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METHODS ARTICLE

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Substitution modeling can coherently be used in attributional life cycle assessments

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Abstract

Most life cycle assessment (LCA) studies use the attributional methodology. This approach attributes a share of global environmental impacts to one or multiple functions provided by a normatively circumscribed system. Multifunctional systems that are not technologically subdivisible between co-functions are frequently encountered in LCA studies. It then becomes necessary to resort to co-production modeling techniques, like the substitution approach. The use of substitution modeling in attributional LCA (ALCA) is, however, discouraged amongst practitioners, due to the alleged violation of central requirements of the attributional methodology. The objective of this research is to shed light on common misconceptions about the compatibility of substitution with ALCA. The first misconception is that the use of substitution in ALCA violates the conservation of total environmental impacts. We find that this idea arises from a confusion regarding the attribution of impacts to the secondary product(s). The second misconception stipulates that substitution is not coherent with the state-descriptive characteristic of ALCA. We conclude that we can describe a given system *as resulting* from an inferred (substitution) change, rather than *as disrupted* by this change. Finally, we discuss the choice of the substituted technology, and argue there is a logic to marginal substitution in ALCA. We therefore recommend accepting substitution modeling in ALCA.

KEYWORDS
attributional, co-production, industrial ecology, life cycle assessment, multifunctionality, substitution

1 | INTRODUCTION

1.1 | Perspectives on LCA questions and on multifunctionality

Life cycle assessments (LCAs) investigate the link between the provision of functions by the economy (typically through the consumption of goods, products, or services) and environmental impacts. By studying networks of economic activities, the LCA community predominantly asks two types of questions and therefore developed two distinct methodologies: questions as to the consequences of a decision, with the consequential LCAs

(CLCAs), and questions of attribution of burden, with the attributional LCAs (ALCA) (Schaubroeck et al., 2021). An ALCA aims to impute a share of anthropogenic environmental impacts to one or multiple functions provided by a system through the modeling of all the resource extractions and the emissions in the functions' value chains (Ekvall & Weidema, 2004; UNEP/SETAC, 2011). This approach essentially asks an *accounting* question, striving to associate each function with an environmental footprint, such that the sum of the footprints of all final consumptions[1] would theoretically add up to total anthropogenic impacts (Tillman, 2000; UNEP/SETAC, 2011). According to Bamber et al. (2019), based on the review of 2687 LCA studies published between 2014 and 2018, the majority follows an attributional approach (94%). The present study focuses on ALCA and on the compatibility of modeling choices with its methodological requirements.

The economy presents many multifunctional processes, or co-productions. Co-productions typically pose a problem when the goal of the study is to model the environmental impacts of one of the co-products without the other(s). The following allocation hierarchy is provided in the International Organization for Standardization (ISO) 14044 standard, one of the main methodological references that frame LCA co-production modeling (Hermansson et al., 2020; Moretti et al., 2020), to solve multifunctionality issues, without specifying any distinction for its implementation in attributional and consequential studies (International Organization for Standardization, 2006):

a. Avoiding allocation by
   1. subdivision;
   2. system expansion;
b. Partition following underlying physical relationships;
c. Partition based on other relationships.

If co-products are technologically independent, despite being apparently produced in the same process, it is clearly advantageous to subdivide the multifunctional process into distinct sub-processes with additional data collection to separate the value chains of each co-product without the need for assumptions or modeling (option a1). However, as many co-production processes are not technologically subdivisible, the hierarchy then prioritizes system expansion (option a2). Rather confusingly, two different modeling techniques are considered in the literature as "expanding" the system. On the one hand, the "functional unit expansion" approach, as termed by Schaubroeck et al. (2022), refers to "avoiding the multifunctionality problem by broadening the system boundaries and introducing new processes and several functional units" (Wardenaar et al., 2012), and thus maintaining "all function(s) corresponding to the multiple products involved in the multifunctionality issue" (Heijungs et al., 2021). On the other hand, the "substitution approach" also expands the scope of the system under analysis. This co-production modeling procedure assigns all impacts of the system to the primary (or determining; Weidema, 2000) product, defined as the "co-product that determines the production volume of that process" (Weidema, 2003), minus the impacts avoided through the displacement of primary productions by the secondary (or dependent; Weidema, 2000) product(s) (Heijungs et al., 2021; Schrijvers et al., 2016b). Substitution is not explicitly part of the ISO 14044 hierarchy, but Amendment 2 describes the methodological procedure for system expansion as the integration of "the product system that is substituted by the co-product […] in the product system under study" (International Organization for Standardization, 2020). The amendment also acknowledges the "functional unit expansion" as a form of system expansion: "The concept of expanding the product system to include additional functions related to the co-products can also be referred to as system expansion […]" (International Organization for Standardization, 2020). The equivalence of substitution and functional unit expansion, implied in Amendment 2 of the ISO 14044 standard, was demonstrated by Tillman et al. (1994), who showed that these two approaches give commensurate results in a comparative study (see Section SI-1 of the Supporting Information for a mathematical demonstration). LCA practitioners, long before the publication of Amendment 2, already widely used substitution and functional unit expansion as system expansion approaches, often interchanging nomenclature (Heijungs, 2013; Moretti et al., 2020).

Functional unit expansion is not always practical, as it requires all co-products to be studied together in their co-production ratio, which can compromise the achievement of the initial objectives of the study (see Section SI-2 of the Supporting Information for a demonstration of the resulting aggregation of co-functions). This problem is especially acute when the multifunctionality occurs far upstream of the final consumption under study. For example, a mine co-producing copper and gold can avoid allocation by calculating the LCA of its output of "copper-together-with-gold," but that footprint is of little use as part of an LCA calculating the footprint of an electric car containing the copper without the gold. Substitution avoids the aggregation of the initial functional unit with all the co-functions in the value chain of the final studied product (Heijungs et al., 2021). Another difference between functional unit expansion and substitution pertains to the selection of processes included in standalone systems. The former only includes flows physically linked to the value chains providing the functional units, whereas the latter also incorporates the value chains of the primary production(s) substituted by the secondary product(s) of the multifunctional process(es) in the system (Heijungs et al., 2021; Schaubroeck et al., 2021; Schrijvers et al., 2020) (see Figure 1).

[1] A final consumption is defined "as a product that is directly consumed by humans and not used in the life cycle of another product" (Schaubroeck et al., 2021).

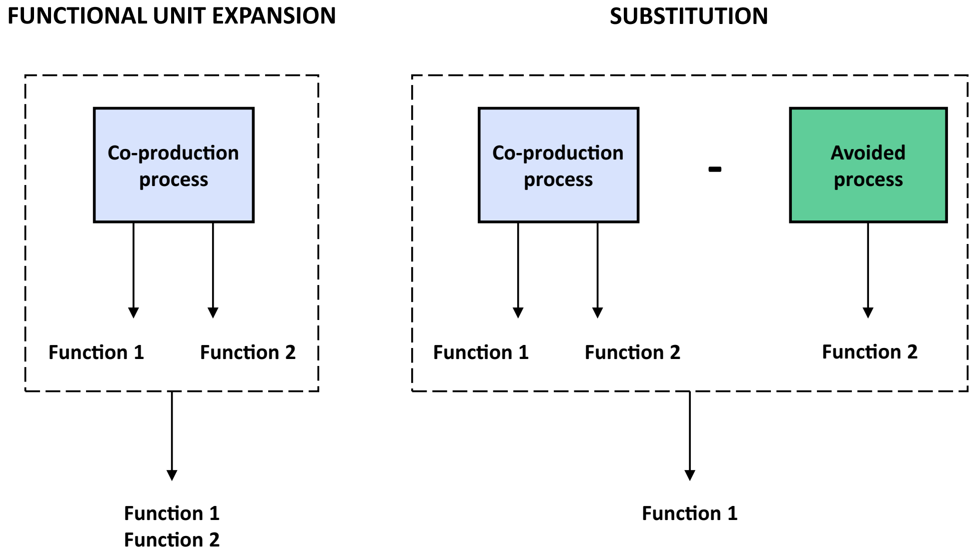

FIGURE 1 Illustration of the differences between the functional unit expansion and the substitution approaches. The investigated process is the co-production process, providing the primary function 1 and the secondary function 2. The avoided process is a monofunctional process providing function 2. The expansion of the functional unit in the functional unit expansion approach leads to a multifunctional unit, providing functions 1 and 2, while the subtraction of the avoided process from the co-production process in the substitution approach leads to a system providing only function 1.

