Stepwise guidance for tackling multifunctionality challenges in prospective life cycle assessment

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RESEARCH

Stepwise guidance for tackling multifunctionality challenges in prospective life cycle assessment

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Abstract
Prospective life cycle assessment (pLCA) is increasingly used to assess the potential environmental impacts of product systems under future scenarios. However, addressing uncertainties arising from future variability in multifunctional processes remains a methodological challenge. For example, waste heat that is considered nonfunctional at the laboratory scale may become functional at larger scales. While some pLCA case studies have addressed these issues, a systematic and comprehensive approach for identifying and handling multifunctional processes remains lacking. This paper introduces a structured, stepwise guidance that builds upon and complements existing methods for addressing multifunctionality under future scenario development in pLCA. Focusing on the uncertainty due to choices and epistemic uncertainties, the guidance covers the identification of relevant inventory parameters such as flow types, the number of functional flows, substituted products, substitution ratios, and allocation factors. Applying this framework to a case study on novel incinerator bottom slag valorization reveals that pLCA results are sensitive to future assumptions regarding potential variability of these inventory parameters. The proposed approach allows for a more comprehensive and transparent assessment of multifunctionality in pLCA, thereby supporting consistent environmental decision-making.

Keywords Multifunctional processes · Prospective life cycle assessment · Uncertainty · Scenario development · Stepwise guidance · Industrial ecology

1 Introduction

Prospective life cycle assessment (pLCA) is increasingly used to explicitly assess the potential environmental impacts of product systems in the future, considering temporal changes and technological development (Arvidsson et al., 2023). Relevant literature guiding methodological decisions in pLCA focuses on challenges such as modeling foreground and background systems, data sourcing, comparability, uncertainty, and temporal mismatches (Arvidsson et al., 2018; Cucurachi et al., 2018; Moni et al., 2020; Thonemann et al., 2020; van der Giesen et al., 2020).

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A crucial methodological challenge in both conventional life cycle assessment (LCA) and pLCA studies is the handling of multifunctional processes—involving multiple functional input or output flows (Guinée et al., 2004; Pelletier et al., 2014). Guinée et al. (2021) proposed a systematic four-step approach to identify and handle such processes. Additional methodological guidance covers allocation principles (Suh et al., 2010), rationales for different procedures (Pelletier et al., 2014), substitution methods in recycling (Vadenbo et al., 2017; Zink et al., 2016), and selecting methods aligned with study goals and scope (Ijassi et al., 2021; Schrijvers et al., 2020).

Identifying and handling multifunctional processes introduces uncertainties from methodological choices and data variability, such as determining flow type, allocation factors, or substitution credits (Igos et al., 2019; Mendoza Beltran et al., 2016). In pLCA, epistemic uncertainties—stemming from limited knowledge and the need to model inherently uncertain future system states—are particularly pronounced (Bisinella et al., 2021; Björklund, 2002; Mendoza Beltran et al., 2018).

Current literature addresses different multifunctionality challenges in pLCA. Corona et al. (2018) address the variability in identifying multifunctional processes arising from future technological efficiency changes altering the number of functional flows (see Fig. 1). Handling-related variability is addressed with respect to substituted products, substitution ratios (Adrianto et al., 2023; Thonemann et al., 2022), or external factors such as coproduct prices used to derive allocation factors (van den Oever et al., 2023). Additional challenges occur when flow functionality changes over time—for example, waste heat treated as a waste flow today may become a valuable product in future scenarios (Moni et al., 2020). Consequently, the identification and handling of multifunctional processes in pLCA is often inconsistent, incomplete, or entirely lacking (Thonemann et al., 2022). These sources of variability, such as uncertain flow types and alternative substitution scenarios (see Fig. 1), underscore the need to explicitly address epistemic uncertainties to improve decision reliability in complex product systems.

Incorporating future scenarios into LCA is an established approach to address epistemic uncertainties (e.g., Mendoza Beltran et al., 2018; Zacharopoulos et al., 2023). However, a review by Bisinella et al. (2021) found that only one quarter of 514 studies consistently applied scenario theory. Addressing this, Langkau et al. (2023) introduced the SIMPL approach, which supports consistent future scenario development in pLCA. Yet, the uncertainties associated with methodological choices on how to handle multifunctionality are explicitly not covered in the SIMPL approach (Langkau et al., 2023). Given that tackling multifunctionality challenges in pLCA is often inconsistent, incomplete, or entirely lacking, a research gap persists regarding a systematic and comprehensive approach to address those challenges.

Therefore, this article provides stepwise guidance for the consistent application of future scenarios for pLCA, with a particular focus on identifying and handling multifunctional processes. It systematically addresses variability in flow types, the number of functional flows, the substituted products, substitution ratios, and allocation factors.

The article is structured as follows: In Sect. 2, the stepwise guidance for tackling multifunctionality challenges in pLCA is proposed. In Sect. 3, the guidance is applied to a case study of a novel valorization process for incinerator bottom slag (see Fig. 1). Section 4 discusses the findings, and Sect. 5 concludes with main insights.

