When do allocations and constructs respect material, energy, financial, and production balances in LCA and EEIO?

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Abstract

Conservation of mass and energy are essential to physical accounting, just as price and market balances are essential to economic accounting. These principles guide data collection and inventory compilation in industrial ecology. The resulting balanced surveys, however, can rarely be used directly for lifecycle assessment (LCA) or environmentally extended input-output analysis (EEIO); some modeling is necessary to recast coproductions by multifunctional activities as monofunctional unit processes (a.k.a. Leontief production functions or technical "recipes"). This modeling is done with *allocations* in LCA and *constructs* in IO.

In this article, we ask how these models respect or perturb the balances of the original inventory. Which allocations or constructs, applied to what type of dataset, have the potential to simultaneously respect its multiple physical, financial, and market balances?

Our analysis builds upon the recent harmonization of allocations and constructs and the ongoing development of multilayered supply and use inventory tables. We derive the necessary and sufficient conditions for balanced models, investigate the role of data aggregation, and clarify these models' relation to system expansion.

We find that none of the modeling families in LCA and EEIO are balanced in general, but special data characteristics can allow for the respect of multiple balances. An analysis of these special cases allows for clear guidance for data compilation and methods integration.

1 Introduction

1.1 Aim of study

The conservation of mass and energy is fundamental to our physical understanding of the world. Similarly, a financial balance is essential to our economic reasoning;

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the value of any product must equal the production costs plus profits. We also need markets to balance, as each product consumed must be produced, and vice versa. A complete record of the flows of any closed system necessarily respects all these balances, and any imbalance would indicate inaccurate or incomplete measurements.

These balanced inventories, however, generally cannot be used directly in life-cycle calculations. Some modeling steps are necessary to recast our observations of the world into models we can apply to product systems, be it in an environmentally extended input-output (EEIO) analysis or a lifecycle assessment (LCA). The main point of issue comes down to coproduction. Activities with multiple functions are allocated to generate monofunctional unit-processes (in LCA parlance), or constructs are applied to generate a symmetric transaction matrix (in input-output (IO) parlance).

What we seek to answer here is *how do allocations and constructs affect the balances of the original inventory in LCA and EEIO? When can the resulting system descriptions respect the same balances as their source data, and when are physical and economic realism partly sacrificed?* Recent work has revived this issue, not least because we are seeing more precise and balanced inventories in both fields and a novel convergence of modeling practices.

1.2   Scientific context

Both LCA and EEIO analyze direct and indirect consequences of human activities (Heijungs and Suh, 2002; Miller and Blair, 2009). As their perspectives and data sources are complementary (Norris, 2002; Mongelli et al., 2005; Majeau-Bettez et al., 2011), multiple hybrid analyses take advantage of the completeness of EEIO and the specificity of LCA (Suh et al., 2004; Suh and Huppes, 2005; Strømman et al., 2009; Lenzen and Crawford, 2009; Peters and Hertwich, 2006; Suh, 2004, 2006; Nakamura and Kondo, 2002; Nakamura et al., 2008, 2011).

A complementarity of perspectives has also long been recognized between these models and material flow analysis (MFA) (Bouman et al., 2000). Multiple MFAs extend their system descriptions with lifecycle emission intensities (e.g., Venkatesh et al., 2009; Graedel et al., 2012; Pauliuk et al., 2013). Similarly, Waste-IO extends traditional EEIO models with MFA capabilities (Nakamura and Nakajima, 2005; Nakamura et al., 2011, 2008).

LCA, EEIO, and MFA are also converging in terms of data compilation and inventory/survey structures (Weidema, 2011). The LCA community is increasingly adopting inventory structures that are articulated in terms of both products and activities, notably with the ecospold 2 data format (Weidema, 2011). This structure is similar to that of supply and use tables (SUTs), which explicitly describe both commodities and industries and have long been the structure of choice for EEIO surveys (United Nations, 1968, 1999; European Commission, 2008). Similarly, recent EEIO projects increasingly record physical aspects of product flows in addition to their economic dimensions, which better aligns their data compilation with that of LCA and MFA (Schmidt et al., 2010; Merciai et al., 2013). This additional data collection makes it possible to represent a system in multiple *layers* (e.g., mass layer, energy layer, monetary layer). LCA and EEIO communities thus seem to be converging towards compatible, multilayered, multi-unit, balanced SUT

frameworks for their inventory records.

Until recently, however, this convergence of data compilation had not been matched by an equivalent harmonization of coproduction modeling practices. In the LCA community, coproductions are typically tackled with system expansion, partitioning and substitution approaches (Guinée 2002; ISO 2006). EEIO practitioners rather generate symmetric transaction tables with system-wide models called *constructs*, notably the industry technology construct (ITC), the European system construct (ESC), the commodity technology construct (CTC), the byproduct technology construct (BTC) (Stone, 1961; Jansen and ten Raa, 1990; ten Raa and Rueda-Cantuche, 2007; European Commission, 2008).

