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METHODS, TOOLS, DATA, AND SOFTWARE

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A practice-based framework for defining functional units in comparative life cycle assessments of materials

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Abstract

In comparative life cycle assessment (LCA) studies of materials, there is a mismatch between the current practice and existing guidelines regarding functional unit definition. The purpose of this study is to develop a practice-based framework for defining functional units in comparative LCAs of materials and provide guidance regarding in which situations different functional unit types are relevant. A literature review of comparative LCAs of materials identified three types of functional units: (i) the reference flow functional unit, (ii) the property functional unit, and (iii) the performance functional unit. These functional unit types, of which only the latter strictly complies with LCA guidelines, represent varying degrees of functional equivalence and technological maturity. The most relevant functional unit type depends on the goal of the study. We suggest that screening assessments of whether materials have comparable environmental impacts can apply reference flow functional units. Material comparisons for certain application areas with some important properties can apply property functional units. For comparisons of end products, performance functional units can be applied. However, even in such cases, complete functional equivalence can hardly be achieved due to more or less relevant product differences. The applicability of the framework is demonstrated for the case of comparing cemented carbide and polycrystalline diamond hard materials.

KEYWORDS

cemented carbide, functional unit, industrial ecology, life cycle assessment (LCA), polycrystalline diamond, prospective life cycle assessment (LCA)

1 | INTRODUCTION

The use of materials in various technologies constitutes a foundation for the current way of life in contemporary societies (Graedel et al., 2015). Materials with properties such as strength, hardness, conductivity, resistance, insulation, and permeability have enabled numerous applications. At the same time, the use of materials causes large environmental and resource impacts. Choosing materials that perform better from these perspectives is crucial for a transition to a more sustainable society.

Life cycle assessment (LCA), the most well-developed tool for environmental assessment of products[1] (Finnveden et al., 2009; Ness et al., 2007), is commonly applied to assess environmental and resource impacts as well as to identify potential trade-offs between different environmental impacts (Baumann & Tillman, 2004). An important part of the goal and scope definition of an LCA is to define a functional unit, which is a measure of the performance of the functional outputs of a product system (ISO, 2006) and constitutes the basis for product comparisons. At the same time, several studies have highlighted challenges in defining the functional unit. These challenges include (i) functions difficult to quantify (Cooper, 2003; Reap et al., 2008), such as the aesthetics of meals; (ii) to adequately represent a product with several functions (Cooper, 2003; Reap et al., 2008), such as computers; and (iii) emerging technologies with partly unknown future functions (Hetherington et al., 2014; Moni et al., 2020; Thonemann et al., 2020), such as nanomaterials.

Some responses to these challenges include having a clear goal definition and defining multiple functional units focusing on different functions (Collado-Ruiz & Ostad-Ahmad-Ghorabi, 2010; Cooper, 2003; Hetherington et al., 2014; Moni et al., 2020; Thonemann et al., 2020). There also exist several international standards and LCA guidelines that provide guidance on the definition of the functional unit. The ISO (2006) standard provides a general definition of the functional unit concept, but does not provide guidance on how the functional unit should be constructed in practice for specific products. Several LCA guidelines emphasize end-use function(s) (Curran, 2012; European Commission, 2010; Guinée, 2002; Hauschild et al., 2018; Jolliet et al., 2016; Weidema et al., 2004). Typically, these guidelines prescribe that the functional unit should consider obligatory properties, that is, features that an end product must have in order to be perceived as a product by the user, but also so-called positioning properties, such as price and comfort. In addition, the importance of functional equivalence in comparative LCAs is commonly highlighted since the lack of equal functions might render comparisons unreasonable and unfair (Curran, 2012; Guinée, 2002; Hauschild et al., 2018; Jolliet et al., 2016; Weidema et al., 2004). Functional equivalence is sometimes even stated as a requirement for comparative LCAs (European Commission, 2010). The possibility to reach complete functional equivalence is seldom questioned, although some guidelines acknowledge that this might be difficult to achieve in some cases (Curran, 2012; Jolliet et al., 2016).

When it comes to comparing materials using LCA, it can be quite challenging to define functional units. Since the materials compared generally have at least partly different properties, different performances and/or bring additional functions, it is hardly possible to have complete functional equivalence. Consequently, if the requirement of complete functional equivalence was to be followed strictly, it would make it difficult to conduct comparative LCAs of materials at all. The identification of the end-use function(s) of a product, for example, in terms of obligatory and positioning properties as emphasized in LCA guidelines, might not always be possible due to the unknown future applications of novel materials.

Thus, international standards and other LCA guidelines, as well as the scientific literature on LCA methodology, opt for an approach to functional unit definition that might not always be feasible in comparative LCAs of materials. Concrete recommendations on how to define and construct functional units, or what functional unit to apply in different situations, such as in early comparisons of novel materials, are typically not provided. Furthermore, the difficulty of establishing complete functional equivalence in comparative LCAs of materials is rarely acknowledged, but functional equivalence is rather considered a prerequisite for such studies.