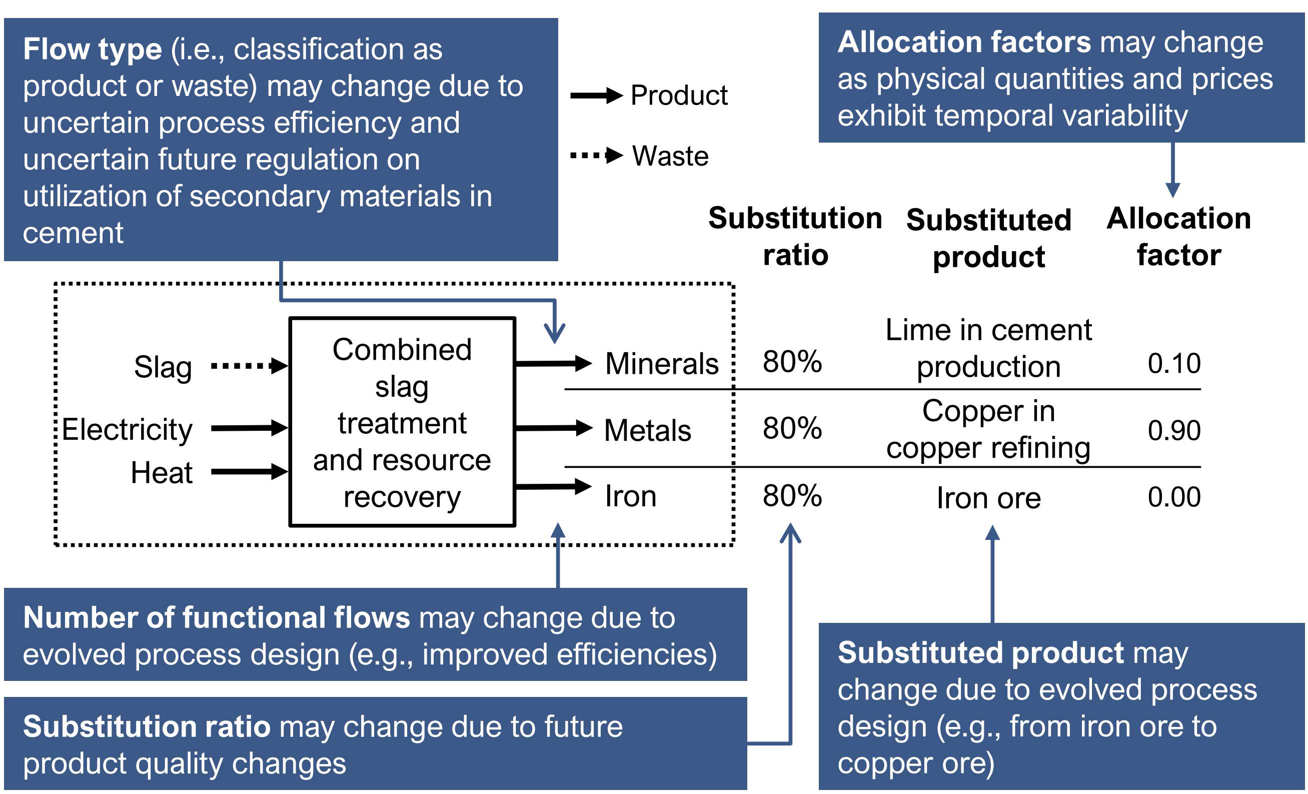

Fig. 1 Example of a multifunctional process and sources of future variability in the flow type, the number of functional flows, the substituted product, the substitution ratio, and the allocation factor (blue boxes). The functions of the process are incinerator bottom slag treatment and the recovery of secondary minerals, metals, and iron. This novel process is further discussed in the case study in Sect. 3

2 Addressing multifunctionality in prospective LCA: a stepwise guidance

Multifunctional processes fulfil multiple functions through interlinked functional flows, and their identification and handling are subject to variability and uncertainty (Guinée et al., 2004; Pelletier et al., 2014). This is particularly important in pLCA, where long-term forecasts and data estimates are inevitably uncertain (French & Geldermann, 2005). Uncertainty manifests in various forms, yet no unified categorization has emerged across disciplines. French (2023) identifies nine types of uncertainty to illustrate this diversity. Huijbregts (1998) categorized uncertainty into parameter uncertainty, *model uncertainty*, and *uncertainty due to choices* (e.g., selection of a procedure to handle multifunctionality), to which Björklund (2002) added *epistemic uncertainty* and *mistakes*. **Epistemic uncertainties** stem from limited knowledge and the need to model inherently uncertain future system states (Bisinella et al., 2021; Björklund, 2002; Mendoza Beltran et al., 2018). In pLCA, limited knowledge is caused by future **variability** that is denoted by the inherent physical randomness (French, 1995) of LCA input data, which Huijbregts (1998) categorized as temporal, spatial, and inter-object variability.

Inventory parameters that are relevant for identifying multifunctional processes include the flow type (product or waste) and the number of functional flows, and for handling multifunctionality, these are the substituted product, substitution ratios, and allocation factors.

Allocation factors denote the proportion of the quantity of an individual functional flow relative to the aggregated quantities of all functional flows, based on a selected criterion (e.g., total mass or revenue). Consequently, the sum of all allocation factors equals 1.

Inventory parameters are influenced by the external context (macroenvironment) comprising political, economic, social, technological, environmental, and legal (PESTEL) factors, as well as by the product system itself (Fahey & Narayanan, 1986; Issa et al., 2010). External elements that strongly influence the inventory parameters are defined as **key factors** (Langkau et al., 2023). Key factors can impact both the foreground system, and the background system, including indirect processes such as resource extraction and energy supply (European Union, 2010).

While all types of uncertainty should be considered in a pLCA of multifunctional processes, this guidance focuses on the uncertainty due to choices and epistemic uncertainties. Epistemic uncertainties are introduced by the unknown future development of external key factors and by temporal variability, encompassing short-term fluctuations (e.g., weather-related electricity mix fluctuations) and long-term shifts (e.g., commissioning of power plants).

To systematically address epistemic uncertainties in identifying and handling multifunctional processes in pLCA, this stepwise guidance builds on the *four-step approach* by Guinée et al. (2021): 1: distinguishing of product and waste flows; 2: identification of functional flows; 3: identification of multifunctional processes; and 4: handling of multifunctionality (see blue-framed boxes in Fig. 2). The approach is further developed through sub-steps that complement the SIMPL approach, which integrates inventory modeling with prospective scenario development in three iterative steps (Langkau et al., 2023): A: identification of relevant inventory parameters and key influential external factors, B: formulation of future assumptions, and C: development of future scenarios. These steps are adapted to emphasize relevant inventory parameters for multifunctional processes (see Fig. 2):

- 1.A: Identify key factors influencing the flow types and the number of functional flows.
- 1.B: Develop future assumptions regarding the type of each flow and the number of functional flows.
- 1.C: Integrate these assumptions into consistent future scenarios for the product system to address epistemic uncertainty in identifying multifunctional processes.
- 4.A: Identify key factors that influence the relevant inventory parameters for handling multifunctionality.
- 4.B: Develop future assumptions regarding relevant inventory parameters for handling multifunctionality.
- 4.C: Develop future scenarios addressing epistemic uncertainty in handling multifunctional processes.

This stepwise guidance provides a methodology for incorporating potential variability in parameters relevant to multifunctionality in pLCA. As a complement to the SIMPL approach, it supports consistent scenario development for the overall product system under investigation and the systematic integration of multifunctionality within the three iterative steps of prospective scenario development (see green boxes in Fig. 2). Therefore, it is recommended to apply the SIMPL approach to develop a consistent storyline of a future scenario, where multifunctionality challenges are systematically tackled through the proposed sub-steps of this guidance.

Guidelines are employed for crucial steps of this guidance to help identify the key factors and relevant economic flows that may alter the process's multifunctionality compared to the base-case.

These guidelines should be used collaboratively with stakeholders and experts to identify relevant choices and sources of uncertainty affecting the outcome and interpretation of the pLCA study. In this article, the guidelines are shown in a condensed version. The comprehensive guidelines and examples from pLCA case studies in the literature