1.2 | Agreement of multifunctional models with the attributional perspective

Functional unit expansion is fully compatible with all the defining requirements of ALCA (Majeau-Bettez et al., 2018; Schrijvers et al., 2016b). After all, the scope of the system under analysis can be defined as narrowly or as expansively as desired while retaining an attributional perspective. One is always free to analyze a bundle of functions rather than a single functional unit.

By contrast, substitution is strongly associated with CLCA (Schrijvers et al., 2016a), and its use in ALCA is controversial (Moretti et al., 2020). A defining characteristic of ALCA is its aforementioned accounting perspective (UNEP/SETAC, 2011). Brander and Wylie (2011) show an instance in which substitution modeling leads to a net loss of impacts relative to the total net emissions of the unallocated system description because of the "inclusion of a credit for environmental burdens that do not occur" (Brander & Wylie, 2011). Based on this counterexample, Majeau-Bettez et al. (2018) conclude that substitution is not compatible with the accounting characteristic of ALCA. This led to a first criterion for the compatibility of multifunctional models with the attributional perspective:

- ***Characteristic A: Additivity criterion***—*"Preserv[ation] of total burdens when model [is] applied to total consumption" (Majeau-Bettez et al., 2018).*

Heijungs and Guinee (2007) also express concerns about speculating as to "what would have happened" scenarios with the substitution method. This reasoning rests on a broadly accepted defining characteristic of ALCA: it describes the state of a system (the "actual physical burdens" [Brander & Wylie, 2011], a "snapshot of the impacts as they are" [Camillis et al., 2013], "the absolute impacts of a product system at/up to a given point in time" or a "static situation" [Pelletier et al., 2014]), not a perturbation to this system. Consequently, Majeau-Bettez et al. (2018) defined a second criterion to assess the methodological compatibility of multifunctional modeling techniques and ALCA:

- ***Characteristic B: State-description criterion***—*"Co-production modeling should not rely on perturbation logic" or "perturb the production balance"*(Majeau-Bettez et al., 2018).

The UNEP/SETAC definition of the attributional approach includes a specification on which processes should be included in the studied systems: "The systems analysed ideally contain processes that are actually directly linked by (physical, energy, and service) flows to the unit process that supplies the functional unit" (UNEP/SETAC, 2011). A third desirable characteristic for co-production modeling in attributional systems was thus defined by Majeau-Bettez et al. (2018):

- ***Characteristic C: Responsibility for impacts within the system follows flows of the different production chains***—*"Co-production modeling should not create links between emissions and activities that are not mediated by product or service flows"* (Majeau-Bettez et al., 2018).

The inclusion of activities that compete with secondary productions within the boundaries of the studied systems seemingly violates this characteristic (Majeau-Bettez et al., 2018). Contrary to the necessity of the two first characteristics, which follows fundamentally from the question of attribution of a *share* (Characteristic A) of a total *observable* (Characteristic B) impact, the necessity of Characteristic C was never demonstrated and seems more a matter of convention in the definition of environmental footprints. We further discuss Characteristic C in Section 5.

Hence, two axiomatic criteria, Characteristics A and B, seem to be transgressed when using substitution modeling in ALCA. For these reasons, studies conclude that the use of substitution should be avoided in attributional studies (Brander & Wylie, 2011; Chenet al., 2010; Schrijvers et al., 2016a, 2020; Weidema, 2014). However, these alleged incompatibilities are often disregarded in practice, as shown by Moretti et al. (2020), who found 31% of the self-declared ALCAs from a text-mining process on 532 multifunctional studies use substitution to solve multifunctionality issues.

1.3 | Objective

There is a major contradiction in guidance on the use of substitution in ALCA. On the one hand, the literature holds that substitution and functional unit expansion demonstrably yield commensurate results and are equivalent. On the other hand, as discussed in Section 1.2, these two methods presumably differ in their respect of ALCA requirements; with functional unit expansion fully compatible with the fundamental characteristics of ALCA, and substitution violating the conservation of total environmental burden (Brander & Wylie, 2011; Majeau-Bettez et al., 2018) and the state-descriptive nature of attributional studies (Brander & Wylie, 2011; Camillis et al., 2013; Heijungs & Guinee, 2007; Majeau-Bettez et al., 2018; Pelletier et al., 2014). Both cannot simultaneously be true: functional unit expansion and substitution cannot be methodologically equivalent *and* differ in their fundamental compatibility with ALCA. The objective of this paper is to shed light on two misconceptions about the compatibility of substitution and ALCA, at the root of this contradiction:

- ***Misconception 1****: The use of substitution in ALCA violates the conservation of environmental impacts.*

We refute Misconception 1 by revisiting the counterexample of Brander and Wylie (2011) in Section 2.

- ***Misconception 2****: Because ALCA describes a system in a given state and substitution describes a change in state (a perturbation, something avoided), the two cannot logically and coherently be mixed.*

Rectifying Misconception 2 and identifying the logical role of substitution in a state-descriptive ALCA in Section 3 will raise the question of *which* type of substitution can contribute coherently to this description. As a corollary to our demonstration in Section 3, we find that:

- ***Corollary 1***: There is a logic to marginal substitution in ALCA.

In Section 4, we thus argue that a marginal substitution fits more logically than a substitution of an average production mix, even though ALCA value chains rightly rely on average mixes for all other parts of their system description.

1.4 | Disclaimer and limitations to the scope of this study

Before analyzing Misconceptions 1 and 2, it is necessary to clarify which issues are *not* addressed by this research, considering that co-production modeling in LCA, and particularly the use of substitution in ALCA, are controversial topics.

1. This research does not aim to prove or disprove the usefulness of ALCA, or to compare its relevance with other approaches such as the consequential perspective.
2. This research aims to determine whether substitution modeling can be *compatible or not* with an ALCA. It does not aim to rank the conceptual or methodological relevance of substitution among other co-production modeling approaches that are known to be compatible with ALCA, such as partition.
3. The substitution co-production modeling approach is still under methodological development, and some important challenges need to be addressed to improve its operationalization. Some of the most important challenges are the identification of the substituted technological mix (Finnveden et al., 2009; Mathiesen et al., 2009; Saraiva et al., 2018; Weidema, 2000) and the quantification of the substitution potential according to functionality and market/price indirect and rebound effects (Vadenbo et al., 2017). This research does not aim to address these challenges, which require separate and elaborated reflections carried out jointly with consequential practitioners.