To address this situation, the purpose of this study is to develop a practice-based framework for defining functional units in comparative LCAs of materials and provide guidance regarding in which situations different functional unit types are relevant. A literature review is conducted to investigate how functional units are defined and constructed in practice for the purpose of material comparisons (Section 2). The review constitutes the foundation for the practice-based framework, which contains three approaches to functional unit definition (Section 3). The case of comparing cemented carbide (WC-Co) and polycrystalline diamond (PCD) hard materials is then applied to illustrate the applicability of the framework (Section 4). The article ends with a concluding discussion where some aspects of the practice-based framework are discussed in more detail (Section 5).

2 | LITERATURE REVIEW

The literature on the practice of functional unit definition in comparative LCAs of materials was reviewed by applying the search string TITLE-ABS-KEY((“life cycle assessment*” OR “LCA*”) AND (“material substitut*” OR “material compar*” OR “material replace*”)) in the Scopus database (2020-05-11), resulting in 92 studies. Only comparative LCAs of materials[2] with the functional unit(s) clearly stated were included in the literature review. Based on this, 29 relevant studies were identified. Considering the difficulty of covering all relevant studies using search terms, 11 additional highly relevant studies about nanomaterials, nanocomposites, and insulation materials were also included in the literature review (Bi et al., 2018; Hervy et al., 2015; Hicks & Theis, 2017; Khanna & Bakshi, 2009; Kim & Fthenakis, 2012; Kono et al., 2016;Lloyd & Lave, 2003; Pourzahedi et al., 2017; Roes et al., 2007; Upadhyayula et al., 2017; Wu et al., 2020). In total 40 studies are summarized in Table 1 and described in Sections 2.1–2.3, where they are grouped based on the approach used for the functional unit construction and assessed in terms of their compliance with LCA guidelines. The 40 studies are also presented with more details in the Supporting Information.

[1] Note that materials are also products, that is, product flows.

[2] For example, comparative LCAs of different waste treatment systems or different processes for producing the same material were excluded. Also, comparisons of materials used for energy generation, rather than as materials, were not included in this review (e.g., fossil vs. biomass energy).

TABLE 1 Summary of the studies included in the literature review, showing the materials compared, functional unit(s) applied and the approaches to functional unit construction

Study	Materials compared	Functional unit(s)
Studies applying simple functional unit construction		
Bi et al. (2018)	Silver-enabled and conventional polymeric material	97 g polymeric material
García-Gusano et al. (2015)	Cements with various shares of other materials	1 ton cement
Hicks and Theis (2017)	Silver-enabled fabric and conventional fabric	145 g fabric
Hossain et al. (2016)	Natural and recycled aggregates	1 ton material
Kim and Fthenakis (2012)	Several nanomaterials and some conventional materials	1 kg material
Li et al. (2019)	Conventional wooden material and a novel wooden composite material	100 kg material
Ott and Ebert (2018)	Timber construction components of varying composition	1 m^2 of construction area of the component
Rossi (2014)	Stainless steels of various chemical compositions	1 kg stainless steel flat coil or quarto plate product
Valderrama et al. (2013)	Clinkers with various shares of alternative material	1 kg clinker
Wang et al. (2019)	Four cathode materials	1 kg material
Bribián et al. (2011)	Bricks and tiles, insulation materials, cement and concrete, wood and other common building materials	1 kg material
Zimele et al. (2019)	Foam concrete, aerated concrete blocks, and hollow ceramic blocks	1 m^3 material
Studies constructing the functional unit based on material properties		
D'Errico and Ranza (2015)	Magnesium, carbon-fiber-reinforced polymer and steel	1 floor pan component with certain strength, size and geometry
Fitch and Cooper (2005)	Metallic components, plastic components	786 vehicle components of equal mechanical properties
Geyer (2008)	Mild steel, advanced high strength steel and aluminum	Vehicle components with equal mechanical properties
Grant et al. (2014)	Building envelope combinations of aluminum, brick or wood walls and green, thermoplastic or ballast built-up roofs	1 building envelope with certain insulation
Hervy et al. (2015)	Nanocellulose-reinforced polymer composites, glass-fiber-reinforced polypropylene and polylactide	The equivalent mass of material with equal tensile stiffness
Khanna and Bakshi (2009)	Carbon nanofiber polymer composites and steel	(i) 1 plate component with equal stiffness (ii) Automotive body panels with equal stiffness
Kono et al. (2016)	Cellulose fiber, fiberboard, foam glass, stone wool, and polyurethane	The equivalent mass of material with equal thermal properties
Kua (2015)	Sand and sand with a certain share of steel slag	The equivalent mass of material with equal volume
Kua (2013)	Sand and sand with a certain share of copper slag	The equivalent mass of material with equal volume
Lloyd and Lave (2003)	Nanocomposites, steel and aluminum	Vehicle body panels with equal stiffness
Palazzo and Geyer (2019)	Steel and aluminum	All light vehicles produced in North America between 2012 and 2050 with equal material properties
Pittau et al. (2019a)	Bio-based and synthetic insulation materials	1 m^2 of wall with an equivalent insulation thickness with equal thermal transmittance

(Continues)

TABLE 1 (Continued)