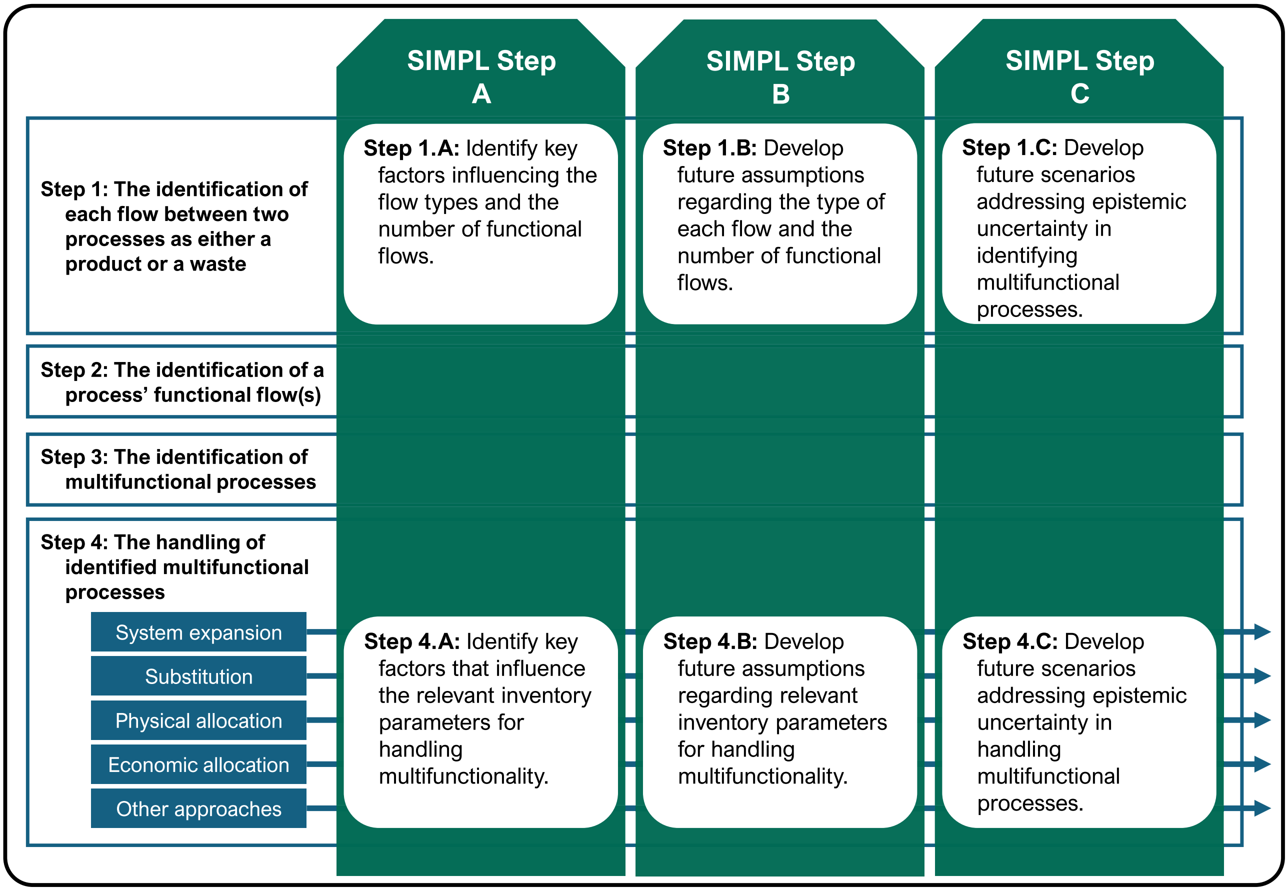

Fig. 2 The proposed stepwise guidance builds on the four-step approach from Guinée et al., (2021) to identify and handle multifunctional processes in pLCA (boxes with blue frame). To address the identified research gap regarding multifunctionality under future scenario development in pLCA, this four-step approach is integrated into the three steps of the SIMPL approach by Langkau et al., (2023) (green boxes), resulting in sub-steps in Step 1 and Step 4 (white boxes). In Step 4, specific guidance is provided for each option to handle multifunctionality (blue boxes)

to illustrate their application can be found in Supplementary Information SI1.

2.1 Step 1: The identification of each flow between two processes as either a product or a waste

In Step 1, the guidance addresses additional epistemic uncertainty in identifying multifunctional processes. Therefore, guidance is provided to develop an exploratory set of potential future process scenarios with distinct multifunctional characteristics regarding the flow type (product/waste) and the number of flows in a pLCA. Guinée et al. (2004) recommend distinguishing product and waste flows based on their economic value as follows:

product: economic value ≥ 0
waste: economic value < 0

Step 1.A: Identify key factors influencing the flow types and the number of functional flows.

This step is to evaluate potential changes in the number or type of economic flows and to identify external key factors that cause these changes.

Recommended guidelines include:

1. Identify factors that may alter the number (count) of waste input (i.e., waste treatment as a function) or product output flows, considering process modifications, upscaling, or technological advances.
2. Identify factors that may alter the economic value of the flows of the process under investigation and check whether this could result in a change in flow types.
3. Consider factors related to the background system that may influence flow types in the process, ensuring systematic evaluation of external drivers such as market, regulatory, or technological changes.

Step 1.B Develop future assumptions regarding the type of each flow and the number of functional flows.

Future assumptions should be developed based on the key factors identified in the previous Step 1.A, to consider future variability in flow numbers or types.

These assumptions can explore potential process improvements, such as hypothesizing the transformation of a current waste stream into a valuable coproduct and assessing its impact on multifunctional process evaluation. If such changes yield relevant environmental benefits, process development can prioritize strategies to enable this transition.

Step 1.C: Integrate these assumptions into consistent future scenarios for the product system to address epistemic uncertainty in identifying multifunctional processes.

The output of this step is a set of quantitative future assumptions regarding the types and numbers of economic flows, defining their potential variations from the baseline scenario. Therefore, the future assumptions developed in Step 1.B are systematically integrated into a manageable number of consistent future scenarios of the product system. Assumption combinations are selected based on logical consistency and distinctiveness (Langkau et al., 2023), ensuring scenario reliability and comprehensive coverage of uncertainties without redundancy.

2.2 Step 2: The identification of a process's functional flow(s)

Each functional flow represents a function of the processes investigated, which is either the production of a product or the treatment of waste. Therefore, all **product output flows**, or **waste input flows,** are **functional flows** (Guinée et al., 2021).

2.3 Step 3: The identification of multifunctional processes

All unit processes with more than one functional flow are classified as multifunctional.

A graphical representation facilitates the application of the first three steps of the guidance (Fig. 3). Identifying waste and product flows of both baseline and future scenarios in Step 1 enables straightforward identification of the functional flows in Step 2 and multifunctional processes in Step 3.

For further investigation, relevant scenarios must be selected, ensuring that the chosen scenarios either have distinct multifunctional characteristics or are nonfunctional. The three basic types of multifunctional processes—coproduction (only functional output flows), combined waste processing (only functional input flows), and recycling (functional input and output flows)—along with their possible combinations, can be used for a distinct selection (Guinée et al., 2021).

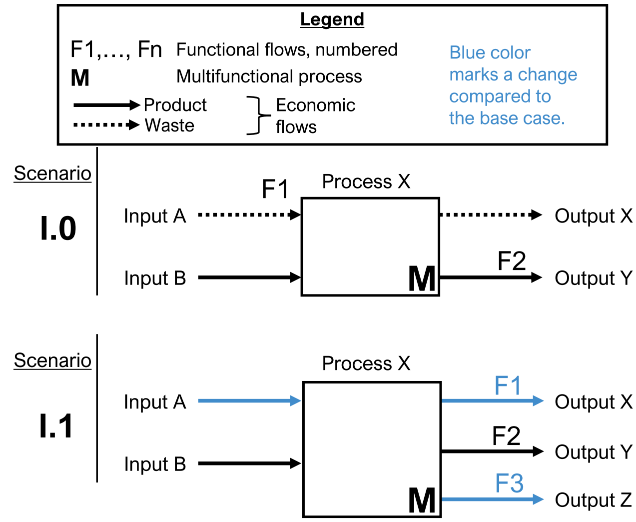

Fig. 3 Illustrative example of a base-case (I.0) and a future scenario (I.1). In **Step 1** product flows are marked with solid arrows and waste flows with dashed arrows; In **Step 2** functional flows are marked with capital F plus an ascending number; In **Step 3** multifunctional processes are marked with a bold capital M. Blue color marks a change in flow type and number of functional flows compared to the base-case

2.4 Step 4: The handling of identified multifunctional processes

Step 4 addresses the additional challenges in handling multifunctional processes in pLCA by adapting three SIMPL approach steps for future scenario development (A, B, C).