4. A substitution logic is not applicable in every co-production context, regardless of the attributional or consequential perspective. The arguments supported in this paper are only applicable to situations where substitution can logically be used. To say that the consumption of a final product leads to the substitution of a primary production assumes that (1) the volume of production of a co-producing activity responds proportionately to the demand for this final product, and that (2) this volume of production forced onto the market a secondary co-product, and that this co-product has a functional equivalence and is directly competing with the substituted primary product such that this primary production will be proportionally reduced. Therefore, conditions for the applicability of the substitution co-production modeling approach (both in ALCA and CLCA) include:
   4.1 A primary product and the secondary product(s) that are substituting primary production(s) can be unambiguously identified. This condition is explained into more details in Section 2.2.
   4.2 Co-products must be technologically coupled (in a partial-joint or full-joint production, as defined in Majeau-Bettez et al., 2018), that is, they are produced together in a (more or less) fixed ratio.
   4.3 For each secondary production, there must exist a competing primary production whose output is functionally equivalent and that can diminish their production. This is not necessarily the case for so-called “exclusive byproducts” (Majeau-Bettez et al., 2018).

2 | MISCONCEPTION 1: THE USE OF SUBSTITUTION IN ALCA VIOLATES THE CONSERVATION OF ENVIRONMENTAL IMPACTS

2.1 | Importance of the additivity criterion (Characteristic A) in ALCA

Additivity constitutes the essence of the attributional perspective, as this approach aims to evaluate the share of total past, present, and future anthropic emissions that every final product is accountable for (Finnveden et al., 2022; Heijungs, 1997; Sandén & Karlström, 2007). By including extraction and emission flows involved in a product’s value chain (Majeau-Bettez et al., 2018), the ALCA practitioner makes a “normative” (Weidema et al., 2018) allocation and defines an “initial sphere of responsibility” (Brander et al., 2019) for a particular consumption. This allocation of responsibility can be used to promote sustainability by designing policies (Brandão et al., 2014), for example, taxing emitters according to normative emission allocation rules. ALCA must therefore avoid double-counting emissions or leaving emissions unallocated.

2.2 | Incoherence in the attribution of impacts to secondary products

Heijungs (1997) legitimately express concern about a potential erroneous use of substitution modeling: one could apply substitution by treating one co-product as the primary product, and then apply the same substitution modeling but this time treating the other co-product as the primary product. Such a procedure would yield two processes that embed contradictory assumptions and whose sum would not yield the original impacts of the multifunctional process (Heijungs, 1997). The example of a co-generation process co-producing steam and electricity is given: “If we subtract a steam production process when considering pure electricity, and an electricity production process when we considering pure steam, it is unlikely that the sum of these two systems yields the original multiple process” (Heijungs, 1997). However, we would argue that this demonstration does not prove a general incompatibility of substitution with ALCA. It is rather a reminder that a primary product must be unambiguously identifiable for substitution modeling to be internally consistent (Cherubini et al., 2011), as previously argued in disclaimer 4.1, because only secondary products can substitute primary productions. The demand for the primary product determines the size of the multifunctional process’ production, while the secondary products are forced on the market due to their technological coupling with the primary product. Under the assumption of an inelastic demand for secondary products, they substitute primary productions.

The counterexample of Brander and Wylie (2011) constitutes a central argument against the use of substitution in ALCA footprint calculations. This study concludes that substitution, contrary to functional unit expansion and partition, does not conserve the total net emissions of the unallocated co-production of wheat ethanol (primary product) and dried distillers grains (secondary product). Upon closer inspection, we find that an assumption introduced by these authors fully explains this discrepancy: they assume that the secondary product is burden free with substitution modeling. In other words, their results rest on the assumption that the attribution of impacts to the secondary product(s) is “not applicable” as “substitution avoids allocation” (Brander & Wylie, 2011). In fact, this assumption necessarily leads to double-counting the benefits of co-production; a credit is *explicitly* given to the primary product by subtracting the emissions of the substituted process, and a benefit is *implicitly* given to the secondary product by rendering it burden free. Figure 2a illustrates this erroneous application of substitution compared to functional unit expansion and partition.

A parallel can be drawn with co-production modeling in recycling processes. As illustrated in Figure 3a, the recycled content approach attaches zero environmental burden to the production of recycled material input, but does not give any credit for end-of-life recycling. (Frischknecht, 2010). The end-of-life substitution approach (Figure 3b) gives a credit for end-of-life recycling (substitution of virgin material), but attributes the

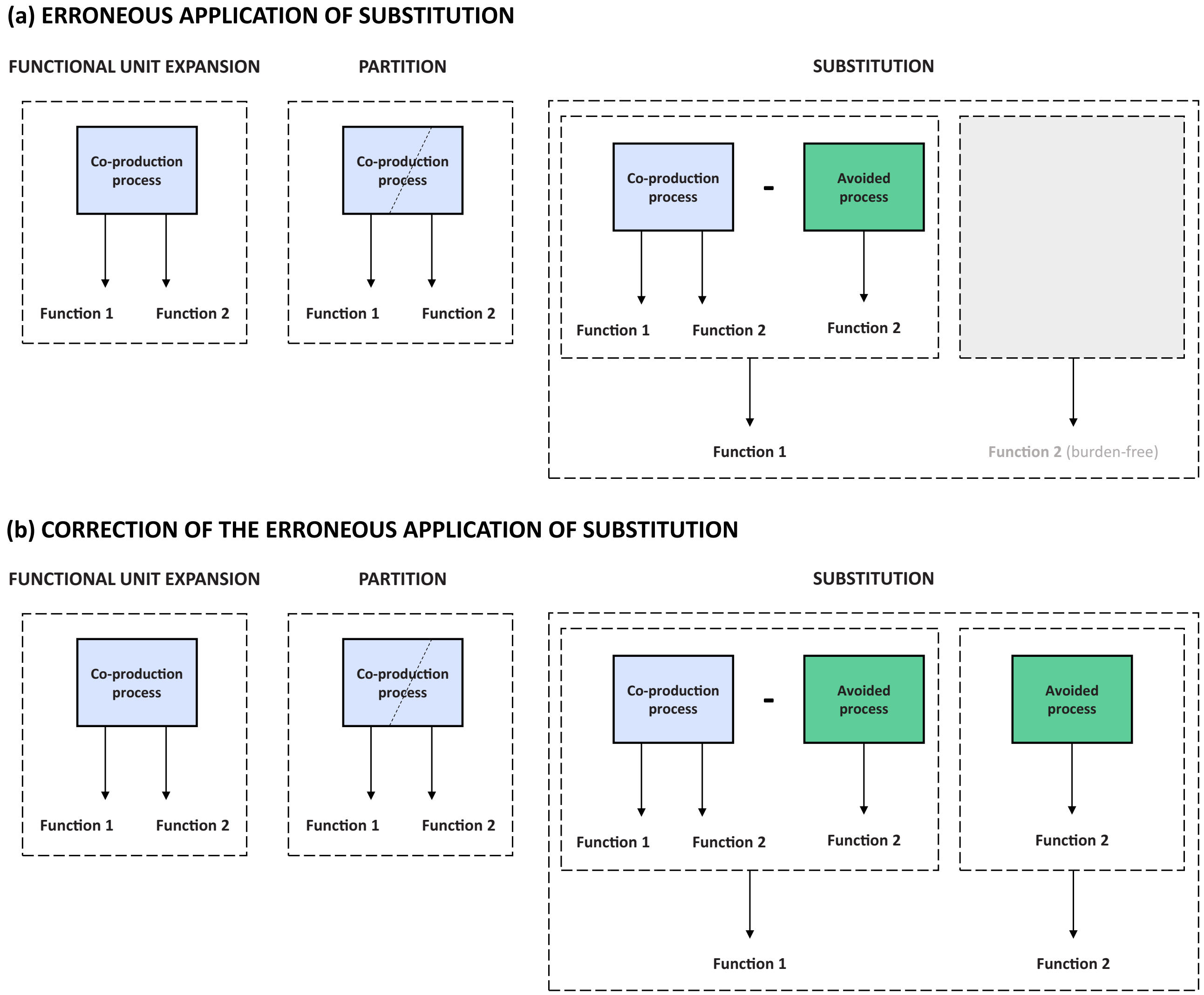

FIGURE 2 (a) Illustration of the comparison of the functional unit expansion, partition, and substitution approaches, as described by Brander and Wylie (2011). This application of substitution is erroneous, and leads to double-counting the benefits of substitution, with a credit attributed to the co-production process for substituting function 2 and a burden-free system attributed to function 2. (b) Correction of the erroneous application of substitution in the worked example of Brander and Wylie (2011). The system attributed to function 2 must be the avoided process to conserve the impacts of the initial unattributed co-production process.

