	↗ 82.1%
Recovery efficiency RKEF purification	88.0%	88.0%	↗ 88.7%	↗ 89.4%
Recovery efficiency FS refining	90.0%	90.0%	↗ 90.5%	↗ 91.0%
Recyling efficiency	90%	90%	↗ 94%	↗ 98%
Material efficiency	nan	+ 0%	↗ + 3%	↗ + 13%
Energy efficiency	nan	+ 0%	↗ + 3%	↗ + 13%
Reductant substitution	0% processes	10% processes	20% processes	30% processes
Inventory background parameters				
Background scenario	SSP2-NDC	SSP2-NDC	SSP2-PkBudg1150	SSP2-PkBudg500

Fig. 6 Scenarios resulting from step C and the respective quantification of parameters

4.2.3 Step C: Combine assumptions into future scenarios

To perform the consistency check (step C1), the Excel template provided by the SIMPL approach was used (see SI 2.3). The distinctness-based selection of scenarios (step C2) is also presented in SI 2.3 and resulted in the three scenarios shown in Fig. 6.

The three scenarios considered are consistent with the REMIND model assumptions. In the NDC scenario, battery demand increases due to decarbonization efforts, with LFP chemistries (nickel-free) dominating the market at 70% by 2050. HPAL production pathways are favored over RKEF routes, although some RKEF plants remain operational. China strengthens its market dominance, while Other Asia (primarily Indonesia) expands production. In the <2 °C scenario, more ambitious decarbonization targets drive a major increase in battery demand, encouraging the adoption of sodium-ion batteries (SIB) and solid-state batteries (SSB) due to their performance advantages, both of which contain nickel. By 2050, RKEF technologies are no longer in operation, with China maintaining dominance and Other Asia gaining additional market share. In the <1.5 °C scenario, the strongest decarbonization efforts result in the highest battery demand. LFP remains the leading chemistry, but SIB and SSB advance faster than expected, substantially reducing the share of NMC batteries. HPAL fully replaces RKEF production, and the surge in demand drives value chain diversification, with operations expanding in CAZ and Other Asia, while China continues to dominate.

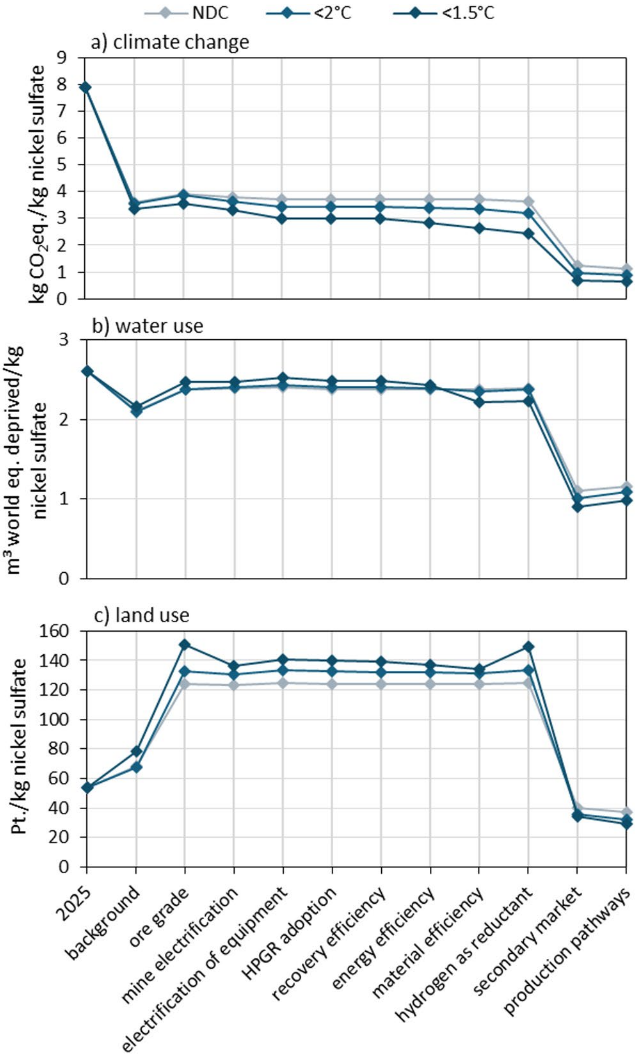


Fig. 7 Effects of parameter changes on (**a**) climate change, (**b**) water use and (**c**) land use impact results for the three scenarios. Parameters are calculated consecutively, which means that the preceding parameter is influenced by the parameter before

4.3 Impact assessment and interpretation

Figure 7 shows the climate change, water use, and land use impact results in 2025 and the effect of parameter changes by 2050 for the NDC, < 2 °C, and < 1.5 °C scenarios. Parameters were applied and results calculated consecutively, so each preceding parameter influences those that follow.