Initially, the practitioner needs to choose at least one procedure to handle multifunctionality (e.g., physical allocation). It is recommended to select several alternative procedures to analyze the influence of this choice (uncertainty due to choices) on the pLCA results (ISO, 2006). Then, for each procedure, key factors influencing relevant inventory parameters for handling multifunctional processes are identified (Step 4.A). Next, future assumptions are developed for these parameters (Step 4.B). Finally, these assumptions are systematically combined into consistent future scenarios for each chosen procedure to consider the epistemic uncertainties (Step 4.C).

Step 4.A: Identify key factors that influence the relevant inventory parameters for handling multifunctionality.

Step 4.A establishes the foundation for effectively addressing the additional epistemic uncertainty in handling multifunctional processes in pLCA. In this step, key factors influencing the relevant inventory parameters—specifically, the substitution ratio, the substituted product, and the allocation factor—are identified. Guidelines structure the identification process and ensure consideration of all critical aspects.

In the following, guidance is provided separately for each handling procedure: system expansion (Step 4.A.i), substitution (Step 4.A.ii), physical allocation (Step 4.A.iii), and economic allocation (Step 4.A.iv).

Step 4.Ai: Handling multifunctionality by system expansion.

System expansion requires redefining the study's goal and system boundaries to include all functions of the process within the goal and functional unit (Guinée et al., 2021; Schaubroeck et al., 2022).

Consequently, in a non-comparative study, this procedure is independent of time-varying parameters regarding multifunctionality handling, since only the functions of the studied system are analyzed, and no reference systems are included. In this case, the epistemic uncertainty remains similar in conventional LCA and pLCA, rendering additional challenges in pLCA minor. However, this only applies to the challenges related to handling multifunctionality in a non-comparative study, not to uncertainties in general. Nonetheless, it is recommended to verify that the goal and scope align with future scenarios.

In contrast, in a comparative study, system expansion can be used to make two systems comparable by expanding at least one of the systems to include an additional process (ISO, 2012). For example, comparing combined heat and power generation with a gas turbine (functional unit: heat and power generation) may involve adding a heat pump process inventory to the gas turbine system. This procedure is mathematically equivalent to substitution, as both incorporate additional process inventories with positive (adding) or negative (subtracting) signs (Heijungs, 2014).

Therefore, when conducting a comparative study, it is recommended to account for variations in the inventory of the additional process, as discussed in detail in the following section.

Step 4.Aii: Handling multifunctionality by substitution.

Several authors (e.g., Brander & Wylie, 2011; Schrijvers et al., 2016; Weidema, 2014) argue that substitution should be avoided in attributional LCA, whereas Provost-Savard and Majeau-Bettez (2024) show that it can be applied coherently in attributional studies under specific conditions. Furthermore, established guidance such as the ILCD Handbook (European Union, 2010) explicitly permit substitution in attributional LCAs. Reflecting this debate, this guidance considers substitution as one of the methods for handling multifunctionality in general, acknowledging its context-dependent suitability.

When applying substitution, a substituted process is virtually included with a negative sign in the product system to model coproduct displacement. For example, assessing power generation (coproduct A) from a process also producing heat (coproduct B), the function of a monofunctional heat production process (substituted product) is virtually added to the system model with a negative sign. This procedure results in a virtually monofunctional process model.

If the functionality of the coproduct and the substituted product is equivalent, then the substitution ratio is equal to 1. However, discrepancies in quality may result in a substitution ratio that deviates from 1 (similarly for comparative system expansion; see Step 4.A.i). Vadenbo et al., (2017) define the substitution ratio according to Eq. (1) as the ratio of the functionality of the coproduct over the functionality of the substituted product. Accordingly, a ratio greater than 1 indicates that less than one unit of the coproduct is required to provide the same function as one unit of the substituted product; a ratio less than 1 indicates that more than one unit of the coproduct is needed; and a ratio of 0 denotes that the coproduct cannot substitute the function of the substituted product at all.

$$\text{substitution ratio} = \frac{\text{functionality of the coproduct}}{\text{functionality of the substitute product}} \tag{1}$$

Therefore, when handling multifunctionality by substitution in pLCA, the future functionality of the coproduct and the substituted product must be considered.

The following guidelines address variability in relevant inventory parameters for substitution by supporting the identification of key factors that influence both the substitution ratio and the substituted product.

4. Ensure genuine substitution and verify that the function is provided by a monofunctional process rather than relying on pre-allocated database data (Heijungs & Guinée, 2007; Pelletier et al., 2014). Consider the influence of demand elasticity and potential rebound effects (Earles & Halog, 2011; Provost-Savard & Majeau-Bettez, 2024; Vadenbo et al., 2017).
5. Account for future variability in the substitution ratio by examining impacts from coproduct quality and input composition changes.
6. For each functional flow, determine whether future quality variations may change the substituted product.
7. Analyze how macroenvironmental changes could lead to alternative applications, thereby changing the substituted product.
8. Incorporate process efficiency changes or changed production technology of the substituted product. The premise software can be useful in this context (Sacchi et al., 2022).

Step 4.Aiii: Handling multifunctionality by physical allocation.

If physical allocation is used, a physical criterion such as the mass or energy content of the functional flows is applied to determine the allocation factors. These factors are used to partition the life cycle inventory of the multifunctional process into the individual functions. In pLCA, it is important to acknowledge that the physical ratio between functional flows may vary over time.

Recommended guidelines include:

9. Evaluate how future **technology setups** could alter physical relationships between functional flows, by collaborating with technology developers and modeling alternative configurations (Cucurachi et al., 2018; van der Giesen et al., 2020).
10. Model changes in physical relationships between functional flows due to **process upscaling**, utilizing learning curves, economies of scale, and alternative input flow compositions (Cucurachi et al., 2018).

Step 4.iv: Handling multifunctionality by economic allocation.

Economic allocation uses the relative revenue of functional flows—determined by physical quantity and unit price—to establish allocation factors that partition the multifunctional process inventory. In pLCA, both physical quantities and prices are susceptible to diverse factors such as political events, economic shifts, technology diffusion, patents, and inflation (Ma et al., 2024). Despite this, many pLCAs apply static revenue ratios (e.g., Georgiades et al., 2023; Liptow et al., 2015; Tuomisto et al., 2022; van der Meide et al., 2022), overlooking dynamic market realities exemplified by divergent copper, gold, and silver price trends in cathode production (Hait et al. (2009); see Figure S1 in Supplementary Informations SI3 and SI6).

Studies addressing revenue variation remain limited: Zuiderveen et al. (2021) used historical price sensitivity analysis, while van den Oever et al. (2023) applied best/worst-case scenarios assuming parallel coproduct price movements with static physical ratios—both approaches oversimplifying complex market dynamics. Identification of factors altering the revenue ratio is therefore recommended.

Guidelines include:

11. Identify relevant price developments and analyze the elasticity of supply and demand for coproducts, using price forecasts for commodities or economic theory to anticipate possible price fluctuations.
12. Consider the possible influence of patents and technology diffusion, as expiration of patents or increased diffusion typically leads to price reductions through heightened competition and lower production costs (Towler & Sinnott, 2013).