LCA allocations and EEIO constructs bear little resemble in their formulation and outcome; the former untangles the requirements of coproducts of a given industry, whereas the latter models an economy-wide average production technology for each product. Though potential links were identified early on between the SUT and LCA frameworks (Heijungs, 1997), it is only with Kagawa and Suh (2009) and Suh et al. (2010) that equivalences between LCA allocations and EEIO constructs were identified. Majeau-Bettez et al. (2014) then provided a formal harmonization of LCA allocations and EEIO constructs, deriving the different models of both fields from a single, generalized equation.

Both the LCA and EEIO communities have independently invested important research efforts to assess the strengths and weaknesses of their respective models. Pure and hybridized IO constructs have been evaluated in terms of their capacities to respect axiomatic criteria (Jansen and ten Raa, 1990; Rueda-Cantuche and ten Raa, 2009), their generation of negative coefficients (ten Raa and Van der Ploeg, 1989; Almon, 2000; Suh et al., 2010), and their representation of different types of coproduction (ten Raa and Chakraborty, 1984; Londero, 1999; Bohlin and Widell, 2006; Smith and McDonald, 2011). Similarly, the LCA allocation problem has been discussed in terms of the different model's level of subjectivity, transparency, data requirements, compliance with ISO standards, and physical realism (Frischknecht 1994; Weidema 2000; ISO 2006; Heijungs and Guinée 2007; Cherubini et al. 2011; Ardente and Cellura 2012; Jung et al. 2012, among others). Allocation choices pertaining to waste treatment and recycling have been evaluated somewhat separately, both in the ISO standard (ISO 2006; Weidema 2014) and in the literature (Ekvall and Tillman, 1997; Ekvall, 2000; Huppes, 2000; Werner and Richter, 2000; Finnveden, 1999; Johnson et al., 2013).

Some of these evaluations of allocations and constructs focused specifically on the respect of balances. Jansen and ten Raa (1990) and Rueda-Cantuche and ten Raa (2009) assessed the financial and production balances of monetary IO tables resulting from different constructs. Weidema and Schmidt (2010) presented an illustrative example in which some LCA models respect all physical balances and others do not. Yet, despite a growing focus on physically balanced inventories (Schmidt et al., 2010; Merciai et al., 2013; Ecoinvent Centre, 2014), and despite ongoing efforts to track material stocks and flows through lifecycle economic models (cf. Kytzia et al., 2004; Nakamura et al., 2011), the literature remains fragmented as to the ability of allocated or constructed models to simultaneously conserve material, value, and product balances.

This fragmentation of the literature leaves many apparent contradictions unresolved. Is it possible for substitution to be physically balanced (Weidema and

Schmidt, 2010; Weidema, 2011) if it "requires the equivalence of things that are not necessarily equal" (Heijungs and Guinée, 2007)? Can BTC be equivalent to system expansion (Suh et al., 2010) whilst violating production balance (Jansen and ten Raa, 1990)? If partition allocation is expected to leave intact only the balance of the property that defines the allocation (Weidema and Schmidt, 2010), why is the classic example of a combined heat and power (CHP) plant always carbon-balanced regardless of the choice of partitioning property?

In view of the current convergence of LCA and EEIO, a systematic analysis of balances in coproduction models seems required in order to resolve these — apparent or real— contradictions. Perhaps most importantly, this analysis should inform a reflection as to whether these balances constitute axiomatic, universal requirements, or whether they only play meaningful roles for a limited set of industrial ecology questions.

1.3 Scope and structure of study

A first objective of this study is thus to determine which allocations and constructs, under what conditions, will lead to system descriptions that simultaneously respect the different financial, physical and production balances initially found in a multilayered SUT inventory. We then extend this analysis to discuss which balances seem required for what type of industrial ecology investigation.

There are clear benefits to jointly analyzing LCA allocation models and EEIO product-by-product constructs because of their common roots (Suh et al., 2010; Majeau-Bettez et al., 2014). Conversely, because industry-by-industry constructs do not explicitly represent product groups (European Commission, 2008; Rueda-Cantuche and ten Raa, 2009), these models are too far removed from the allocation problem and are beyond the scope of this analysis.

Allocation and construct choices are, of course, not the only potential source of imbalance in industrial ecology systems. The vast literature on balancing algorithms (e.g., Lenzen et al., 2007, 2009) is made necessary by important discrepancies and gaps in the raw data collection. Similarly, data aggregation causes inhomogeneous product mixes and aggregation errors (Viet, 1994; Konijn and Steenge, 1995; Lahr and Stevens, 2002; Olsen, 2000), which can be an important source of imbalances in lifecycle studies (Weisz and Duchin, 2006; Merciai and Heijungs, 2014). To better focus on the specific contribution of coproduction modeling choices, however, this article only discusses these other sources of error in situations where they are relevant to the choice of allocation or construct (see sections 6.3 and SI-7).