environmental burden of virgin material production to the input, regardless of its actual recycled content (Bergsma & Sevenster, 2013; Schrijvers et al., 2016b). These two approaches cannot be combined (see Figure 3c) without erroneously double-counting the environmental benefits of recycling (Schrijvers et al., 2016a), similarly to the double-counted benefits of substitution by Brander and Wylie (2011).

2.3 | Intuitive rebuttal of the violation of the additivity criterion

An intuitive solution emerges from the incoherence presented in Section 2.2: to preserve the total impacts of the unallocated multifunctional process, the environmental impacts attributed to the secondary product(s) must be set equal to those of the substituted (or avoided) primary production(s). In other words, if the impacts of the substituted primary production(s) are both *subtracted* from the footprint of the primary function and *added* as the footprint of the secondary (substituting) function, the total impacts are obviously conserved. Figure 2b illustrates this intuitive solution applied to the worked example of Brander and Wylie (2011) (see Section SI-3 of the Supporting Information for a mathematical correction). This subtraction-and-addition approach is used to distribute impacts between the primary and secondary products, but has no influence on the total emissions of the system. This reasoning follows from the well-established modeling of substitution in CLCA, instigated by Weidema (2000) and Ekvall and Weidema (2004), and is consistent with the method put forward by Moretti et al. (2020) and Cherubini et al. (2011), who point to

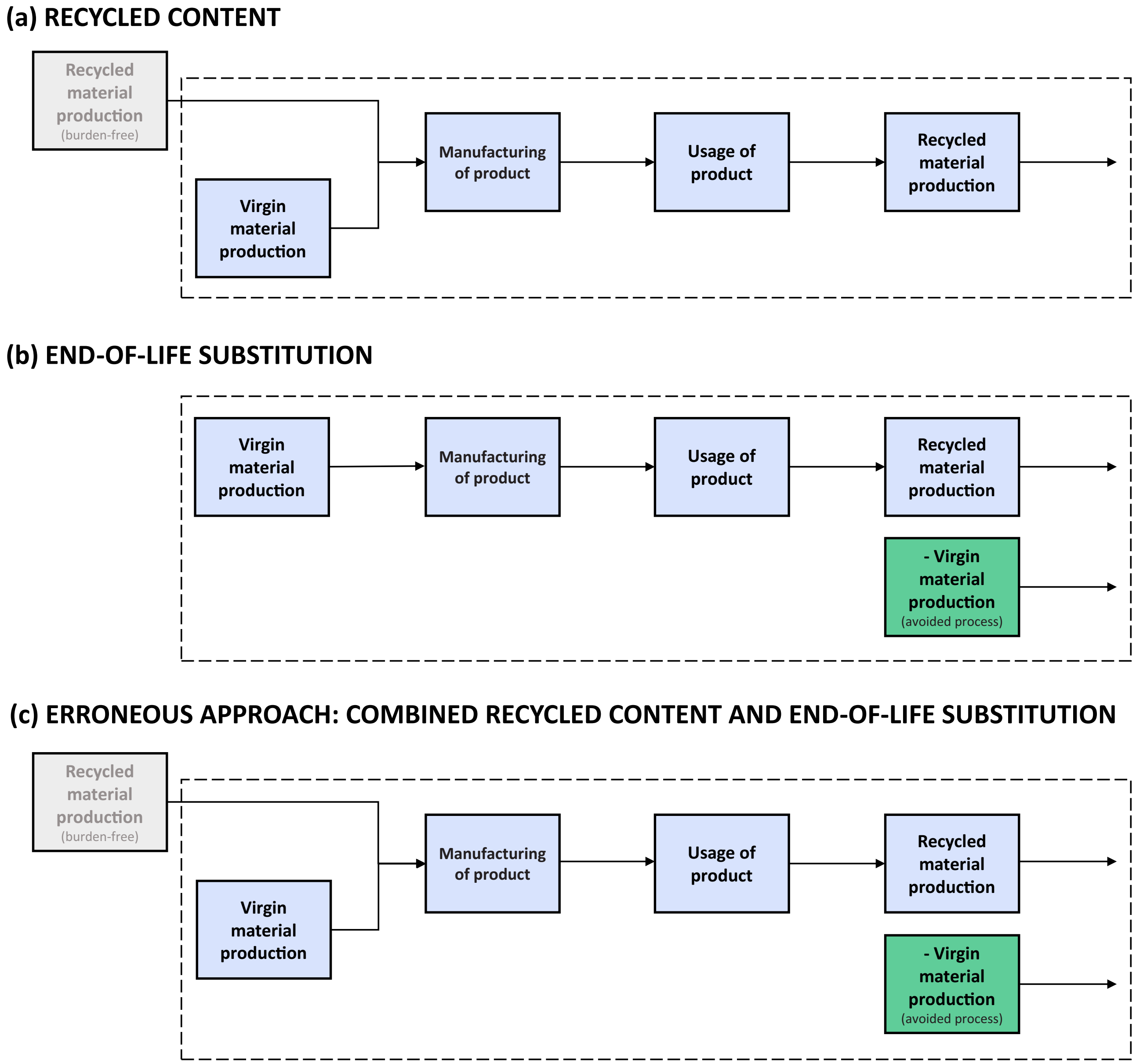

FIGURE 3 (a) Illustration of the recycled content approach. The recycled material input is considered burden free. (b) Illustration of the end-of-life substitution approach. A credit is attributed for the substitution of virgin material production by the production of recycled material output. The material input is considered to be 100% virgin. (c) Erroneous combination of the recycled content and of the end-of-life substitution approaches.

this possibility in an attributional framework: "with substitution, the impact of a by-product should equal that of the product it substitutes, and so is independent on the actual process that produces it" (Moretti et al., 2020).