Step 4.B: Develop future assumptions regarding relevant inventory parameters for handling multifunctionality.

Quantitative future assumptions shall be developed, defining the potential variation compared to the baseline scenario. Table 1 summarizes all guidelines and influencing factors related to the specific procedures to handle multifunctionality that should be considered.

Additionally, when economic allocation is applied, it is recommended to develop the same future assumptions as for physical allocation and additionally consider different future price developments to calculate the relative revenue ratio between the functional flows. If available, price forecasts for commodities should be used to support the quantification of future assumptions.

Step 4.C: Develop future scenarios addressing epistemic uncertainty in handling multifunctional processes.

This step complements the future scenario development based on SIMPL by adding an uncertainty analysis regarding the choice of different procedures to handle multifunctionality. Future assumptions from Step 4.B expand the scenarios developed in Step 1.C. These scenarios are further developed for each handling procedure selected by the practitioner. Therefore, Step 4.C consistently incorporates future variability in substitution ratios, allocation factors, and substituted processes in the future scenarios.

Consequently, a scenario that addresses the challenges and uncertainties in identifying multifunctional processes is further developed into scenarios that also account for potential changes in the application of the selected handling procedure. The structure of scenario development is exemplified in Fig. 4.

Numerous combinations of future assumptions generate substantial challenges through excessive potential scenarios, which are further compounded by the comparison of multiple handling procedures. Rather than reducing the number of scenarios at the outset, a wider range of scenarios should first be generated and assessed; relevant ones are then selected and refined through iterative specification. Rapid impact assessment of scenario combinations can be supported by tools such as superstructure approach or parametric modelling (Douziech et al., 2023; Steubing & Koning, 2021).

To select a manageable set of meaningful scenarios, suitable cut-off criteria can be applied (e.g., eliminating scenarios with less than a 5% impact variation from baseline or retaining only the three most distinct scenarios). A selection of one to four scenarios per multifunctionality handling procedure is recommended as a practical complexity management strategy (Kosow & Gaßner, 2008; Pesonen et al.,

Table 1 Summary of the core methodology of the proposed guidance structured along the three steps of the SIMPL approach (green columns) which is complemented by the four-step approach from Guinée et al. (2021) as well as respective sub-steps (lines) to identify and handle multifunctional processes in pLCA

		Step A		Step B	Step C
		Identify factors that may alter	Consider	Develop future assumptions to vary the	Develop consistent future scenarios to
Step 1	Guideline 1	Number of functional flows	Process modifications, upscaling, or technological advances	• Number of functional flows • Flow type (i.e., classification as product or waste)	Address epistemic uncertainty in identifying multifunctionality
	Guideline 2	Flow types (i.e., classification as product or waste)	Process under investigation		
	Guideline 3		Macroenvironment		
Step 2 **Step 3**	No specific recommendations			No specific recommendations	No specific recommendations
Step 4 System expansion	No specific recommendations	Goal and scope	Future scenarios In case of a comparative study consider the same guidelines as for substitution	No specific recommendations	Expand the scenarios developed in Step 1.C, addressing epistemic uncertainty in identification and handling multifunctionality
Step 4 Substitution	Guideline 4	Genuine substitution	Demand elasticity and potential rebound effects	• Substituted products • Substitution ratio • Product system of the substituted product	
	Guideline 5	Substitution ratio	Coproduct quality, input composition changes, and upscaling		
	Guideline 6	Substituted product	Quality variations		
	Guideline 7		Macroenvironment		
	Guideline 8	Process efficiency or production technology of the process that provides the substituted product	Shifts in energy supply, efficiency, and technology adoption		
Step 4 Physical allocation	Guideline 9	Physical relationships between functional flows	Technology setups	• Technology setup • Scale of the process.	
	Guideline 10		Process upscaling		
Step 4 Economic allocation	Guideline 11	Economic value	Elasticity of supply and demand	Same as for physical allocation plus • Economic value	
	Guideline 12		Patents and technology diffusion		