There exist two popular notation conventions for calculating lifecycle requirements and impacts: the Leontief (1936, 1970) requirement matrix method, and the technology matrix and scaling vector method (Heijungs, 1997). These two representations resolve the same linear algebra problem and calculate equivalent results (Peters, 2006). Most LCA allocation methods have been formalized in both notations (cf. Heijungs and Suh, 2002; Jung et al., 2013; Majeau-Bettez et al., 2014), but IO constructs are only defined and related to allocations in the former. For this reason, and to build upon the literature on balanced SUTs, we align our sign convention with the Leontief approach.

We urge our readers to familiarize themselves with the terminology and nota-

tion of this article, presented in supporting information (SI) (section SI-1). To not overburden the main text, the mathematical proofs are also presented in SI.

Section 2 presents the defining characteristics and balances of a multilayered SUT. We then derive in sections 4 and 5 the necessary and sufficient conditions for the respect of these balances by the different LCA and EEIO models. This allows for a complete overview of modeling options, notably for representing waste treatment and exclusive secondary products, in section 6. We then explore practical implications for various research questions in section 7.

2 SUT inventory

2.1 Mixed-unit SUT

Both LCA and EEIO inventories describe the technosphere in terms of a set of activities ($*$) and a set of products ($\bullet$). The supply of these products by these activities may be conveniently regrouped in a product-by-activity supply table ($\mathbf{V}_{\bullet *}$). The requirements of these activities are then recorded in two separate tables: a use table ($\mathbf{U}_{\bullet *}$)[1] for product requirement and an extension table ($\mathbf{G}_{**}$) for use of factors of production ($\star$) (United Nations, 1999). This extension table then describes all requirement flows that cannot be fulfilled by the technosphere within a given time period (Duchin, 2009), such as the use of capital services (Pauliuk et al., 2014), mineral ores, skilled labor, O_2, and the dilution of pollutants (emissions). A column vector ($\mathbf{h}$) tabulates final consumption of products by households, governments, and capital stock formation (European Commission, 2008; Pauliuk et al., 2014).

The main benefit of such a SUT accounting framework is that inputs and outputs of industries may be recorded as observed, without embedded allocation assumptions (European Commission, 2008; United Nations, 1999; Lenzen and Rueda-Cantuche, 2012). For example, the supply of electricity and heat by a CHP plant would be recorded as separate flows in the supply table, and the total use of fuel by this plant would simply be noted as one entry in the use table, without having to decide what share of the fuel should be ascribed to what coproduct. This modeling decision can thus remain fully dissociated from the observation phase for greater transparency and flexibility (Suh et al., 2010).

Most inventories in LCA and EEIO mix multiple different units in the same system description. EEIO typically describes product flows in monetary terms and environmental extensions in physical terms. Even more so, mixed-unit IO (Hawkins et al., 2007) and LCA inventories can be a real patchwork of units, with each product described with the most suitable *functional unit* (Guinée, 2002).

The obvious disadvantage with mixed-unit SUT inventories is that the system is never completely described in terms of any of its dimensions. Flows described uniquely in terms of mass cannot be included in cost calculations; flows accounted only in terms of their energy content cannot be used to check the carbon balance,

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[1] Optionally, recording the specific supplier for each use flow —i.e., recording traceable product flows— adds an extra dimension to the use table (Majeau-Bettez et al., 2014). Instead of a commodity-per-industry table ($\mathbf{U}_{\bullet *}$), it becomes a SourceIndustry-per-commodity-per-industry table ($\mathbf{U}_{* \bullet *}$).

etc. A more complete representation is achieved with multi-unit, multilayered SUT inventories.

2.2 Multilayered SUT

In a multilayered SUT inventory, each flow is spelled out explicitly in terms of its different dimensions (Schmidt et al., 2010; Ecoinvent Centre, 2014). The carbon content of the fuel used in a CHP plant, for example, is recorded in the carbon layer of the use table $\left(u_{fuel,CHP}^{carbon}\right)$, whilst the economic value of this same fuel input would be found in the monetary layer $\left(u_{fuel,CHP}^{monetary}\right)$.[2]

Upgrading a mixed-unit inventory to a multi-unit inventory is performed by acquiring additional data on the composition of each product and factors of production. These may be described in terms of their mass, elementary content, energy content, or economic value. We refer to such dimensions of products and factors of production as *properties*. If it is expected that these properties are conserved —i.e., that they survive the transformation of the products or factors without alteration to their quantity— these properties are characterized as *conservative*. For the sake of this article, mass, energy, elementary content and value are all *conservative properties*.

Let us record the different properties ($\triangle$) of products and factors of production in a property-per-product table ($\mathbf{\Lambda}_{\triangle\bullet}$) and a property-per-factor table ($\mathbf{\Lambda}_{\triangle\star}$), respectively, with each property normalized relative to the unit used in a mixed-unit SUT. Assuming homogeneous product groups (Weisz and Duchin, 2006),[3] these property tables enable the definition of each layer of a multi-unit SUT inventory from a mixed-unit layer by simple unit conversion. For example, the carbon-content of the use of fuel by a CHP plant ($u_{fuel,CHP}^{carbon}$) is simply given by $\lambda_{carbon,fuel} u_{fuel,CHP}$.