2.4 | Illustrative example of the correction of Misconception 1 with a combined heat and power process

An example of the application of the proposed solution is the attributional representation of a small-scale combined heat and power (CHP) plant using pellet sawdust from forest biomass combustible, based on the study of Havukainen et al. (2018). The co-generation plant has two distinct functions: producing electricity and producing heat. In this study, the authors identify the electricity as the co-product that determines the production volume of the CHP process (primary product), and the technologically linked heat production as the secondary product that substitutes primary heat production. For each MJ of total energy produced, the plant generates 0.21 MJ of electricity and 0.79 MJ of heat for the district heating network. In the context of the study, the avoided heat production technology mix is natural gas combustion (Havukainen et al., 2018). In other contexts, there could be a substitution of another primary heat production technology or of a mix of technologies (Schaubroeck et al., 2021). Results show that the climate change impacts of the CHP process are 62 gCO_2-eq/MJ of total energy produced. The avoided heat production from natural gas generates 72 gCO_2-eq/MJ of heat produced. To obtain the independent global warming potential (GWP) footprint of the electricity production ($GWP_{\text{primary function, electricity}}$), we need to subtract the impacts of the substituted natural gas heat production from the total net impacts of the multifunctional process using Equation (1):

$$GWP_{(\text{primaryfunction,electricity})}\left[\frac{gCO_2\text{-eq}}{MJ_{\text{electricity}}}\right] = \frac{\left[62\left[\frac{gCO_2\text{-eq}}{MJ_{\text{total energy}}}\right] - 72\left[\frac{gCO_2\text{-eq}}{MJ_{\text{heat}}}\right]\times 0.79\left[\frac{MJ_{\text{heat}}}{MJ_{\text{total energy}}}\right]\right]}{0.21\left[\frac{MJ_{\text{electricity}}}{MJ_{\text{total energy}}}\right]} = 24.38\left[\frac{gCO_2\text{-eq}}{MJ_{\text{electricity}}}\right] \quad (1)$$

We then allocate the avoided impacts of the natural gas heat production to the footprint of heat generation by the CHP process ($GWP_{\text{secondary function, heat}}$), using Equation (2):

$$GWP_{\text{secondary function, heat}}\left[\frac{gCO_2\text{-eq}}{MJ_{\text{heat}}}\right] = 72\left[\frac{gCO_2\text{-eq}}{MJ_{\text{heat}}}\right] \quad (2)$$

Subsequently, we can recalculate the impacts of the unallocated multifunctional process ($GWP_{\text{multifunctional process, CHP}}$) from the footprints of both co-functions, for 1 MJ of total energy produced, with Equation (3):

$$GWP_{\text{multifunctional process,CHP}}\left[\frac{gCO_2\text{-eq}}{MJ_{\text{totalenergy}}}\right] = 24.38\left[\frac{gCO_2\text{-eq}}{MJ_{\text{electricity}}}\right]\times 0.21\left[\frac{MJ_{\text{electricity}}}{MJ_{\text{total energy}}}\right] + 72\left[\frac{gCO_2\text{-eq}}{MJ_{\text{heat}}}\right]\times 0.79\left[\frac{MJ_{\text{heat}}}{MJ_{\text{total energy}}}\right] = 62\left[\frac{gCO_2\text{-eq}}{MJ_{\text{total energy}}}\right] \quad (3)$$

The total impacts are conserved, illustrating the validity of the approach discussed in Section 2.3 in this specific case. This mathematical demonstration is translated into matrices in Section SI-4 of the Supporting Information.

2.5 | Mathematical generalization of the agreement of substitution with the additivity criterion

We generalize the example above, to show it generally holds for situations where substitution is applicable, with the framework illustrated in Figure 4. The symbols used in this figure and their signification are presented in Table 1.

In Figure 4a, the value chains included in an attributional study (system *A*) are represented as a portion of the global system of all value chains (technosphere *T*). A multifunctional process (Process M) is part of the value chain providing the final product of system *A* (product *o*). This multifunctional process produces a primary product (product *m*) and a secondary product (product *q*). System *T-A* contains all the processes, flows of products, and environmental flows that are part of system *T*, but not part of system *A*. Hence, technosphere *T* is a system respecting the additivity criterion, with no double-counted or unrepresented impact.

For more generality, we choose to not put process M at the final end of the value chain (i.e., directly satisfying the functional unit under study). It is however possible that the primary product flow of Process M directly satisfies the final function of system *A* ($p_{m,M} = p_{o,M} = f_{o,A}$); the processes downstream of the production of product *m* illustrated in Figure 4a are inexistent in this case. The same principle applies to the secondary production. Elseway, system *A* includes all the processes between the production of product *m* and of product *o*, to include the whole value chain of the final studied product, and all the processes between the production of product *q* and of product *s*, to reach the point of substitution, defined as "the point where the by-product can—without further treatment—substitute a reference product as an input to an activity" (Weidema, 2018). For example, taking an old corrugated cardboard recycling process as the attributional studied system (primary function: waste management; secondary function: production of recycled corrugated cardboard) the sorted old corrugated cardboard flow exiting a material recovery facility cannot directly substitute a primary corrugated cardboard production, and has to go through some reprocessing steps before reaching the point of substitution. These reprocessing steps have to be included in the attributional studied system.

The final demand vector of product flows ($\boldsymbol{f_k}$) is of dimension *N*, where *N* is the number of final demand products in system *k*. Each position in the vector corresponds to a different product, and the value of each element indicates the product flow demanded in system *k*. In system *A*, only the first position (associated with product *o*) and the second position (associated with product *s*) of $\boldsymbol{f_A}$ are not null:

$$f_A = \left[f_{o,A},\ f_{s,A},\ 0,\ \ldots\right] \quad (4)$$

Figure 4b illustrates the application of the proposed substitution modeling approach within the framework. Process S provides a flow of product *s'* ($p_{s',S}$), which is functionally equivalent (≡) to the substituting secondary product flow originating from Process M ($f_{s,A}$). We subtract Process S and all its upstream processes from system *A* to obtain the system allocated to the final studied function (A_{FINAL}). To follow the subtraction-and-addition

TABLE 1 Symbols used in the general framework representing the substitution modeling approach that allows for a conservation of total impacts in attributional studies.

Symbol	Signification
Sets	
$\mathcal{S}$	Set of systems; $\mathcal{S} = \{T, A, A_{FINAL}, A_{SECOND}\}$
$\mathcal{P}_i$	Set of processes in system *i*; $i \in \mathcal{S}$
$\mathcal{C}_i$	Set of products (commodities) in system *i*; $i \in \mathcal{S}$
Systems (comprising processes, flows of products and environmental flows)	
T	System comprising the entire (past, present, and future) technosphere; $T \in \mathcal{S}$
A	Attributional system comprising the value chain providing the final studied function and the associated substituting secondary function(s); $A \in \mathcal{S}$
A_{FINAL}	System allocated to the final studied function independently from the associated substituting secondary function(s); $A_{FINAL} \in \mathcal{S}$
A_{SECOND}	System allocated to the substituting secondary function independently from the associated final studied function; $A_{SECOND} \in \mathcal{S}$
Processes	
M	Multifunctional process in the value chain of the final studied function; $\mathrm{M} \in \mathcal{P}_T$; $\mathrm{M} \in \mathcal{P}_A$
O	Process providing the final studied function; $\mathrm{O} \in \mathcal{P}_T$; $\mathrm{O} \in \mathcal{P}_A$
N	Process providing the substituting secondary function; $\mathrm{N} \in \mathcal{P}_T$; $\mathrm{N} \in \mathcal{P}_A$
S	Process providing the substituted secondary function as a primary function; $\mathrm{S} \in \mathcal{P}_T$
Products	
m	Primary product of Process M $m \in \mathcal{C}_T$; $m \in \mathcal{C}_A$
q	Secondary product of Process M $q \in \mathcal{C}_T$; $q \in \mathcal{C}_A$
o	Product providing the final studied function; $o \in \mathcal{C}_T$; $o \in \mathcal{C}_A$
s	Product providing the substituting secondary function; $s \in \mathcal{C}_T$; $s \in \mathcal{C}_A$
s'	Primary product of Process S; $s' \in \mathcal{C}_T$
Product flows	
$\mathrm{p}_{i,j}$	Flow of product *i* produced by process *j*; $i \in \mathcal{C}_T$; $j \in \mathcal{P}_T$
$\mathrm{f}_{i,j}$	Flow of final demand product *i* produced by system *j*; $i \in \mathcal{C}_T$; $j \in \mathcal{S}$
Vectors	
$\boldsymbol{f}_k$	Final demand vector of product flows of system *k*; $k \in \mathcal{S}$ $\mathbf{f}_k = [\mathrm{f}_{i,j}, \ldots]$
$\boldsymbol{e}_i$	Vector of environmental flows of system *i*; $i \in \mathcal{S}$
Variables	
α	Substitution ratio
π	Market response