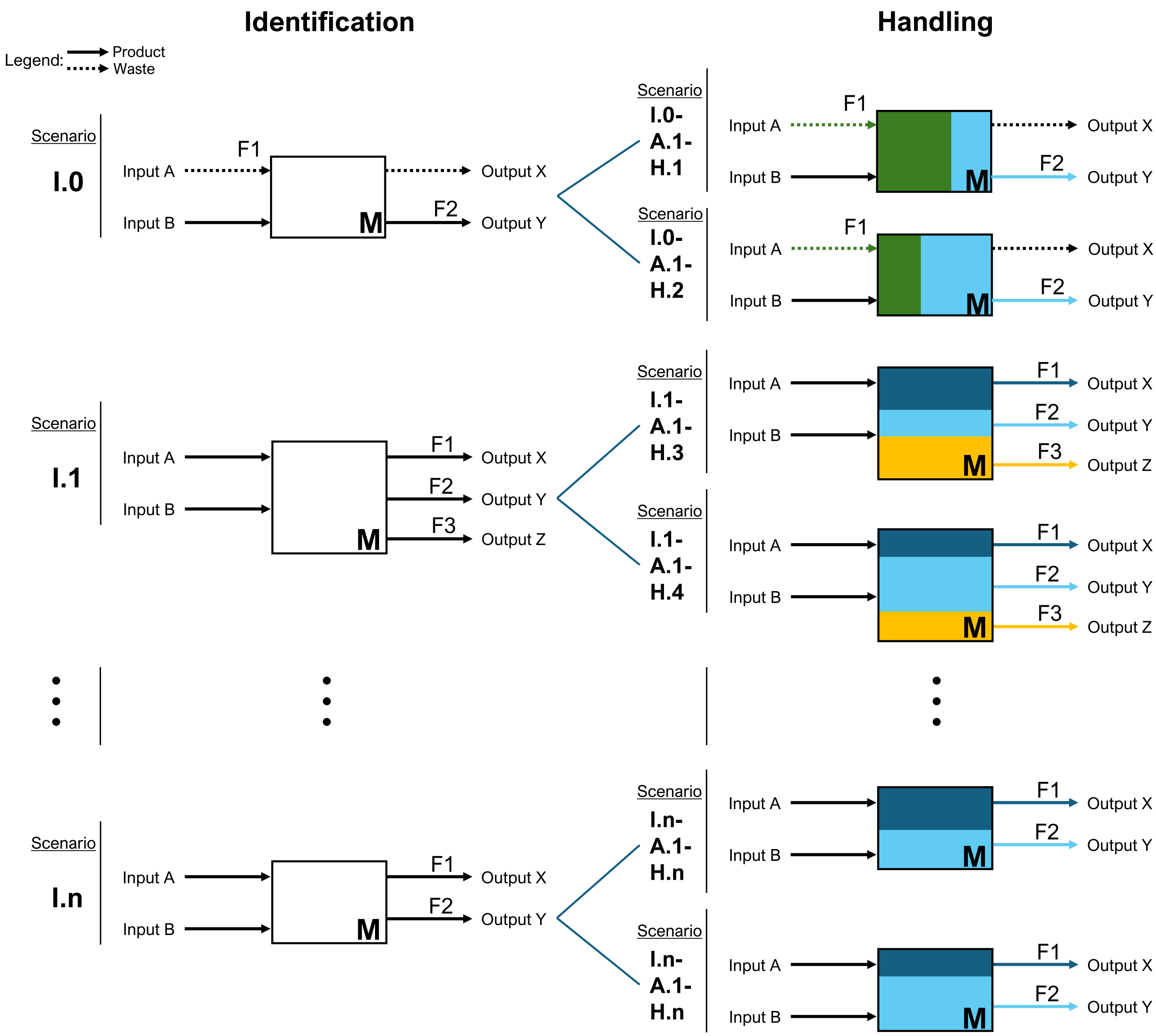

Fig. 4 Illustration of the structure of the scenario development. In Step 1.C, different scenarios are developed that address potential changes over time in the identification of multifunctional processes (scenarios I.0, I.1, …, I.n). In Step 4, multifunctionality is handled for example, with allocation (A.1). In addition, the scenarios from Step 1.C are extended in Step 4.C to consider the potential changes over time when applying the chosen procedure to handle multifunctional processes (H.1, H.2, …, H.n). The coloring of the processes is intended to represent the allocation factors for the functional flows by the size of the area, depending on the scenarios developed. Dashed arrows represent waste flows, and solid arrows product flows

2000). These heuristics improve operationality but do not remove the need for expert judgement, and scenario selection therefore remains partly subjective and intuitive (Kosow & Gaßner, 2008).

Using the SIMPL approach, this yields a small set of scenarios with consistent storylines that integrate multifunctionality alongside other aspects, prioritizing distinctness in multifunctional characteristics, handling procedures, and LCA results.

A summary of the core methodological aspects of the proposed guidance can be found in Table 1.

3 Case study of incinerator bottom slag valorization

In Germany, incinerator bottom ash (IBA), also called incinerator bottom slag, is primarily used in landfill construction (ITAD, 2024). However, that slag contains minerals and metals that cannot yet be economically recovered. To recover valuable minerals and metals as high-quality secondary raw materials, a novel slag valorization process was developed in a research project.

3.1 Innovative treatment of waste incineration slag as a multifunctional process

The valorization process's key step is the selective milling of slag, as detailed by Adhiwiguna et al. (2024), facilitating efficient component separation. Following milling and magnetic separation, eddy current and density separation yield three fractions—minerals, iron, and non-ferrous metals (Adhiwiguna et al. (2025); see Fig. 1). The minerals can substitute natural resources in cement production, reducing CO_2 emissions as the pre-calcinated CaO substitutes $CaCO_3$. Recovering metals such as copper, gold, and silver provides additional potential economic benefits.

Since the overall process has only been studied discontinuously at laboratory-scale, potential scaling effects must be considered in the pLCA. As industrial-scale operation is unlikely before 2030, this year is selected as the reference. The system boundary is cradle-to-grave, and the functional unit is defined as *1 megagram (Mg, i.e., 1 metric ton) of treated slag*. The impact assessment category climate change (characterization factor: GWP100) is analyzed in this simplified case study. The Activity Browser model and all data are provided in Supplementary Informations SI7 (Zacharopoulos 2025) and SI2.

3.2 Scenario development for pLCA

A scenario workshop was conducted to apply the guidance from Sect. 2 to develop future process scenarios. Participants included one representative from the waste incineration industry, two from the slag processing industry, two from plant engineering, and two from the cement industry. Participants represent a cross-section of the German IBA market, suggesting low sensitivity to alternative industry actors. Divergent interests were resolved by adopting the slag processing industry's perspective for best/worst-case modeling. The workshop placed particular emphasis on addressing epistemic uncertainties related to the identification and handling of multifunctionality during scenario development. The following section presents the guidance application and selected results.

Step 1 (Identification of each flow type): Three waste flows and nine product flows are identified (see Table 2).

Step 1.A (Identify key factors): key factors influencing both the type and the number of flows are identified. For example, "Minerals for cement" (currently classified as waste due to German construction regulations) may become a product via improved metal separation or regulatory changes allowing its use as cement raw meal. "Iron 20% Fe" classification depends on quality: landfilling (waste) versus copper production use (product), given comparable copper concentrations to ore (see Table 2).

Step 1.B (Future Assumptions): It is assumed that the "Minerals for cement" flow will change from waste to product and will be used as raw meal for cement production in all future scenarios. For the "Iron 20% Fe" flow, best-case (utilization as copper ore) and worst-case (processing as waste) assumptions were developed. All future assumptions are summarized in Table 2.

Step 1.C (Future Scenarios): The future assumptions are combined into a future best-case and a future worst-case scenario. As a result, two consistent and distinct scenarios regarding the future flow types and numbers are developed.

Steps 2 and 3 (Functional Flows & Multifunctional Processes): The base-case scenario has six functional flows; both future scenarios have seven. All scenarios thus contain multifunctional processes.

Step 4.A and 4. B (identification of key factors and future assumptions): In the scenario workshop, key factors that influence the relevant parameters for handling multifunctional processes and the derived future assumptions were discussed. A summary of the important results of Step 4.A and Step 4.B is given in Table 3.

Step 4.C (Future Scenarios): The scenario development process combined best-case and worst-case assumptions for consistency and distinctness, with all data detailed in the SI. In the workshop, three process scenarios were developed:

Base-case 2023: Average values for the year 2023 represent typical operational parameters of the project. The process uses natural gas for heat supply, with a specific energy consumption of 19.947 GJ/h.

Best-case 2030: Efficient IBA combustion and storage yields high CaO content and low residual moisture, reducing natural gas consumption in the mill to 16.234 GJ/h.

Worst-case 2030: Inefficient IBA treatment lowers CaO content and increases residual moisture, raising natural gas consumption to 23.829 GJ/h.

Subsequently, these scenarios were expanded with specific assumptions for identifying and handling multifunctionality.

For **substitution**, the best- and worst-case scenarios from Step 1.C were combined with the respective assumptions from Step 4.B, resulting in "Substitution: Base-case 2023," "Substitution: Worst-case 2030," and "Substitution: Best-case 2030." Likewise, for **physical allocation**, the worst-case and best-case mass balance (see Table 3) was combined with the respective scenarios from Step 1.C, yielding the same three scenario variants.

Table 2 Summary of Step 1 and Step 2, including sub-steps, applied to the case study on novel slag valorization

		Step 1	Step 1.A	Step 1.B	Step 1.C		Step 2		
Flow name	Econ. value per FU [€]	Flow type	Key factors influencing the flow type and flow number	Future assumptions	Future scenarios		Functional flows		
		Base-case 2023			Best-case 2030	Worst-case 2030	Base-case 2023	Best-case 2030	Worst-case 2030
Inputs									
Slag	−25	w	G.3 Increasing demand through processing	Waste in the future	w	w	F1	F1	F1
Electricity	3	p			p	p			
Heat	7	p			p	p			
Conveyor belt	> 0	p			p	p			
Industrial machine	> 0	p			p	p			
Outputs									
Minerals for cement	−10	w	G.2 Improved separation of undesired metals q.3 future regulatory changes	Minerals will be used as a raw material in the future	p	p		F7	F7
Minerals for concrete	0	p	G.2 Quality and quantity of precious metals on an industrial scale	Product in the future	p	p	F2	F2	F2
Metals, aluminum	0	p	G.2 The quality and quantity of the flow on an industrial scale	Product in the future	p	p	F3	F3	F3
Metals, copper	12	p			p	p	F4	F4	F4
Iron 40% Fe	0	p			p	p	F5	F5	F5
Iron 20% Fe	−3	w	G.2 The quality and quantity of iron on an industrial scale G.1 If this flow could be used as a product, it would coincide with the flow “Iron for copper ore”	Best-case: no waste flow; Worst-case: remains waste	–	w			
Iron for copper ore	0	p			p	p	F6	F6	F6