By convention (European Commission, 2008), a positive supply denotes an output from an activity, a positive use denotes an input, and vice versa for negative values. In this article, let us extend the sign convention for product use ($\mathbf{U}$) to the use of factors of production ($\mathbf{G}$): a positive factor use denotes a net input from the environment, whereas a negative factor use denotes an emission.

A multilayered SUT with this sign convention can elegantly represent the supply of waste treatment and other "functional input" flows. Indeed, the provision of all functional flows is recorded in the supply table, regardless of whether they constitute an input or output in a given property layer. Thus, if a waste-treatment activity *outputs* a valuable service by taking *in* waste, the provision of this same service would be recorded in $\mathbf{V}$ as a positive entry in the monetary layer and a negative entry in the mass layer (see section SI-5).[4]

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[2] Similarly, the concept of *value added*, essential to financial balance (European Commission, 2008), is simply the monetary dimension of the use of factors of production ($\mathbf{G}_{\star\star}^{monetary}$) (Duchin, 2009).

[3] In addition to simplifying notation, the assumption of homogeneous product groups ensures that allocations and constructs are the only sources of imbalances in this study, which allows us to focus on the specific contribution of these modeling choices to balance issues. The sensitivity of our results to this fundamental assumption of LCA and EEIO (Viet, 1994; Konijn and Steenge, 1995; Weisz and Duchin, 2006) is discussed in section SI-7.

[4] The conversion between a mixed-unit layer and property layers of different signs is simply performed by allowing for negative values in property tables $\mathbf{\Lambda}_{\triangle\bullet}$.

Thus, even in the presence of waste-treatment, the explicit description of requirement ($\mathbf{U}$, $\mathbf{G}$) and supply flows ($\mathbf{V}$) in terms of their different properties (layers) and direction (input/output, by sign conventions) embodies enough information to represent the technosphere in a physically and economically consistent manner.

2.3   Balances in multilayered SUT

One of the greatest appeals of the multilayered SUT is that it allows for critical quality checks (European Commission, 2008), with balances that should hold across its columns and rows in terms of multiple properties, as illustrated in figure 1 with a mass and a monetary layer (pale and dark gray) derived from a mixed-unit layer (hatched).
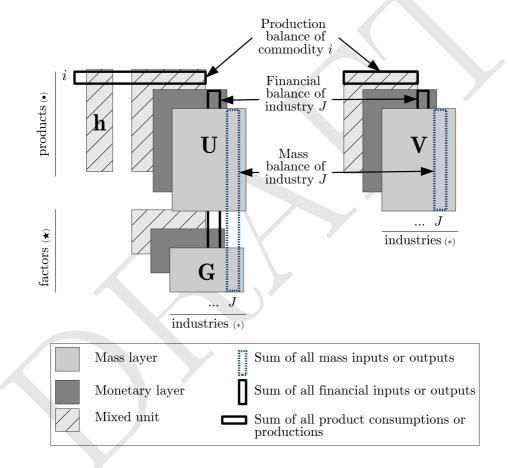

Figure 1: Multilayered supply ($\mathbf{V}$) and use ($\mathbf{U}$) inventory tables (SUT), with environmental extensions ($\mathbf{G}$) and final consumption ($\mathbf{h}$), derived from a mixed-unit layer (hatched). Column-sums in the different layers assess the financial and mass balances in the different industries, and row-sums in the mixed-unit layer assess production balance (a.k.a. market balance) for the different commodities.

The column sums within a given layer should balance if the different industries conserve this layer's defining property (Schmidt et al., 2010). In each layer m, the total amount of m in the requirements sourced by industry J from the economy $\left(\sum_{i \in \bullet} u_{iJ}^m\right)$ and from the environment $\left(\sum_{c \in \star} g_{cJ}^m\right)$ should equal the sum of m in its

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supplied functional flows $\left(\sum_{i \in \bullet} v_{iJ}^m \right)$.

Column-balance of activity J in layer m of a multilayered SUT:

$$\underbrace{\sum_{i \in \bullet} u_{iJ}^m + \sum_{c \in \star} g_{cJ}^m}_{\text{total amount in requirement flows}} = \underbrace{\sum_{i \in \bullet} v_{iJ}^m}_{\text{total amount in supply flows}} \qquad m \in \triangle, J \in * \qquad (1)$$

For greater convenience, each industry's balance may be reformulated in terms of the original mixed-unit SUT ($\mathbf{U}$, $\mathbf{V}$, $\mathbf{G}$) and the unit conversion tables ($\mathbf{\Lambda}_{\triangle \bullet}$, $\mathbf{\Lambda}_{\triangle \star}$).