Study	Materials compared	Functional unit(s)
Poulikidou et al. (2015)	Fiber-reinforced polymer composites, aluminum, and steel	1 truck roof with equal stiffness under geometrical constraints
Pourzahedi et al. (2017)	Carbon nanotube-enabled composites and conventional aluminum sheets and composites	1 satellite shield with certain shielding effectiveness
Pushkar (2019)	Natural perlite, coal bottom ash and fly-ash-based aggregates	1 m^2 of roof with equal thermal transmittance
Roes et al. (2007)	(i) Polypropylene nanocomposite and polypropylene, (ii) polypropylene nanocomposite and polyethylene, and (iii) polypropylene nanocomposite and glass-fiber-reinforced polypropylene	(i) Equal amount of packaging film needed for 1000 bags of candies with equal mechanical properties (ii) Equal amount of agricultural film with equal mechanical and barrier properties needed to cover a greenhouse (iii) Car body panels with equal mechanical properties
Studies constructing the functional unit based on performance		
Kayo and Noda (2018)	(i) wood and cement, (ii) wood and concrete, (iii) wood and asphalt, (iv) wood and steel, and (v) wood and concrete	(i) 1 m^2 piling area with piles stored permanently in the ground (ii) 1 dam with infinite lifetime (iii) 1 m^2 walkway paving area with 10 year lifetime (iv) 1 m roadside earth embedded guardrail with 10 year service life (v) 1 m noise barrier with 30 years lifetime
Maywald and Riesser (2016)	Glass and so-called ETFE foil membrane	1 m^2 of transparent roof with a lifetime of 30 years
Pasetto et al. (2017)	Pavements with various shares of the industrial by-product steel slag	1000 m motorway with a service life of 20 years
Pittau et al. (2019b)	Timber and reinforced concrete with masonry	1 m^2 of heated floor area of an existing residential building with a specified design
Scott and Cullen (2016)	Molybdenum, graphene, and graphite	Back contacts necessary for 1 GW of photovoltaic energy capacity
Stripple et al. (2008)	Three plastic materials	1-year treatment of a patient with catheters
Upadhyayula et al. (2017)	Graphene-reinforced poly(ether imide) coating and conventional hot-dipped galvanized zinc coating	Corrosion resistance for a steel surface during its 60-year life
van der Harst et al. (2014)	Polystyrene, bioplastic, and a composite material	1 disposable beverage cup fit for serving 180 ml hot drinks by vending machines
Wang et al. (2017)	Lithium-rich cathode material and a cathode material containing cobalt	1 lithium-ion battery providing 16 kWh of energy in one discharge and a specified total driving distance over the battery's lifetime
Wigger et al. (2017)	Hard chromium and nano-tungsten-carbide-cobalt (nano-WC-Co)	1 substrate with a coated area of 1 m^2 with a thickness of 300 μm and a specified service life
Studies applying several approaches to functional unit construction		
Amarakoon et al. (2018)	Cadmium sulfate and zinc sulfate	(i) Simple construction: 1 kg input material (ii) Construction based on performance: lifetime output in kWh of 1 m^2 of copper indium gallium (di)selenide photovoltaic cell
Wu et al. (2020)	Carbon nanotube-supported polyethylenimine and conventional monoethanolamine	(i) Simple construction: 1 kg material (ii) Construction based on performance: mass of material required to adsorb 1 kg CO_2

Note that some functional units have been shortened for clarity and are therefore not identical to the wordings in the studies.

2.1 | Studies applying simple functional unit construction

In 14 of the studies (Table 1), the approach used for functional unit construction is simply to compare materials based on a certain amount of material, setting the functional unit equal to the selected LCA reference flow, often 1 kg. These studies commonly apply a cradle-to-gate system boundary. Several studies compare novel materials with conventional ones, for example, novel versus conventional cathode materials for lithium-ion batteries

(Wang et al., 2019) and novel nanomaterials versus conventional materials like aluminum (Kim & Fthenakis, 2012). Also, the studies often compare various construction materials, see, for example, Ott and Ebert (2018). Material properties generally vary between the compared materials in these studies, such as between stainless steels with different mechanical strengths (Rossi, 2014). However, such variations in properties are not considered in the functional unit definitions, which consequently do not reflect the function(s) of the materials. Simple constructions of functional units based on reference flows are thus not strictly compliant with ISO (2006) or with LCA guidelines. For example, Curran (2012) stated that a simple functional unit definition in terms of physical output can be used when the goal of a study is to develop an environmental profile for a single product, but not in comparative LCAs. However, the 14 studies applying simple functional unit construction do conduct material comparisons. Thus, there is a clear mismatch between LCA guidelines and practice in these studies.

Most of the 14 studies use simple functional unit constructions for screening assessments involving novel materials. Although not considering the functions of the materials, the results from such early assessments can still inform decision-makers and manufacturers about the relative environmental impacts of materials. For example, Kim and Fthenakis (2012) concluded that nanomaterials, while being generally more energy intensive than conventional materials, could still be environmentally beneficial if added in smaller quantities that improve product performance considerably. Thus, a simple functional unit can reveal the performance increase needed for novel materials to be environmentally preferable over some conventional materials. However, Kim and Fthenakis (2012) also exemplify a less suitable application of this functional unit construction approach when they also compared materials with completely different envisioned and realized applications, such as carbon nanotubes (mainly used in electronics and composites) with titanium dioxide nanoparticles (mainly used in sunscreen). Such comparisons become much like comparing apples and oranges. While some studies, like the one by Kim and Fthenakis (2012), acknowledge the limitations of their results and/or comment on their usefulness, other studies compare materials with varying properties but do not problematize this fact nor provide guidance on the context within which the results can be applied. For example, Wang et al. (2019) provided a ranking of cathode materials with different electrochemical properties in terms of environmental impacts, but did not provide guidance on how to interpret these results in light of the difference in properties. This is problematic since the lack of such guidance can have implications on the further use of the results.