G.1 to G.3 denote respective guidelines. w: waste, p: product, F1 to F7: functional flows (numbered per base-case 2023). The economic (Econ.) value represents the costs and revenues per functional unit (FU). Revenues are calculated based on the prices of coproducts. Both future scenarios include one additional functional flow. The iron fraction consists of the flows “iron 40% Fe,” “iron 20% Fe,” and “iron for copper ore;” the metals consist of “metals, aluminum” and “metals, copper;” the mineral fraction is further divided into “minerals for cement” and “minerals for concrete” (for a simplified illustration of the treatment process Figure S2 in Supplementary Information SI3)

Table 3 Summary of identified key factors and varying parameters in Step 4.A; and developed future assumptions in Step 4.B

Handling procedure	Key factor	Varying parameter	Flow	Future assumption
	Step 4.A		Step 4.B	
System expansion	No factors considered	–	–	–
Substitution	- Input composition of slag - scale effects	Substitution ratio of all product flows	All flows except "Metals, copper."	Best-case: substitution ratio 100%; worst-case: 20%
	output product quality	- Additional recovery of platinum/palladium from "Metals, copper." - Substitution of copper ore or iron ore by "Iron for copper ore."	"Metals, copper" "Iron for copper ore"	Best-case: substitution ratio 85%, including recovery of platinum and palladium; worst-case: 20% Best-case: substitutes copper ore; worst-case: substitutes iron ore
			All flows except "Metals, copper."	Best-case: substitution ratio 100%; worst-case: 20%
Mass allocation	Scale of the model	Lab-scale and industrial-scale mass balances differing in the iron separation rate	All flows	Lab-scale mass balance = worst-case; industrial-scale mass balance = best-case Detailed mass balance is listed in the SI
Economic allocation	Economic context and market conditions	The economic value of input slag, "Metals, copper," and "Minerals for cement" flows	Waste flows	Worst-case: economic value €15/Mg; best-case: €100/Mg
			"Metals, copper"	Future prices of precious metals based on public forecasts, defining best and worst-cases
			"Minerals for cement"	Value greater than zero only in the best-case, linked to avoided CO_2 emission certificate costs

Detailed documentation of Step 4 application can be found in Supplementary Information SI2. Resulting foreground scenarios difference files are available in Supplementary Information SI4

For **economic allocation**, mixed scenarios were developed to address the uncertainty of different price trends, resulting in three scenarios: "Economic Allocation: Basecase 2023," "Economic Allocation: Mix 1 2030" (Input low/Output high value), and "Economic Allocation: Mix 2 2030" (Input high/Output low value).

Furthermore, three **future background scenarios for 2030** were developed using the tool premise, version 2.2.9 (Sacchi et al., 2022) based on ecoinvent 3.10, cut-off (ecoinvent Association [dataset], 2023), and REMIND (Baumstark et al., 2021; Wernet et al., 2016):

- "Best-case 2030": human well-being is based on sustainable practices and renewable energies; global warming is limited to 1.5 °C and reaches 1.2 °C by 2100.
- "No Policy 2030": current socio-economic trends continue, and no additional climate policies are implemented; the steady increase in global warming, reaching 2.6 °C in 2100.
- "Worst-case 2030": economic growth is based on fossil fuels and natural resources; global warming increases at the same rate as in the past and reaches 4.8 °C by 2100.

In total, 10 foreground scenarios (system expansion: 1; substitution: 3; physical allocation: 3; economic allocation: 3) were each combined with the three background scenarios, resulting in 30 scenarios overall. These were modeled and evaluated using the superstructure approach (Steubing & Koning, 2021) within the Activity Browser (Steubing et al., 2020).

3.3 Results

Figure 5 presents the best- and worst-case scenario combinations for foreground and background scenarios across different procedures to handle multifunctionality and reveals substantial variation in global warming impact (GWI; kg CO_2-eq per Mg slag).

Within a single foreground scenario, the variation due to different background datasets is at most 12 kg CO_2-eq/Mg slag. In comparison, the difference between different foreground scenarios applying the same multifunctionality procedure within the same background scenario shows greater variation: 109 kg CO_2-eq for substitution and 30 kg CO_2-eq for economic allocation. Furthermore, the selection of the foreground scenario in substitution can even reverse the results, shifting from negative GWI to net CO_2-eq emissions (see substitution best-case 2030).

This demonstrates that methodological assumptions related to allocation and substitution can have a greater