Balance of property m in activity J, expressed in terms of a mixed-unit layer:

$$\underbrace{\sum_{i \in \bullet} \lambda_{mi} u_{iJ} + \sum_{c \in \star} \lambda_{mc} g_{cJ}}_{\text{total amount in requirement flows}} = \underbrace{\sum_{i \in \bullet} \lambda_{mi} v_{iJ}}_{\text{total amount in supply flows}} \qquad m \in \triangle, J \in * \qquad (2)$$

Contrary to their mass or energy contents, products are not themselves conserved; they are created by industries and destroyed by other industries or final consumers. They are subject to another type of balance, however: the consumption of any product must be matched by an equal production by the various industries (Miller and Blair, 2009). This balance between production and consumption (production balance for short, or market balance), is most conveniently assessed with the row-sums of the mixed-unit layer. In balanced markets, the total supply of commodity i across all industries $\left(\sum_{J \in *} v_{iJ} \right)$ must be met by an equal total consumption, either intermediate $\left(\sum_{J \in *} u_{iJ} \right)$ or final (h_i) (equation (3)).

Production balance (row balance) of commodity i in the inventoried system:

$$\underbrace{\sum_{J \in *} u_{iJ} + h_i}_{\text{total consumption}} = \underbrace{\sum_{J \in *} v_{iJ}}_{\text{total supply}} \qquad i \in \bullet \qquad (3)$$

Multilayer SUTs thus allow for crucial quality checks, in addition to dissociating observation from allocation or construct modeling. This is our starting point. We now turn to assess how LCA and EEIO models respect or perturb the row and column balances of such inventories.

3 From SUT to technical recipes

Both LCA and EEIO rely on system descriptions that are articulated in terms of "recipes", also known as Leontief production functions (Miller and Blair, 2009).

Defining such recipes from the inventory of a multifunctional activity constitutes a challenge, however, because such an inventory describes not the production of a single, homogeneous product but rather the coproduction of multiple products, potentially used in different ratios by different industries (Guinée, 2002).

It is nevertheless sometimes possible to define Leontief production functions from coproducing activities without introducing additional assumptions. If the multifunctionality artificially results from aggregation, disaggregating the coproduction with additional data will reveal that each commodity is in fact produced independently, each with its own distinct recipe (Guinée 2002; ISO 2006). Alternatively, if all the coproducts of an activity are always purchased together *in a constant ratio*, it is possible to represent all coproducts as *bundled* together, as is done with classical system expansion for final consumption (Wardenaar et al., 2012; Heijungs, 2013) and with matrix pseudo-inversion for intermediate consumption (Heijungs and Frischknecht, 1998). Because these representations depend on a fixed ratio between coproducts regardless of the purchaser, the bundle of all functions can then be regarded as the single, homogeneous product for which a recipe is defined.

In all other cases, however, LCA and EEIO practitioners turn to modeling to *artificially* generate monofunctional recipes from multifunctional activity descriptions, introducing assumptions, modeling choices, and, potentially, imbalances.

In this article, we regroup under the term *allocation* all models that extract, from the joint requirements of a multifunctional activity, the recipe for the production of a single commodity.[5] Allocation models —notably partition allocation (PA), product substitution allocation (PSA) and alternate activity allocation (AAA)— thus all start from the joint product use flows of an activity J ($\mathbf{U}_{\bullet J}$) to model the product requirements for the production of individual products (i, j, $k \ldots \in \bullet$) by this specific activity, that is, allocated product flows $\mathbf{Z}_{\bullet Ji}$, $\mathbf{Z}_{\bullet Jj}$, and $\mathbf{Z}_{\bullet Jk}$.[6]

$$allocation : \mathbf{U}_{\bullet J} , \mathbf{V}_{\bullet J} \rightarrow \mathbf{Z}_{\bullet J\bullet} \tag{4}$$

Whereas allocations are models applicable to individual activities, constructs are rather applicable to complete system inventories. In this article, the term *construct* designates the modeling of a symmetric, self-contained[7] and complete system of monofunctional recipes from a SUT inventory. In other words, a construct transforms a whole SUT into a system of product interdependencies, which can be represented as a square flow matrix ($\mathbf{Z}$) and normalized to a square technical coefficient matrix ($\mathbf{A}$). Various aggregation constructs — notably the CTC, ITC, ESC, and BTC — thus produce product-by-product representations (equation (5)) based

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[5] It must be noted that this definition of *allocation* is broader than that of the ISO14044 standard (ISO 2006) and explicitly includes substitution modeling. Guinée (2002) and Heijungs and Guinée (2007) point to the confusion surrounding the term "allocation", which is sometimes used, in the narrow sense, to mean "partitioning" and sometimes, in the broader sense, to designate the modeling response to a multifunctionality problem.

[6] Similarly, for factors of production, allocations start from a joint use by activity J ($\mathbf{G}_{\star J}$) to model factor requirements for the production of individual commodities by this activity, i.e., $\mathbf{G}_{\star Ji}$, $\mathbf{G}_{\star Jj}$, etc. *factor allocation* : $\mathbf{G}_{\star J}$, $\mathbf{V}_{\bullet J} \rightarrow \mathbf{G}_{\star J\bullet}$

[7] In a product-by-product $\mathbf{A}$-matrix, for example, the production of each commodity is individually described by a technical recipe, and in turn each recipe is expressed in terms of the commodities of this system.

on different assumptions (United Nations, 1999; European Commission, 2008).[8]

$$aggregation\ construct : \mathbf{U}_{\bullet *}, \mathbf{V}_{\bullet *} \to \mathbf{Z}_{\bullet \bullet} \qquad (5)$$

From functions 4 and 5, it is clear that the concept of allocations and constructs are intimately related. Both convert descriptions of industries ($\mathbf{U}$, $\mathbf{V}$) into recipes for the production of commodities ($\mathbf{Z}$, $\mathbf{A}$). In doing so, how are the balances of the SUT preserved or discarded?