2.2 | Studies constructing the functional unit based on properties

In 16 of the studies (Table 1), the functional unit is constructed based on material properties relevant for a certain application. In some studies of building materials, the functional unit in terms of mass or thickness of the materials compared was varied to account for the materials' thermal properties, see, for example, Kono et al. (2016), Pittau et al. (2019a), and Pushkar (2019). Kono et al. (2016) defined the functional unit (*f.u.*) as the mass in kg of an insulation material required for certain thermal properties:

$$f.u = \lambda \rho R A \tag{1}$$

with λ being the thermal conductivity [W/mK], ρ the density [kg/m^3], R the thermal resistance [m^{2}K/W], and A a certain surface area [m^2].

Several other studies compared conventional and lightweight materials in vehicles by considering material properties such as mechanical strength. Commonly, these studies apply Ashby's material indices (often abbreviated MI) to ensure equivalent mechanical properties of the compared materials, see, for example, Fitch and Cooper (2005), Khanna and Bakshi (2009), and Palazzo and Geyer (2019). These indices provide a general approach for comparing material components based on certain strength and/or stiffness constraints (Ashby, 2011; Ashby & Jones, 1980). For example, in the case of comparing panels under equal stiffness (Khanna & Bakshi, 2009), the index is defined as:

$$\mathrm{MI} = \frac{E^{1/3}}{\rho} \tag{2}$$

where E is Young's modulus [GPa], a measure of stiffness. Ashby's material indices can thus be applied to calculate the required thickness of the materials given a strength and/or stiffness constraint. In addition, geometrical constraints are sometimes considered (Poulikidou et al., 2015).

Studies applying a functional unit construction based on material properties do not consider the function of materials in specific end products and are thus not strictly compliant with LCA guidelines either. Studies applying this approach thus further demonstrate a mismatch between LCA guidelines and practice. However, the reviewed literature suggests that insights for decision-makers can still be obtained from such studies. For example, Roes et al. (2007) investigated whether a novel polyprolylene nanocomposite had environmental advantages over conventional plastics. Specific results could not be obtained due to the unknown performance of the composite in specific end-use products, but potential material reductions based on the relative strength of the composite could be estimated (approximately −9% for packaging films, −37% for agricultural films, and −1% for automotive panels). Although more specific studies would be required to confirm the results for specific products, they indicate a potential of the novel composite to reduce environmental impacts when it replaces polymers with less favorable material properties.

TABLE 2 Practice-based framework for defining the functional unit in comparative life cycle assessments (LCAs) of materials

	Reference flow functional unit	Property functional unit	Performance functional unit
Description	Represents a certain amount of material	Represents the main relevant properties of the material for a certain application area	Represents the performance of the material in a specific end product
Typical goal	Generic comparison of environmental impacts of materials, e.g., for ecodesign purposes	Comparison of environmental impacts of materials based on relevant properties for an application area	Comparison of the environmental impacts of materials in specific end products
Typical example	1 kg material	1 kg material with certain properties	1 end product with a certain performance
Procedure for functional unit construction	Equal to the LCA reference flow	Relevant properties are combined in some way, e.g., Ashby's material indices	Performance data is estimated from, e.g., experiments
Data requirement[a]	Low: might require material composition data	Medium: requires quantitative data about the material's main relevant properties	High: requires quantitative data about the end product's performance

[a]Data requirement should here be interpreted from a fundamental perspective, not necessarily from an LCA analyst's perspective; end product performance data might be easily available to the LCA analyst in some cases, but might still have taken years to obtain through multiple experiments.

With this approach, it becomes important to describe transparently how the functional unit is constructed based on the material properties, such as in Equation (1). Several of the reviewed studies do not provide equally transparent descriptions. For example, Palazzo and Geyer (2019) conducted a comparative LCA of materials for vehicle components to assess the benefits of a lightweight solution. They considered so-called material replacement coefficients, in turn based on physical material properties and design constraints (e.g., geometric and economic). Unfortunately, exactly how the material replacement coefficients were derived was not transparently described.

2.3 | Studies constructing the functional unit based on performance

A third approach to functional unit construction, applied in 12 of the reviewed LCA studies (Table 1), is based on product performance in clearly specified end-use applications. These studies often compare well-developed products for which much data were available. For example, van der Harst et al. (2014) applied the functional unit of one disposable beverage cup fit for serving 180 ml hot drinks by vending machines when comparing polystyrene, bioplastic, and composite cup materials. Another study by Pasetto et al. (2017) applied the functional unit of 1000 m motorway with a service life of 20 years in a comparison of pavements with various shares of the industrial by-product steel slag.

This type of functional unit construction based on performance is the only type that considers the end-use function(s) of the compared materials and thus the only type that is strictly compliant with LCA guidelines (Curran, 2012; European Commission, 2010; Guinée, 2002; Hauschild et al., 2018; Jolliet et al., 2016;Weidema et al., 2004). In many cases, this type of functional unit definition is appropriate and straightforward. These studies can, in line with their study goals, inform decisions related to what materials are environmentally preferable to use for the specific end products assessed. However, challenges can appear when considering novel materials with partly unknown performance. For example, Scott and Cullen (2016) compared novel carbon back contact materials to the current molybdenum-based device. The functional unit was the back contacts necessary for delivering 1 GW of photovoltaic energy capacity at United States Army installations. Several unverified assumptions, such as similar conversion efficiencies of the devices, had to be made due to lack of data on carbon back contact performance.