Climate change impacts decrease from 7.9 kg CO₂-eq./kg in 2025 to 1.1, 0.9, and 0.7 kg CO₂-eq./kg in the three scenarios, respectively. This reduction is mainly driven by the decarbonized background system and the increasing share of secondary supply (as secondary supply has up to 90% lower life cycle GHG emissions compared with primary supply). The influence of ore grade decline remains minor (with only + 4% increase in impacts). This limited effect can be explained by the fact that ore grade mainly affects energy-related GHG emissions, and energy supply is assumed to be decarbonized through changes in the background system. Moreover, it should be noted that the influence of ore grade decline might be underestimated due to the assumed linear rather than exponential effect on energy inventory flows (see SI 4). Overall, the individual impact reduction potential of the considered parameters appears minor compared to the effect of considering changes in the background system (which decreases impacts by 55–58%). Nevertheless, when combining the mitigation effects of all the other parameters, climate change impacts decrease by 35–38% across the three scenarios. This highlights the importance of a consistent set of relevant parameters in pLCA, even when individual contributions appear modest. Moreover, if the background system does not achieve the level of decarbonization assumed here, the relative influence of these parameters would be substantially higher. Future electricity mix impacts were modelled using REMIND scenarios, which aggregate countries into supra-regions. As a result, grid decarbonization in countries like Indonesia may be overestimated, increasing the mitigation potential of background changes and reducing the relative importance of other parameters such as changing primary supply market shares. Considering global nickel sulfate demand, total climate change impacts amount to 14.5 Mt CO₂-eq. in 2025, decreasing by 51% by 2050 in the NDC scenario due to a relatively low demand increase, and by 20% in the < 1.5 °C scenario, where high relative emission reductions counter the increase in demand (all impact category results are provided in SI 5).

Water use and land use results illustrate different trends and potential trade-offs, although the underlying impact assessment methods for these categories have substantially higher uncertainty. Water use impacts decrease from 2.6 m³ world eq. deprived/kg in 2025 to 1.2, 1.1, and 1.0 m³ world eq. deprived/kg, largely due to the increasing share of secondary supply (49–53% impact reduction across scenarios), which shows lower water intensity compared to primary supply. Ore grade decline has a more pronounced effect on water use impacts than on climate change, increasing impacts by 12–14%, while considering background scenarios instead reduce impacts by 17–19%. The combined influence of other parameters remains relatively limited.

Land use impacts decrease from 54 Pt./kg in 2025 to 37, 32, and 29 Pt./kg, respectively. Ore grade decline leads to a substantial increase in land use due to larger extraction and tailings disposal areas. The effect of ore grade decline is more pronounced in the < 1.5 °C scenario (+ 134% increase in impacts), where higher nickel sulfate demand exacerbates the decline. However, this effect is largely offset by the increasing share of secondary supply, which decreases impact results by up to 212% for the same scenario.

Applying different background system scenarios can increase land use change by 25–45%. Most other parameters have only minor effects, although reductant substitution with hydrogen causes a notable increase in land use impacts (-28% in the < 1.5 °C scenario) because part of the hydrogen is produced via biomass gasification. Similar trends can be observed in other impact categories where emissions from tailings are the main contributors, such as eutrophication and ecotoxicity.