4 Recipe balances

In this section, we ask when the different models generate recipes that are simultaneously balanced with respect to multiple conservative properties. We first investigate allocation models in sections 4.2 to 4.5. We then extend our analysis to IO constructs in section 4.6, making use of the fact that all constructs can be expressed either as multiple repeated or aggregated allocations (Majeau-Bettez et al., 2014) (see section SI-2.2).

Equation (6) defines the balance of a given property in an allocated recipe. The recipe for the production of commodity j by industry J is balanced in terms of property m when the total amount of m in the supply of j ($\lambda_{mj}v_{jJ}$) equals the net total amount of m in allocated requirement flows, taking into account both flows of commodities (e.g., z_{iJj}) and of factors of production (e.g., g_{cJj}).

Balance of m in allocated recipe for production of j by industry J:

$$\underbrace{\sum_{i \in \bullet} \lambda_{mi} z_{iJj} + \sum_{c \in \star} \lambda_{mc} g_{cJj}}_{m \text{ in requirements allocated to } j} = \underbrace{\lambda_{mj} v_{jJ}}_{m \text{ in supply of } j} \qquad \forall j \in \bullet \qquad (6)$$

Since equation (6) — which mirrors equation (2) for unallocated flows — explicitly includes the unit conversion coefficients (λ_{mi}, λ_{mc}, and λ_{mj}), variables z, g, and v can be conveniently defined in mixed-units.

4.1 Numerical examples

To illustrate the necessary and sufficient conditions for the respect of balances in allocated recipes, two fictional examples are compiled with mixed units in tables 1 and 2. The former presents a CHP plant that requires coal to coproduce heat and electricity. The latter reports the flows associated with raising a dairy cow and raising a steer for slaughter;[9] cow farming coproduces milk and cow meat, whereas steer farming solely produces steer meat.

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[8] along with associated environmental extensions: *factor aggregation construct* $\mathbf{G}_{\star *}, \mathbf{V}_{\bullet *} \to \mathbf{G}_{\star \bullet}$

[9] This fictional example was loosely based on the following sources: Jesse and Cropp (2008); Pettygrove (2010); Roer et al. (2013); College of Agricultural Science (2013).

		Use flows CHP	Supply flows CHP	Factor requirements CHP
electricity	$	0	23.6	
heat	$	0	2.15	
coal	kg	105	0	
CO_2	kg			-328
O_2	kg			238
waste heat	kJ			-1.04×10^3
labor	$			15.8

Table 1: Inventory of a fictional CHP cogeneration plant, in terms of product use flows, product supply flows, and use of factors of production, reported in mixed units

		Use flows		Supply flows		Factor requirements	
		Raising Cow	Raising Steer	Raising Cow	Raising Steer	Raising Cow	Raising Steer
milk	kg	0	0	4170	0		
cow meat	kg	0	0	243	0		
steer meat	kg	0	0	0	304		
feed	kg	29 389	6090	0	0		
manure	kg					$-20\,440$	-5110
respiratory water	kg					-1810	-309
CO_2	kg					-4420	-754
O_2	kg					1690	385
labor	$					1820	320

Table 2: Fictional inventory of product use flows, product supply flows, and use of factors of production associated with raising of a dairy cow and a steer, over the course of their lives, reported in mixed units.

To convert these mixed-unit descriptions to multilayered SUTs, the different products and factors of production are each further described in terms of three properties in table 3.

		energy kJ	value $	carbon kg	dry mass kg
electricity	$^{-1}$	51.4	1.00	0	
heat	$^{-1}$	566	1.00	0	
coal	kg^{-1}	33.0	0.0950	0.850	
CO_2	kg^{-1}	0	0	0.273	
O_2	kg^{-1}	0	0	0	
waste heat	kJ^{-1}	1.00	0	0	
labor	$^{-1}$	0	1.00	0	
milk	kg^{-1}		1.92	0.542	1
cow meat	kg^{-1}		4.85	0.533	1
steer meat	kg^{-1}		6.07	0.623	1
feed	kg^{-1}		0.250	0.402	1
manure	kg^{-1}		0	0.402	1
respiratory water	kg^{-1}		0	0	1
CO_2	kg^{-1}		0	0.273	1
O_2	kg^{-1}		0	0	1
labor	$^{-1}$		1	0	0

Table 3: Fictional properties of products and factors of production associated with the CHP plant (top) and the cattle (bottom) examples, respectively. This table results from the concatenation and transposition of the four Λ matrices (Tables SI-2, SI-3, SI-7 and SI-8), and all properties are normalized relative to the units of inventory for each product/factor in the mixed-unit SUTs (tables 1 and 2).