3 | PRACTICE-BASED FRAMEWORK

The literature review in Section 2 shows a mismatch between guidelines and practice: three different approaches to functional unit definition exist in the literature, while existing guidelines only endorse one of these approaches. To address this mismatch, a practice-based framework for defining the functional unit in comparative LCAs of materials was developed. The framework is presented in Table 2 and includes the three different functional unit types identified in LCA practice: (i) the reference flow functional unit, (ii) the property functional unit, and (iii) the performance functional unit. These three functional unit types, of which only the latter is strictly compliant with LCA guidelines, correspond to the three approaches for constructing the functional unit identified in Sections 2.1–2.3, respectively. These approaches furthermore typically represent varying degrees of functional equivalence, as illustrated in Figure 1.

The reference flow functional unit is often applied in cradle-to-gate comparisons of materials and represents a certain amount of material. Comparative LCA studies applying the reference flow functional unit type often have a low degree of functional equivalence, since they commonly

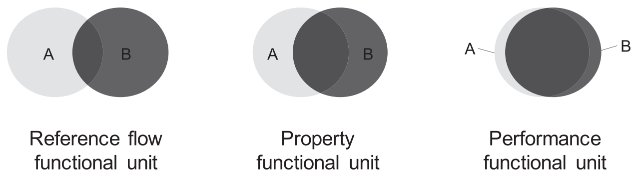

FIGURE 1 Schematic illustration of the varying degree of functional equivalence of the three different functional unit types for two hypothetical materials compared (A and B). The degree of functional equivalence between the compared materials or products increases from left to right, while complete functional equivalence is never achieved

compare materials with notably different properties and performances in specific end products, see, for example, Bribián et al. (2011), Kim and Fthenakis (2012), and Rossi (2014). Although this functional unit type strictly does not comply with the LCA guidelines, we suggest that it can still be useful if the goal is to conduct rough material comparisons, for example, involving novel materials. Results from studies applying this functional unit type reveal the impacts of the materials' production, which might serve as rough indications of the materials' impacts in different applications. However, the materials compared need to at least be envisioned for similar application areas. Rough per-kg impacts then tell which materials have high and low impacts, and such rules of thumb can support ecodesigners with at least some information before complete LCAs of specific end products can be conducted. Ecodesign is a proactive approach often applied in early product development (Pigosso et al., 2015; Tischner & Charter, 2001), when potential applications of a material are uncertain. For example, showing that novel materials have high per-kg impacts tells ecodesigners that the novel materials need to be added in smaller quantities and/or improve the performance of final products considerably to be environmentally preferable to conventional materials.

The property functional unit is sometimes also applied in studies comparing relatively novel materials with some promising properties to conventional materials. Ashby's material index (Equation 2) can be considered an archetype for the construction of property functional units. Although there is some variation in the property functional unit construction among the studies reviewed (Section 2.2), they all attempt to compare materials without considering specific end-use products, while still considering some important material properties relevant for a certain application area. For example, in the application area of electronics, properties like conductivity and resistance are generally important. Results from studies applying this functional unit type can be interpreted as the impacts of providing a certain material property, which might also serve as rough indications of the materials' impacts in different applications requiring that property. The property functional unit is more data intensive than the reference flow functional unit, since it also requires information about the material properties considered. Such information can be known early in the development of novel materials, thus enabling the use of this approach even though information about the performance of specific end products containing the material might be lacking. The functional equivalence in these types of comparisons is higher than for studies applying the reference flow functional unit. However, it is lower than in studies applying the performance functional unit because general material properties, and not specific performance requirements in a specified end product, are considered. Although this functional unit type strictly does not comply with the LCA guidelines either, we suggest it is still useful given the goal of comparing materials for certain application areas requiring certain properties.

The performance functional unit represents the performance of a specific end product. It is more data intensive than the reference flow and property functional unit types, since it requires detailed performance data for the end product. For example, a property functional unit for a conductive material might be based on the property of conductivity, for example, 1 conductivity-weighted kg. A performance functional unit for the same conductive material used in a specific cable might be to provide a certain device with electricity over a certain time. Comparisons applying the performance functional unit have a high degree of functional equivalence and are compliant with the LCA guidelines. Results from studies applying this functional unit type can be interpreted as the impacts of the materials in the specific end products investigated, which is useful given the goal to compare materials used in specific end products. However, the performance functional unit type is typically difficult to apply at an early stage of novel material development when future applications of a material are uncertain or even unknown. An example of this would be the nanomaterial graphene, for which there is a lot of ongoing research due the material's interesting properties, but still potential applications are sparsely commercialized (Reiss et al., 2019).