5 Discussion

5.1 Contribution of SIMPL-M to the field of pLCA

The SIMPL-M approach extends the already more widely used SIMPL approach to develop scenarios for pLCA with mineral raw materials supply specific guidance. It aims to advance the application of pLCA to mineral value chains through three key contributions. First, it provides guidance on the definition of the goal and scope given the unique features of the mining and metals sector. Second, it provides an inventory model blueprint together with a set of relevant inventory parameters, identified through literature and interviews with field experts. The adoption of these two elements could enhance the comparability of future pLCA studies, while simultaneously reducing the time and effort required by practitioners. In contrast to earlier practices, SIMPL-M incorporates a broader and more structured set of parameters to support the harmonization of modelling choices, thereby addressing a major research gap in the literature (Harpprecht et al. 2024). Furthermore, the verification and completeness check of identified parameters through semi-structured interviews with experts ensures that the resulting parameter list is as comprehensive and relevant as possible. Third, it develops a mineral value chain-specific PESTEL checklist and established a CLD that links the identified external factors to the inventory model blueprint and relevant parameters. These developments can be readily applied by practitioners to develop their own scenarios, even if they are not familiar with PESTEL and CLD tools. As noted by Langkau et al. (2023), the significant resources required to apply the SIMPL approach and the unfamiliarity with the use of PESTEL and CLD tools are often perceived as a barrier by practitioners. SIMPL-M therefore contributes to making systematic scenario-based inventory modelling for mineral value chains more accessible. The flexibility of the approach enables its application to a wide range of mineral and metal commodities and scales, from site-specific analyses to regional and global assessments. This increases its relevance for both policy and industry decision-making. Sectors that depend on mineral raw materials (e.g., mobility, energy, and digital technologies) can use SIMPL-M to inform and strengthen their decarbonization strategies.

5.2 Limitations and future research

The SIMPL-M approach also comes with several limitations. Although we identified an extensive list of parameters relevant for prospective modelling, not all of these parameters are equally ready for implementation into inventory modelling. For example, efficiency improvements can be relatively easily incorporated into LCIs, whereas parameters such as reductant and reactant substitution require more detailed process-specific knowledge and potentially additional inventory flows. Furthermore, the list of parameters is biased towards a focus on parameters effecting GHG emissions. This bias stems from the personal focus of interviewed experts (e.g., companies focusing on decarbonization) but also from the fact that other environmental flows are not well represented in current LCI literature. This is the case for, e.g., emissions from tailings disposal, but also water flows representation with tailings management LCIs and process LCIs. More broadly, pLCA relies on scenario data mostly from IAMs with a focus on climate change impacts, which leads to other environmental issues such as toxicity or water scarcity being largely neglected. SIMPL-M also inherits the general challenges of the SIMPL approach regarding uncertainty and scenario quality. Moreover, the nickel sulfate case study used to demonstrate the application of SIMPL-M represents a simplified example, and thus carries limitations associated with such simplifications.

Looking ahead, future work should focus on testing the SIMPL-M framework across a broader range of commodities, value chain configurations, and geographical contexts to further assess its robustness and understand the relative importance of parameters. Some parameters that describe emerging technologies require additional LCI modelling to be effectively integrated into inventories. Therefore, developing LCIs for novel technologies with high future relevance represents an important next step. Additionally, further efforts should aim to quantify correlations between parameters and inventory flows, such as the relationship between ore grade and energy use, to improve modelling accuracy and reliability. Beyond the mineral value chain, SIMPL-M may also serve as a template for extending the SIMPL approach to other sectors.

6 Conclusion

The SIMPL-M extends the SIMPL approach introduced by Langkau et al. (2023) to enable pLCA in mineral value chains. At its core, SIMPL-M provides a generic inventory model blueprint that represents both primary and secondary (cradle-to-gate) mineral supply routes. From a broad set of parameters that influence future environmental performance, the framework identifies a subset of relevant parameters and links them to this blueprint, offering practitioners clear guidance for parameter selection. By promoting consistent and relevant parameter use, SIMPL-M enhances the comparability of pLCA results. It also establishes key macro factors that connect overarching scenarios with parameter assumptions, thereby facilitating the integration of scenario analysis, technology foresight, and value chain dynamics. Together, these features strengthen the robustness and relevance of LCA for forward-looking decision-making in mineral value chains, providing a practical tool for both academia and industry. The framework's applicability is demonstrated through an exemplary case study evaluating future environmental impacts of global nickel sulfate supply for battery production. The results of the case study show the importance of considering parameters beyond background changes, especially for impact categories beyond climate change. Climate change impacts are reduced by 55–58% by applying background scenarios, while the combined effect of all other parameters further reduces impacts by 35–38%. For water use, applying background scenarios only reduces results by up to 19%, while considering secondary supply increases can reduce impacts by up to 53%. The changes are even higher for land use impacts, as the up to 45% increase due to background considerations is far less than the up to 134% increase due to ore grade change, and the 212% decrease due to secondary supply increase. Future research should broaden the testing of SIMPL-M across diverse use cases, ranging from site-specific assessments to global-scale analyses.

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Data availability All data is available in the supplementary information.

Declarations

Competing interests The authors declare no competing interests.

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