The different layers of the multi-unit SUTs of these two examples are presented in section SI-6. As indicated by the absence of residuals, these examples are fully balanced in every property layer.

4.2   Partition allocation

Partition allocation splits the flows of a multifunctional activity. It assigns requirements to each coproduct proportionately to its share of the activity's total supply in terms of a selected "partitioning property" (e.g., economic value, mass, energy content) (Guinée, 2002; Heijungs and Guinée, 2007). In a value-based PA, for example, joint requirements of industry J are split across coproduction flows proportionately to their share of the total economic value.

$$\text{requirements of } j = \text{requirements of } J \times j\text{'s share of partitioning property} \quad (7)$$

We substitute the equations representing partition-allocated flows (equations (SI-7) and (SI-8)) in the equation defining the balance of property m in allocated flows (equation (6)). The resulting equation (SI-24) thus defines the criterion for the balance of property m in partition-allocated flows, and its solution set then necessarily corresponds to all situations where PA leads to balanced recipes. This solution set is expressed in words by proposition 1, with the associated proof in section SI-3.2.

Proposition 1 (PA recipe balance). *All recipes modeled by the partition allocation of the balanced inventory of an activity J will themselves be balanced in terms of property m if and only if the ratio between this property m and the partitioning property is equal for all coproducts supplied by this activity J.*

In other words, the partitioned flows of an industry will be balanced in terms of a property m if and only if this property is found in all coproducts proportionately to the partitioning property, that is, in a constant ratio (α). For example, in the case of a fishing industry co-catching different species of fish, the production functions modeled by mass-based PA will be energy balanced only if all fish species have the same energy density, that is, a constant ratio exists between energy and mass across all coproducts.

A first implication of this proposition is that partitioned flows are guaranteed to be balanced in terms of the partitioning property.[10] Thus, as was pointed out by Weidema and Schmidt (2010), mass-based partition leads to mass-balanced flows, energy-based partition to energy balanced flows, etc.

The other extreme case that guarantees compliance with proposition 1 occurs when a property is completely absent from all coproducts of an activity. In such a case, the ratio between this property and any partitioning property is necessarily constant and equal to zero for all coproducts, which ensures that all modeled production functions will be balanced with respect to this property. For example, the PA of a CHP plant producing electricity and heat will necessarily lead to a system description that is carbon-balanced *regardless of the choice of partitioning property*, as none of its supply flows contain carbon.

Let us examine the *value-based partition allocation* of the example CHP plant. According to proposition 1, any property that is found in a fixed proportion to the financial value (partitioning property) in all coproducts will be balanced in the allocated flows. Trivially, the financial value is proportionate to itself and should be conserved in this allocation. In addition, table 3 shows that the carbon content of electricity and heat is "proportionate" to financial value, with a proportionality factor of $\alpha = 0$, and therefore the allocated recipes should also respect carbon balance. Conversely, the ratio between energy content and economic value is different for heat and electricity (comparing columns 1 and 2 of table 3), and therefore the value-based PA should necessarily lead to an energy imbalance.

The partitioned recipes for electricity and heat production are represented as layers of value, energy and carbon flows in table 4. As expected, the economic and carbon layers are balanced, but the energy layer presents a residual. The value-based PA thus leads to recipes with inputs and outputs that are well matched in terms of value and carbon content but not energy content; the modeled electricity production seems to "destroy" energy, whilst the modeled heat production seemingly "creates" energy.

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[10] In this case, the ratio between property m and the partitioning property is necessarily constant ($\alpha = 1$) for all coproducts, as these two properties are one and the same.

PA	Value Layer ($)		Energy Layer (kJ)		Carbon Layer (kg)	
	electricity	heat	electricity	heat	electricity	heat
Supply	1.0	1.0	51	566	0	0
Product requirements:						
electricity	0	0	0	0	0	0
heat	0	0	0	0	0	0
coal	0.39	0.39	135	135	3.5	3.5
Factor requirements:						
CO_2	0	0	0	0	−3.5	−3.5
O_2	0	0	0	0	0	0
waste heat	0	0	−40	−40	0	0
labor	0.61	0.61	0	0	0	0
Residual	0	0	43	−471	0	0

Table 4: Flows allocated with value-based PA to electricity and heat generation, and further split in terms of their monetary, energy and carbon content layers. The presence of a residual indicates an imbalance.

The "surplus method" is a special case of PA that is based on the property of being a primary product or not (Heijungs and Suh, 2002). With such a binary partitioning property, requirements are partitioned such that they are fully ascribed to the primary product, leaving secondary products burden-free. From proposition 1, such modeling can only be balanced for properties that are proportionate to the partitioning property, that is, properties that are fully absent from any secondary product.