4 | THE CASE OF CEMENTED CARBIDE VERSUS POLYCRYSTALLINE DIAMOND

Hard materials have several important properties, including hardness, toughness, compressive strength, and wear resistance, which affect their function in specific end products. The conventional hard material WC-Co is currently the most important tool material in the manufacturing industry (Fang et al., 2014). However, there is a trend toward an increased use of superhard materials in cutting tools, such as PCD (Bobzin, 2017), which thus competes with WC-Co in applications where high hardness is important (Konstanty, 2005). The case of comparing WC-Co and PCD hard materials is used here to illustrate the applicability of the practice-based framework for defining functional units in comparative LCAs of materials (Table 2). The impact category climate change is used for the illustration.

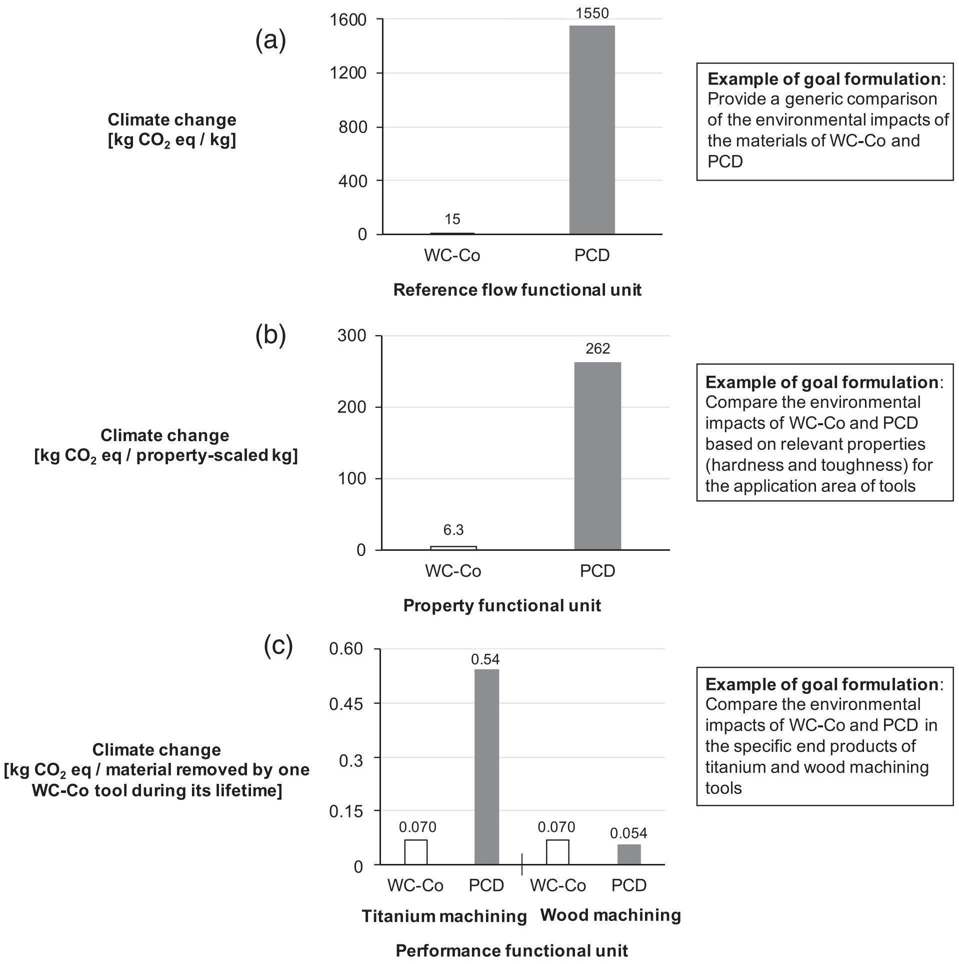

FIGURE 2 Climate change results [kg CO_2 eq/functional unit] for the comparison of cemented carbide (WC-Co) and polycrystalline diamond (PCD) with different functional unit types: (a) the reference flow functional unit of 1 kg WC-Co versus 1 kg PCD, (b) the property functional unit of 0.43 property-scaled kg WC-Co versus 0.17 property-scaled kg PCD, and (c) the performance functional unit, comparing 4.7 g WC-Co to 0.35 and 0.035 g PCD based on the materials' performance as tools for titanium and wood machining, respectively. Data from Table S2 in the Supporting Information

In some cases, data availability is low and the performance of specific end products, or even important application-specific properties of materials, are unknown. In such a screening study of WC-Co and PCD, with the goal to provide a generic comparison of the environmental impacts of these materials, it would be relevant to apply a reference flow functional unit (Table 2). Importantly, a reference flow functional unit can be relevant in this case since the compared materials have a common application area. The functional unit was defined here as the selected reference flow of 1 kg material. While the data requirements are low in these types of comparisons, knowledge about the material compositions might still be required. For this case study, previously derived cradle-to-gate results for WC-Co and PCD production were used in this comparison (Furberg et al., 2019, 2020). Specifically, the "current scenario" from Furberg et al. (2020) was applied so that the following material constituents were used; WC-Co (8 weight-% cobalt) was compared to PCD (6 weight-% cobalt) situated on a WC-Co (13 weight-% cobalt) substrate. The results from the reference flow comparison are provided in Figure 2a.

In other cases, relevant material properties might be known for a certain application area, while the performance of the materials in specific end products are still unknown. In the case of hard materials, the properties of hardness, that is, the resistance to intender penetration, and toughness, that is, the ability of a material to absorb energy before fracture, are particularly important for cutting tools (Prakash, 2014). Some representative values for hardness and toughness of WC-Co and PCD are shown in Table 3. In a study with the goal to compare the environmental impacts of WC-Co and PCD based on relevant properties for a certain application area, such as tools, we suggest that it is relevant to apply a property functional unit (Table 2).