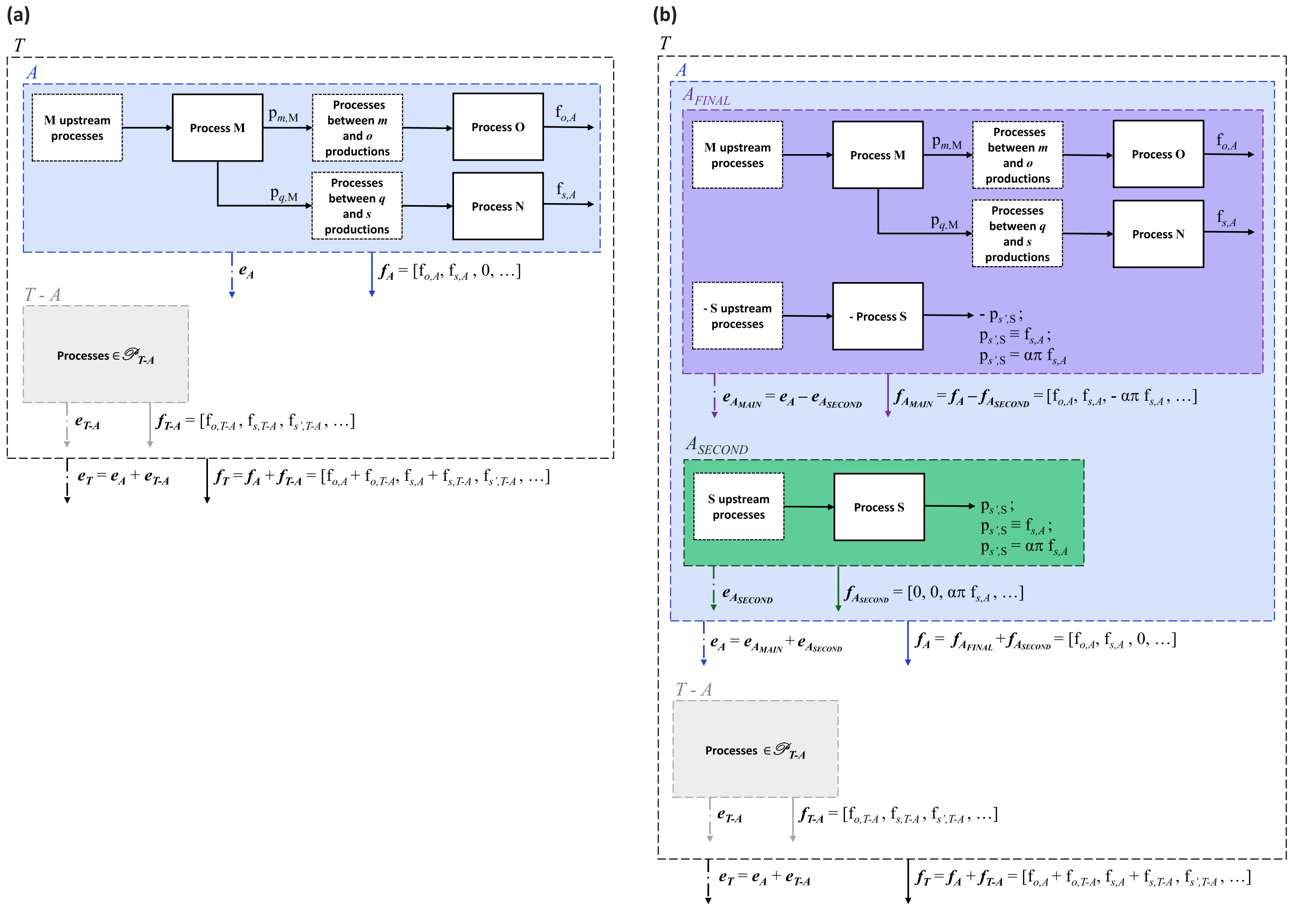

FIGURE 4 Mathematical generalization of the conservation of global impacts when applying substitution modeling to attributional studies. The processes downstream of Process M are optional and determined by the functional unit (in the primary product value chain) and by the point of substitution (in the secondary product value chain). (a) Representation of the global technosphere *T* without substitution modeling. *A* is the attributional multifunctional studied system, providing the primary final demand product flow $f_{o,A}$ and the secondary final demand product flow $f_{s,A}$. (b) Representation of the global technosphere *T* using substitution modeling. The value chain of the substituted flow $p_{s',S}$ is subtracted from the value chain of multifunctional system *A* to yield the system attributed to the studied final product (A_{FINAL}). The system attributed to the secondary product is the value chain of the substituted flow $p_{s',S}$ (A_{SECOND}).

approach described in Section 2.3, Process S and all its upstream processes are added to system *A*, forming the system allocated to the secondary function of system *A* (A_{SECOND} in Figure 4b).

To conserve the global impacts, the vector of environmental flows of system *T* ($\boldsymbol{e_T}$) must remain the same whether substitution modeling is applied or not. The substitution approach only affects system *A*, and consequently it leaves the vector of environmental flows of system *T-A* ($\boldsymbol{e_{T\text{-}A}}$) unchanged. Hence, the vector of environmental flows of system *A* ($\boldsymbol{e_A}$) must also remain the same to conserve the impacts of technosphere *T*. It was postulated that system *T*, illustrated in Figure 4a, respects the additivity principle:

$$e_T = e_A + e_{T-A} \tag{5}$$

In Figure 4b, we split system *A* into two distinct systems (A_{FINAL} and A_{SECOND}):

$$e_T = e_{A_{\text{FINAL}}} + e_{A_{\text{SECOND}}} + e_{T-A} \tag{6}$$

The vector of environmental flows of system A_{FINAL}, using the definition of the substitution modeling approach, is:

$$e_{A_{\text{FINAL}}} = e_A - e_{A_{\text{SUBSTITUTED}}} \tag{7}$$

Where $e_{A_{\text{SUBSTITUTED}}}$ corresponds to the environmental flows of the substituted processes.

Inserting Equation (7) in Equation (6) gives:

$$e_T = e_A - e_{A_{\text{SUBSTITUTED}}} + e_{A_{\text{SECOND}}} + e_{T-A} \tag{8}$$

To respect the additivity principle with the substitution approach illustrated in Figure 4b, Equation (8) must be equal to Equation (5), and we find that:

$$e_{A_{\text{SECOND}}} = e_{A_{\text{SUBSTITUTED}}} \tag{9}$$

In some cases, a primary product that is functionally equivalent to the substituted secondary product of system *A* does not exist. For example, a recycled paper might not have equivalent properties to its virgin alternative. A correction factor, the substitution ratio (α, as defined by Vadenbo et al., 2017), can be employed to represent this technical functional equivalence. Also, a market response factor (π, as defined by Vadenbo et al., 2017) can be used to take into account price elasticities. Hence, $p_{s',S} = \alpha\pi\, f_{s,A}$.