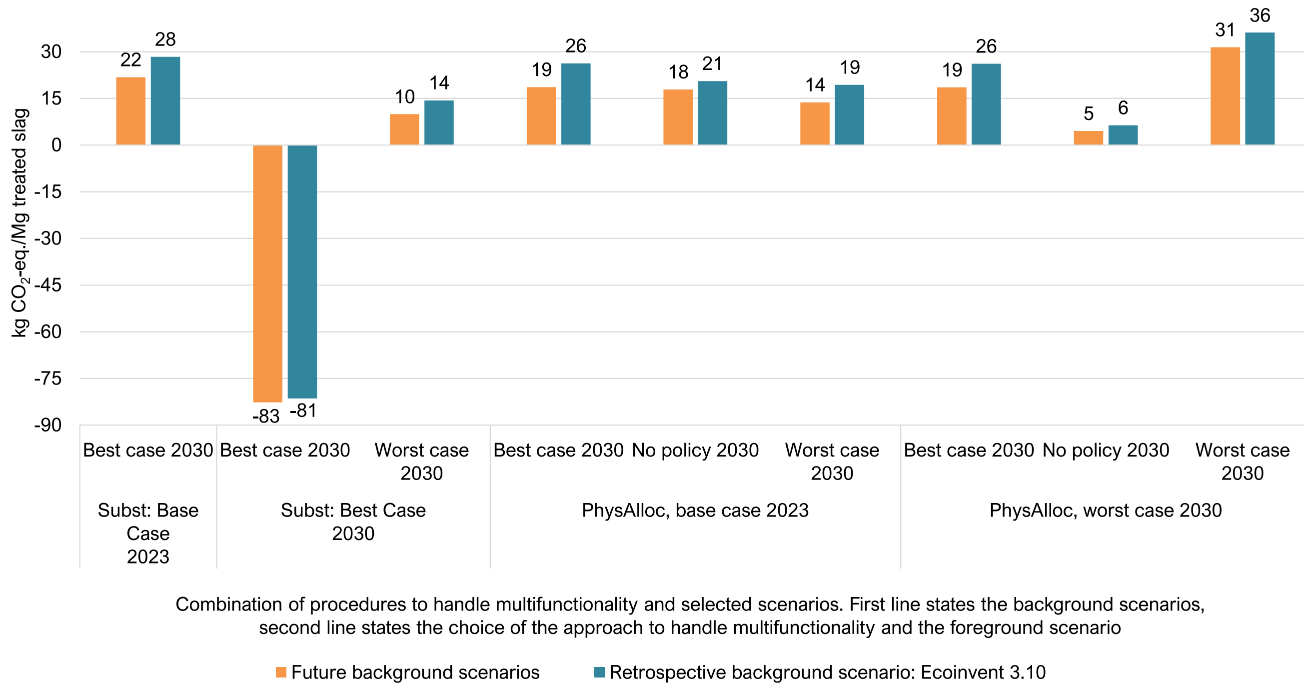

Fig. 5 Comparison of greenhouse gas emissions (kg CO_2-eq/Mg treated slag) across different procedures to handle multifunctionality and best- and worst-Case foreground and background scenario combinations. Various procedures to handle multifunctionality with different underlying rationales are shown. Direct comparisons between different procedures should not be made. The first bar (orange) shows the result considering a future background scenario based on ecoinvent, generated with premise; the second bar (blue) shows the result obtained using the unmodified ecoinvent 3.10 version. Please note that the selected procedure to handle multifunctionality is only considered in the foreground scenarios; the background scenarios are all based on the ecoinvent's cut-off system model. Substitution: Subst., Physical Allocation: PhysicAlloc., Economic Allocation: EconAlloc. Detailed results for all procedures and scenario combinations are available in Supplementary Information SI5

impact on outcomes than the choice of background scenarios. Therefore, transparent examination and reporting of future assumptions related to the method for handling multifunctionality in pLCAs is critical.

4 Discussion

The proposed stepwise guidance offers a transparent, adaptable approach for identifying and handling multifunctionality within pLCA. By integrating multifunctionality considerations directly into the scenario-generation process—rather than treating them as distinct scenario categories—the guidance enhances the SIMPL method by emphasizing variability in parameters relevant for identifying and handling multifunctional processes.

Its applicability is demonstrated through the case study on slag valorization, where the systematic use of the proposed guidelines ensures explicit consideration of future technological, regulatory, and market changes that influence inventory parameters. The study reveals distinct uncertainties tied to each multifunctionality handling procedure: System expansion exhibits lower sensitivity to future variability in inventory parameters but may require careful adjustments to system boundaries. In contrast, substitution is highly sensitive to the selection of substituted products and substitution ratios, which can fluctuate due to technological progress, shifts in coproduct quality, or changes in background systems. Physical allocation is influenced by evolving physical relationships between coproducts, which may change through upscaling, optimization, or input flow variations. In addition to evolving physical relationships between functional flows, economic allocation depends strongly on fluctuating prices, where static price assumptions may misrepresent volatility in commodity markets and thus the revenue ratio between the functional flows.

The results indicate that outcomes are less sensitive to the choice of background scenarios than to the handling of multifunctionality. However, as this finding is derived from a single case study, it should not be generalized. Sensitivity patterns likely vary with the system's characteristics and the temporal scope. Therefore, each pLCA should explicitly evaluate the sensitivity of the results of both the selection of an integrated assessment model (IAM) and associated background scenarios.

The effective application of the guidance depends on technology experts' participation, particularly for defining key factors and formulating plausible future assumptions. This could be a critical aspect if time or the availability of relevant stakeholders are limited. However, practitioners can scale the intensity of stakeholder interaction (Langkau et al., 2023) and model explorative scenarios themselves in case of low participation. Another limitation of the results is that the procedure to handle multifunctionality currently remains unaltered across all background scenarios.

Next, it is important to recognize that the subjective selection of an IAM can substantially influence the development of prospective background data (Bortoli et al., 2025). It is argued that IAMs often rely on optimistic assumptions about rapid technological advances such as large-scale carbon removal technologies, which are highly debated due to various risks, including rebound effects, and uncertain sequestration durability, focusing on economic growth (Bortoli et al., 2025). Therefore, Bortoli et al. (2025) advocate for more diverse IAM selection encompassing economic degrowth trajectories and demand-side solutions, such as energy reduction, when modelling prospective background data.

In the case study, no cut-off criteria were applied to illustrate the full range of possible scenario combinations; in applied pLCAs, however, such criteria are essential to ensure feasibility. To manage complexity, it is recommended to select one to maximal four scenarios for each chosen handling procedure (Kosow & Gaßner, 2008; Pesonen et al., 2000). However, numerous scenario combinations and the need for subjective and intuitive selections remain a practical limitation of the guidance, potentially complicating both the interpretation and communication of results.

Altogether, these limitations can materially influence pLCA outcomes and, consequently, any recommendations derived from them, particularly when different procedures for handling multifunctionality yield diverging results. While this guidance does not prescribe context-specific allocation methods, it supports decision-making by clarifying when such choices are most consequential. Conceptually, systems with strong market interactions, high substitution effects, or rapid changes in the background system (e.g., deep electrification or circular economy approaches) are more sensitive to the choice of handling procedures than systems with stable technologies and well-defined product functions. For these highly dynamic and interaction-intensive systems, recommending a single method is not advisable; instead, results should be interpreted as a range that reflects plausible future system configurations.

5 Conclusion

The proposed stepwise guidance supports the systematic identification and handling of multifunctional processes when generating future scenarios to account for epistemic uncertainties in pLCA. By integrating the four-step approach of Guinée et al. (2021) into the SIMPL framework, the guidance fills an identified research gap (see Fig. 2 and Table 1). It systematically considers uncertainties arising from both the choice of a procedure to handle multifunctionality and future variability in inventory parameters such as flow types, the number of functional flows, substituted products, substitution ratios, and allocation factors.

Application to the case study on innovative slag valorization demonstrates that future assumptions regarding these parameters can substantially influence pLCA results. This underscores the critical need for transparent documentation of future assumptions and methodological choices in pLCA, to support decision-making in technology development and policy measures.

The guidance can also be applied to pLCAs of large transformations, such as the electrification of energy-intensive systems (e.g., steam crackers). In these dynamic and intertwined systems, the framework ensures that functions such as process heat, currently used mainly for internal energy recovery, are consistently treated as potentially marketable functional flows. However, applications to large transformations introduce additional uncertainty, as background system evolution (e.g., electricity mixes or shifts to biobased feedstocks) is strongly scenario-dependent. Consequently, results become more sensitive to the choice of IAM and its underlying assumptions, requiring careful interpretation and transparent communication of choices and uncertainties.

While these comprehensive guidelines improve the reproducibility and comparability of a pLCA involving multifunctional processes, they remain constrained by a lack of harmonized, context-specific standards for pLCAs. This is particularly evident regarding the integration of IAM scenarios and the handling of multifunctionality.

Overall, systematically addressing epistemic uncertainties through this stepwise guidance supports more reliable decision-making. However, pLCA results involving multiple future scenarios are often complex and difficult to interpret. Future work should therefore focus on improving the visualization and presentation of complex results across multiple scenarios and environmental impact categories. This will facilitate clear and transparent communication with decision-makers, who are often not LCA experts.

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Data availability The data that supports the findings of this study are available in the Supplementary Information of this article. The model, as implemented in the LCA software, is openly available as Supplementary Information SI7 in zenodo at https://doi.org/10.5281/zenodo.17083914. The background data are available from ecoinvent. Restrictions apply to the availability of these data, which were used under license for this study.

Declarations

Conflict of interest The authors declare no competing interests.

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