A property functional unit should be constructed to consider the differences in important properties between the materials assessed. In the case of hard materials, established quantitative relationships between the relevant material properties of hardness and toughness could not be identified. Ashby's material indices (Section 2.2) are not relevant for this application area since the tensile strength or stiffness does not reflect

TABLE 3 Property values for the hardness and toughness of cemented carbide (WC-Co) and polycrystalline diamond (PCD) (Prakash, 2014)

Property [unit]	WC-Co	PCD
Hardness (Vickers hardness) [HV]	1350	8000
Toughness (transverse rupture strength) [N/mm^2]	2000	850

the hardness of materials. Instead, the property functional unit was constructed by scaling the reference flow functional unit with the two relevant material properties of hardness and toughness, applying the data in Table 3:

$$f.u_{WC-Co} = f \cdot \left[\frac{P_{H,WC-Co}}{\min(P_H)}\right]^{-1} \cdot \left[\frac{P_{T,WC-Co}}{\min(P_T)}\right]^{-1} \quad (3)$$

$$f.u._{PCD} = f \cdot \left[\frac{P_{H,\,PCD}}{\min(P_H)}\right]^{-1} \cdot \left[\frac{P_{T,\,PCD}}{\min(P_T)}\right]^{-1} \quad (4)$$

where $f.u._{WC-Co}$ [property-scaled kg] is the property functional unit for WC-Co, $f.u._{PCD}$ [property-scaled kg] is the property functional unit for PCD, f [kg] is the 1 kg reference flow applied for both materials, which then becomes scaled by Vicker's hardness (P_H [HV]), and toughness (specifically transverse rupture strength, P_T [N/mm^2]). The parameters min(P_H) and min(P_T) are the minimum Vicker's hardness [HV] and toughness [N/mm^2], respectively, of the compared materials. Equations (3) and (4) thus imply that the 1 kg reference flow (f) for the WC-Co and PCD materials is scaled based on how the two properties compare with those of the other material included in the comparison. For example, if a material is six times harder, which is almost the case for PCD compared to WC-Co, then less material is needed, and a 1 kg reference flow of the material is reduced to 1/6 = 0.17 property-scaled kg. However, if the considered material's properties do not exceed the properties of the material it is compared with, then the 1 kg reference flow remains, since the ratio becomes 1. The calculations resulted in 0.43 property-scaled kg WC-Co and 0.17 property-scaled kg PCD. Climate change results from applying the property functional unit are provided in Figure 2b.

In other cases, specific end products for the considered materials exist and performance data are available. In a study with the goal to compare WC-Co and PCD in specific end products, such as titanium and wood machining tools for which the required performance data are available, a performance functional unit would be relevant (Table 2). To be able to construct this functional unit, extensive knowledge about the end product's performance is required since the performance varies depending on the material properties but also between tool types, such as between a tool for machining of the softer wood and one for the machining of the harder titanium in this case. There are furthermore a number of additional parameters that affect the performance of tools, for example, the cutting speed and the number of cutting edges. In this case study, performance data on the removal of titanium and wood, respectively, by one WC-Co tool during its lifetime were used for the construction of the functional unit. In order to remove as much titanium and wood as one WC-Co tool, 0.1 and 0.01 PCD tools, respectively, are required in order to fulfill the same function (Furberg et al., 2020). That is, when the WC-Co tool wears out, the PCD tool can do another 9 and 99 jobs in titanium and wood machining, respectively. Climate change results for the performance functional unit are presented in Figure 2c.

The results in Figure 2 show that the outcome of the comparison changes considerably depending on the functional unit type applied. In the screening comparison with the reference flow functional unit, WC-Co has the by far lowest climate change impact. This result provides the information to, for example, product developers that the performance of PCD in products must be much higher than that of WC-Co for a substitution to be environmentally preferable. The comparison using the property functional unit shows that thanks to the PCD's much higher hardness, the difference between PCD and WC-Co in terms of environmental impacts become notably smaller with this property functional unit than with the reference flow functional unit, although WC-Co still receives the lowest climate change impacts. This result shows that PCD is probably only environmentally preferable in specific end products where high hardness is of great importance for the performance. WC-Co also has the lowest impact when used as tool for titanium removal, but in the application of wood machining, PCD is the material with lowest impact. These results can inform, for example, tool manufacturers and tool users about which material is environmentally preferable in these specific end products. The comparisons applying the reference flow and property functional units thus indicate that the performance of PCD need to be much higher than that of WC-Co in order for PCD to be environmentally preferable and Figure 2c provides an example of such a specific end-product case (i.e., wood machining tool).

5 | CONCLUDING DISCUSSION

Rather than rejecting many studies because they are not strictly compliant with LCA guidelines, we argue that all three functional unit types can be relevant and provide important insights depending on the goal of the study. Possible further developments of the framework (Table 2) include whether there exist subcategories that can be distinguished within the different functional unit types and which goals such subcategories then fulfil. Aspects not addressed in the developed framework are challenges related to dynamic aspects in the functional unit definition, such as rebound effects, including changes in consumer behavior and growing markets (Kim et al., 2017). Such aspects could potentially be considered together with the framework suggested here, presumably mainly in the performance functional unit type, since an assessment of consumer behavior probably requires a well-defined end product.