This generalization confirms that the final demand and the total emissions of *T* are conserved when applying substitution modeling appropriately. The choice of the substituted process has an influence on the share of impacts attributed to each co-product, but does not affect the total impacts of the studied multifunctional attributional system. The additivity criterion (Characteristic A) is therefore generally respected, which contradicts the first misconception.

3 | MISCONCEPTION 2: BECAUSE ALCA DESCRIBES A SYSTEM IN A GIVEN STATE, AND SUBSTITUTION DESCRIBES A CHANGE IN STATE (A PERTURBATION, SOMETHING AVOIDED), THE TWO CANNOT LOGICALLY AND COHERENTLY BE MIXED

The substitution approach introduces avoided productions in the studied system (Majeau-Bettez et al., 2018). Brander and Wylie (2011) argue that "[t]he values included in corporate inventories are for actual physical emissions or actual physical removals, rather than values for emissions which have not happened." Camillis et al. (2013) state that "[a]s the aim [of attributional studies] is to come up with a snapshot of the impacts as they are, market mechanisms (e.g. substitution) are not captured as they take place over time [...]. For this reason, the substitution technique is not allowed." The "what-if" substitution approach (Heijungs & Guinee, 2007) is thus commonly perceived as a violation of the state-descriptive nature of attributional studies (Characteristic B) (Brander & Wylie, 2011; Camillis et al., 2013; Heijungs, 1997; Heijungs & Guinee, 2007; Majeau-Bettez et al., 2018; Pelletier et al., 2014; Peñaloza et al., 2016). In this section, we argue that this interpretation is overly restrictive.

3.1 | An overly restrictive interpretation

Vadenbo et al. (2017) define the substitution potential as "a measure of the end-use-specific change in consumption of the directly affected products resulting from supplying a co-product [...] to a particular end use or market." Consequently, by its definition, substitution is about change, which appears incompatible with the description of an existing system "as it is," in an attributional manner. In a prospective consequential study, substitution is the expected future change in consumption relative to the current state (or *status quo*), that is caused by a variation in consumption of the final studied product. In this type of study, substitution explicitly describes a perturbation of the *status quo* that is incompatible with an attributional description. For example, if a community decides to increase its consumption of electricity from CHP, we can expect the additional co-produced heat to replace the currently dominant primary source of heat in that locality, for example, natural gas boiler. Substitution fits perfectly with a description of a perturbation. But is consequential modeling the only logical use of substitution within LCA? Is the current state of the system under study the only possible starting point for the modeling of a (substitution) change? Or, following a similar line of inquiry, is a state-descriptive system necessarily described *as disrupted* by a change rather than *as resulting* from a change? A simple mental experiment leads us to answer negatively to all three questions.

3.2 | Intuitive rebuttal of the violation of the state-description criterion (Characteristic B)

It is noteworthy that, once a system has reached a new *status quo*, the substituted flow is being avoided, and therefore, not part of the resulting system. By definition, when a co-production is present in a system, it is not possible to observe the flows that are being substituted by the secondary product(s).. Recalling the example of the municipality where consumption of CHP electricity was increased, we can describe the final state of this town as *resulting from* a substitution, relative to a state where the co-production is less present. It should be noted that we are describing this final state, not perturbing it. In other words, it is possible to describe a given state of a system *in terms* of a (substitution) change.

It is logical to assume that, should the citizens of the municipality not have elected to consume more electricity from CHP, some other industry would have to supply their heating needs. Except in the case of a perfectly elastic demand,[2] any co-production flow can therefore be understood as preventing the existence of a primary production. A co-production, in short, implies some avoidance relative to what would be if the co-production process did not force secondary products on the market.

We can draw an analogy with some state variables in thermodynamics and their quantification in terms of changes from reference states. The enthalpy of 1 kg of a substance, for example, describes its (energetic) state. And yet, the standard enthalpy value is defined in terms of the difference in enthalpy that would occur if we were to produce this state from a hypothetical (reference) system where all the elements (C, N, O, etc.) are isolated in their most stable form at 298 K and 0.1 MPa (Krishnan & Raghavan, 2019). Interestingly, the choice of this specific reference state is entirely arbitrary, and other conventions are found in the literature (Brunner, 2014; Doran, 1995). A thermodynamic system, unchanging and stable in a given state, can nonetheless be described in terms of the change that would have lead to it from another state. Perhaps an ALCA, describing a (stable, given) state, can be described in terms of the (substitution) changes that would lead up to it from another state.

With the substitution approach, the avoidance of a primary production relative to a reference state becomes a property of the system under study, and this property can then logically be integrated within ALCA co-production modeling like any other property (e.g., mass or economic value). It becomes possible, as previously discussed in Section 2, to allocate impacts based on this property. Using substitution does not force us to disrupt the system under study, contrary to what is claimed in Misconception 2. A rebuttal of Misconception 2 applied to the small-scale CHP plant (Havukainen et al., 2018) is provided in Section SI-5 of the Supporting Information. We also use the framework presented in Section 2.5 to generalize the rebuttal of Misconception 2 presented in this section in Section SI-6 of the Supporting Information.

3.3 | A remaining contradiction?

A main and widely accepted distinction between the attributional and the consequential approaches is that the former uses average data while the latter uses marginal data (Ekvall et al., 2005; Finnveden et al., 2009; Plevin et al., 2014; Sandén & Karlström, 2007; Schaubroeck et al., 2021). We employ the terms "average" and "marginal," because these terms typically describe the data used in attributional and consequential studies, but these words are not perfectly defining these data types, as discussed in Schaubroeck et al. (2021). In this work, average data can be defined as "state-descriptive" and marginal data can be described as "change-descriptive." A main methodological aspect that justifies the use of average data in ALCA is the conservation of global impacts. Using average data to describe attributional systems ensures that the emissions of all existing attributional systems providing final products can be added to yield the total global impacts. Heijungs (1997) states that only the "average attribution rule" is compatible with the characteristics of ALCA, including the additivity principle. Then, should we use average data in the reference state and the studied state to respect the additivity principle? After all, CLCA always represents transitions (or perturbations) with marginal mixes. Does our response to Misconception 2 imply that the footprint of the CHP plant should be based on the marginal fuel mix upstream of this plant, which would then lead to a violation of additivity, contradicting our response to Misconception 1? The answer is no. Here again, the distinction is explained by the difference between a change that disrupts the studied system and a change that leads to the studied system. When perturbing the observed system in a CLCA, we are essentially trying to anticipate the introduction of novel productions that has not yet been observed. It makes sense to exclude from this addition any technology that is rigidly constrained or with prohibitive costs. In contrast, for flows that are observable in the state we wish to describe, we do not have to exclude any technology from the average production mixes. Contributors to the observable/average production mixes represent the sum of multiple changes from a reference state: they were all once the "marginal" new additions. And what about the flows that are not observable because they are being avoided, should we take average production mixes or marginal production mixes? This question will be discussed in the next section.

4 | COROLLARY 1: THERE IS A LOGIC TO MARGINAL SUBSTITUTION EVEN IN ALCA

One important aspect that remains to be adressed is the choice of the substituted technologies. As shown in Section 2, this choice will not affect the total impacts of the multifunctional process, but is directly related to the share of impacts attributed to each co-product. In this section, we adress a particular source of confusion when identifying the avoided technologies with the attributional approach: the coherence of substituting marginal processes in ALCA.

[2] If the demand is elastic, rebound effects can occur. For example, direct rebound effects occur when the increased efficiency of a process producing a particular product lowers its price, leading to more consumers purchasing this final product (Earles & Halog, 2011). In this case, substitution might partially happen, or not happen at all.

Schrijvers et al. (2016a) define criteria to evaluate the consistency of different guidelines for co-production modeling in LCA. Through their review of 10 official guidelines, they find that the ILCD handbook (European Commission, 2010), the BP X30-323-0 (AFNOR, 2011), the Greenhouse gas protocol (WBCSD/WRI, 2011), and the PEF Guide (European Commission, 2013) recommend to substitute average data (Schrijvers et al., 2016a). Finnveden et al. (2009) argue that “[t]he major difference between an attributional and a consequential study in this case [substitution by system expansion] is the type of data used. A consequential study would often use marginal data, whereas an attributional study typically would use average data.” Finnveden et al. (2022), also state that “average data [are] being used for substitutions in ALCAs and marginal data for substitutions in CLCAs.” As far as we can tell, however, no compelling argument was ever put forward as to why co-production should substitute an average mix in ALCA. The reasoning seems to have been an extension of the general guidelines of ALCA to the separate question of substitution modeling. Although certainly mathematically possible, we here argue that such a substitution modeling choice makes little internal sense. In contrast, we claim that there is a clear logic to marginal substitution in ALCA that stems from the ideas discussed about Misconception 2 (Section 3).

In addressing Misconception 2, we showed that an attributional state-descriptive multifunctional system can coherently be represented as the result of a transition from a reference technosphere. Substitution modeling thus aims to represent as coherently as possible the (substitution) market mechanism happening during this transition. The average *observable* mixes of the studied system are definitly not good indicators of the *avoided* (and thus inexistent) mixes. Suppose that the current heat mix includes both a natural gas boiler and a rigidly constrained source of heat produced from biogas generated in a landfill. If we say that CHP substitutes the average mix, it implies that it substitutes both natural gas heat and biogas heat. This in turn implies that in the reference state (technosphere *R*) there is more biogas heat than at present, something we just defined as impossible. In other words, we cannot avoid the use of a resource that is constrained and could not be used in greater quantity than in the studied state.

A question that remains concerns the temporal definition of the reference technosphere. Is this reference technosphere a *historical* representation of the world before the existence of the co-production process or a *counterfactual* representation of the world in the same temporal state as the studied attributional system? The second definition of the reference technosphere fits better with the state-descriptive characteristic of attributional studies. The historical marginal substituted mix is not necessarily the same as the marginal substituted mix in the studied state. For example, if when the CHP plant was built, the marginal substituted heat producing technology was coal, and after a while the government decided to prohibit the increase of the use of coal in the municipality, a constrained resource (coal) cannot continue to be the marginal substituted technology. When modeling substitution in ALCA, we thus have to consider the substituted counterfactual unconstrained technological mixes in the studied state. These mixes are composed of the marginal technologies that would respond to the demand for the secondary product(s) if the multifunctional system was inexistent, in the actual studied state. Section SI-7 of the Supporting Information illustrates the temporal evolution of the substituted marginal mix with the example of the CHP process.

The conclusion of this section implies that the observable value chains represented in attributional studies must use average data (as explained in Section 3.3), while the substituted value chains must use marginal data. This complexifies the system modeling, for example, expanding the technology matrix to include average as well as marginal processes.

5 | DISCUSSION

Previous sections showed that substitution modeling can be compatible with two axiomatic characteristics of ALCA. One characteristic of attributional studies (Characteristic C), however, seemingly remains transgressed, because substitution modeling introduces activities that are not directly related to the functional unit by production–consumption flows in the system boundaries. We definitely need a normative convention to attribute responsibility for environmental impacts to functions in ALCA, to harmonize practice and guarantee additivity. However, we argue that Characteristic C should not apply to substitution. In the approach proposed in this manuscript, because the impacts of the substituted activities are simultaneously subtracted from the system providing the primary product, and added to the system(s) providing the secondary product(s), when looking at the total impacts of the multifunctional system, the impacts of these activities are cancelled. Consequently, this method globally does not add to or remove from the studied multifunctional system any impact related to activities that are not part of the value chain. Substitution can be seen as a way to allocate impacts to the primary and secondary products, like partition based on mass, energy, economic value, or other properties. The distribution of impacts with the substitution approach is based on the notions of functional equivalence and competing markets.

In light of the reflections made in this study, it is necessary to revisit and harmonize existing guidelines on three different aspects. First, the guidelines should allow substitution as a suitable method for co-production modeling in ALCA. Second, many guidelines focus on the calculation of the primary product footprint with the substitution modeling approach, but a clear methodology should also be provided for the calculation of the footprints of the secondary products, as presented in Section 2. Third, the different guidelines that recommend to substitute average data (notably the ones identified by Schrijvers et al., 2016a) should also be reviewed to clearly specify that the substituted production mixes should be the counterfactual unconstrained marginal mixes, as explained in Section 4.

When using substitution, we face many practical challenges associated with normative modeling choices. These modeling choices include, for example, the identification of the marginal mixes (Finnveden et al., 2009; Mathiesen et al., 2009; Saraiva et al., 2018; Weidema, 2000) and the quantification of the substitution potential according to functionality and price elasticities (Vadenbo et al., 2017). These challenges do not compromise the axiomatic compatibility of substitution with ALCA, but can affect our capacity to coherently model substitution in specific cases. Despite these challenges, the technological coupling between co-products and the functional equivalence of multiple products in a common market constitute actual properties of the system under study that proved relevant to serve the methodological goals of an ALCA, just like other properties commonly used in partition modeling (e.g., mass, energy, or economic value). As mentioned in Section 1.4, it remains beyond the scope of this study to weigh the advantages and disadvantages of substitution compared to other co-production modeling methods, notably partition, which also brings certain challenges related to normative modeling choices (e.g., the choice of the property on which to perform allocation and the specification of the allocation factors; Heijungs & Guinee, 2007). These modeling choices can have a substantial influence on the results of an LCA using substitution (Viau et al., 2020) or partition (Heijungs & Guinee, 2007). Future work should address more specifically the choice of the substituted mixes in ALCA and CLCA and define clear rules for their identification.

The general approach presented in Section 2.5 ensures applicability to a large variety of ALCA scopes, including the end-of-life reuse and recycling treatments which have historically been considered as requiring distinct co-production modeling guidelines (Weidema, 2000) and are treated separately in the ISO standard (International Organization for Standardization, 2006). The results of this study also have specific implications for the LCA of waste management processes. It questions the dichotomous methodological approaches commonly acknowledged for ALCA (recycled content approach) and CLCA (end-of-life substitution approach). More generally, our results clarify the treatment of multifunctionality in ALCA, questioning the inapplicability of substitution in ALCA, the recommended substitution of average data in ALCA and marginal data in CLCA, and the representation of activities that are not linked to the functional unit by production–consumption flows being restricted to CLCA. The findings of this research do not question the differentiated objectives of ALCA and CLCA, but show that common methodological tools, for example, substitution, can be used in both perspectives to achieve these objectives.

6 | CONCLUSION

Modeling co-production with the substitution approach can be compatible with the fundamental characteristics of an ALCA. First, the use of substitution does allow for a conservation of global impacts and thus respects the additivity criterion if the impacts attributed to the secondary production(s) are the impacts of the substituted primary production(s). Then, a state can be described through its avoidance of a primary production relative to a reference state. Substitution is then the representation of the transition from this reference state to the studied state. Finally, there is a logic to marginal substitution in ALCA, because to realistically represent the transition from the reference state to the studied state, the avoided technological mixes should be the unconstrained marginal mixes. We consequently encourage practitioners to consider marginal substitution as a suitable method for co-production modeling in ALCA.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

Data sharing not applicable—no new data generated.

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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