5.1 | Addressing challenges in functional unit definition

The developed framework can be used to address the challenges related to functional unit definition as identified in the literature (Section 1). For the definition of multiple functional units, which has been suggested as a useful strategy in some cases, the framework provides suggestions of different types of functional units that might be relevant. Regarding the challenge of defining functional units for functions difficult to quantify, it can be addressed by applying a reference flow functional unit in a screening comparison or a property functional unit that accounts for the properties possible to quantify. However, such a comparison is then conducted with the acceptance of a lower degree of functional equivalence. The challenge of defining functional units that adequately represent several functions can be addressed by applying a property functional unit as it offers the possibility to consider several material properties at the same time. The challenge of defining functional units when the function is not yet comprehensively understood, such as for novel materials, can be addressed by applying the reference flow and property functional units with less demand on data availability. In particular, the developed framework contributes to the suggestion in the literature of clarifying the goal of the study (Cooper, 2003; Hetherington et al., 2014; Thonemann et al., 2020) as it distinguishes between different types of functional units and the typical corresponding goals (Table 2). The suggestion in the literature to define multiple functional units when necessary is also in line with the developed framework: multiple functional units can be defined for one of the identified functional unit types, or several functional unit types can be applied. An example of the definition of multiple functional unit types among the reviewed studies can be found in Amarakoon et al. (2018).

The developed framework can furthermore help clarifying functional unit characteristics to LCA practitioners. There are cases when it is unclear what the functional unit represents in the reviewed literature. For example, Carvallo et al. (2013) applied estimates of the relative amount of lightweight materials required to replace the conventional steel material in vehicles based on their own experiences. Such estimations are difficult for a reader to scrutinize. Another study applied weight reduction potentials, in turn based on estimates and assumptions provided by automotive and materials industry experts, in their comparison of vehicle materials (Kelly et al., 2015). What lies behind such estimates, that is, whether they were based on material properties or performance data, is unclear. In fact, few of the reviewed studies studies comment on functional equivalence or discuss functional unit definition to any detail. Applying the functional unit types provided in the developed framework can aid in making the functional unit, and what it represents in terms of underlying data, clearer.

5.2 | Functional equivalence versus application specificity and data requirement

The requirement of comparative LCAs to have a common point of reference, the functional unit, is inherently based on a reduction of an inevitable multifunctionality of products, including materials, to one single quantifiable unit representing the entire functionality. The modeling of this functionality by the construction of a functional unit will always be associated with a certain degree of simplification. For example, a car's multifunctionality is sometimes reduced into the functional unit of person-kilometers, which is a simplification considering that other aspects, such as comfort and safety, might also be considered important by car users. While complete functional equivalence of compared materials can hardly be achieved due to more or less relevant material differences, attempts could be made to achieve functional equivalence by other means, such as by system expansion. In such an approach, a third material, covering for the difference in function between two materials, could be introduced (Fantke & Ernstoff, 2018). The environmental impacts of the third material are then added to the least performing material. However, we have found no example of such a system expansion approach in the literature review of current practices. In addition, it would probably often be difficult to know which material is best suited to cover for inadequacies as well as exactly how much of such a material would be needed. If a system expansion approach were to be applied, a degree of simplification in the functional unit construction would thus still likely be present.

While the functional equivalence typically increases when going from the reference flow functional unit, over the property functional unit, to the performance functional unit, the higher functional equivalence often comes at a cost in terms of increased data requirement. Knowledge about important properties of materials and their specific performance in products can be challenging to acquire, especially if some of the materials are, or contain, emerging technologies (Hetherington et al., 2014; Moni et al., 2020; Thonemann et al., 2020). This is related to the so-called Collingridge dilemma, stating that at an early point in a technology's development, data is scarce but the possibility to alter the technology is high (Collingridge, 1980). As the technology matures, a lot becomes known but the possibility to make alterations is decreasing, due to an increased lock-in from larger investments in knowledge and capital of the technology. For emerging technologies, such as novel materials under development, it might therefore be more motivated to loosen the requirement of stricter functional equivalence and allow for the definition of property and even reference flow functional units. In prospective LCAs (Arvidsson et al., 2018), the definition of the reference flow and property functional units might therefore be extra frequent, since there is typically a considerable data scarcity in these types of studies, and application areas or end products might not yet have been developed.

In addition to high data requirement, performance functional units also make studies more specific, which is a benefit if the goal is to assess some specific end product. However, studies based on product performance functional units may not provide any generic environmental guidance, such as which materials generally have high or low environmental impacts, which can be useful rules of thumb for decision-making and ecodesign. For example, more generic guidance could aid decisions on whether to fund research and innovation related to the development of a material intended for some broad application area, such as the use of carbon nanotubes in electronics. The increased application specificity of performance functional units can thus sometimes also constitute a cost in terms of a lower potential to provide relevant environmental guidance for some decision situations.

In conclusion, we hope the provided practice-based framework will allow for more conscious definitions of functional units in future comparative LCAs of materials, in line with the respective goals of such studies.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

The data that supports the findings of this study are available in the supporting information of this article.

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