4.3 Product substitution allocation

Product substitution allocation isolates a monofunctional recipe for a primary product by assuming that secondary productions substitute other productions outside of the investigated system (Guinée, 2002). Secondary products are thus removed (as they leave the system boundary) and the activity is given credit by recording the avoided primary products as negative requirements.

$$\text{requirements of } j = \text{requirements of } J - \text{products avoided} \qquad (8)$$

For example, requiring one more unit of electricity from CHP without requiring additional heat can be represented as [1] requiring additional electricity in the system and [2] requiring that someone outside of the system reduces their production of heat (hence the negative requirement of heat) (Weidema, 2000; Ekvall and Weidema, 2004). Substitution is often modeled between identical products, products with a common functionality (Weidema, 2000), products of equal value (Werner and Scholz, 2002; Huppes, 2000), or based on broader market analyses and price elasticities (Ekvall, 2000; Dandres et al., 2012).

Although this modeling technique is not identical to the classical definition of system expansion, it is often referred to as such (Wardenaar et al., 2012; Heijungs, 2013), along with another modeling technique (see section 4.4) (Majeau-Bettez et al., 2014). We use different names here to avoid confusion.

To formalize substitution allocation in mathematical terms, an observation of the substitutability between commodities must be recorded in a *substitution matrix*. For example, if each unit of secondary production of j reduces the consumption of i by 0.8 units, a substitution coefficient of 0.8 exists between these two products. We combine the equations that represent substitution-allocated flows (equations (SI-9) and (SI-10)) with the equation defining the balance of property m in allocated flows (equation (6)), and the resulting equation then necessarily represents the criterion for the balance of property m in substitution-allocated flows (equation (SI-30)), as expressed in proposition 2.

Proposition 2 (PSA recipe balance). *The technical recipe modeled by the PSA of the balanced inventory of an activity J will itself be balanced in terms of a conservative property m if and only if this property is found in equal total amount in the secondary supply flows of J and in the substituted flows.*

Because the sufficient and necessary condition for PSA balance is expressed in terms of a sum total amount of m over all substitutions, there is a possibility for multiple imbalanced substitutions to cancel out each other and yield a balanced PSA by sheer coincidence. As this is neither practical nor likely, we focus rather on the set of all *systematically* balanced PSA allocations in corollary 2.1.

Corollary 2.1 (Systematic PSA recipe balance). *The technical recipe modeled by the PSA of the balanced inventory of an activity J will be* systematically *balanced in terms of a conservative property m if and only if, for each secondary production by J, this property is found in equal amount in this secondary production and the production flow that it substitutes.*

In other words, a secondary supply that contains a given amount of m must substitute a primary supply that contains an equal amount of m in order to not cause imbalance to the PSA allocation (proof in section SI-3.3).

In the dairy farm example, milk is the primary product, as it provides the majority of the revenues (Londero, 1999). It should also be noted that cow meat is not exactly identical to steer meat in this example: it has a slightly lower economic value and a lower fat content. This lower mass concentration of lipids leads to an overall lower carbon content in cow meat, as detailed in table 3. Let us assume that \$1 of cow meat can substitute \$1 of steer meat in this fictional market.[11] Given these parameters, we investigate which balances will be respected by PSA in table 5.

From corollary 2.1, the PSA-based recipes will be balanced with respect to a given property if this property is found in equal amount in each secondary product (\$1 of cow meat) and in the product flow it avoids (\$1 of steer meat). Comparing the rows of table 3 quickly reveals that this condition is fulfilled in terms of neither dry mass nor carbon content. Thus, the only dimension for which this substitution will be balanced is the financial layer, which explains the mass and carbon residuals in table 5.

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[11] This is a reasonable substitution assumption, considering how these products are physically similar and how equal willingness to pay is supposed to roughly reflect equal levels of utility. In LCA parlance, they could therefore be assumed to have similar functionality.

PSA	Value Layer ($)		Mass Layer (kg)		Carbon Layer (kg)	
	milk	steer meat	milk	steer meat	milk	steer meat
Supply	1.9	6.1	1.0	1.0	0.54	0.62
Product requirements:						
milk	0	0	0	0	0	0
steer meat	−0.28	0	−0.047	0	−0.029	0
feed	1.8	5.0	7.0	20	2.8	8.1
Factor requirements:						
manure	0	0	−4.9	−17	−2.0	−6.8
respiratory water	0	0	−0.43	−1.0	0	0
CO_2	0	0	−1.1	−2.5	−0.29	−0.68
O_2	0	0	0.41	1.3	0	0
labor	0.44	1.1	0	0	0	0
Residual	0	0	0.012	0	2.0×10^{-3}	0

Table 5: Flows allocated with PSA and further split in terms of their monetary, mass, and carbon content layers. The presence of a residual indicates an imbalance.

4.4 Alternate activity allocation

We can identify a third allocation technique, which we refer to as alternate activity allocation. This modeling technique, which has also been referred to under the umbrella term "system expansion" along with PSA, assumes technical recipes for secondary products and assigns the remainder of the joint requirements to the primary product (Majeau-Bettez et al., 2014). The technology assumptions for secondary products are based on the technological description of alternate, primary productions, hence the name.

$$\text{requirements of } j = \text{requirement of } J − \text{assumed requirements for coproducts} \tag{9}$$

For example, it could be assumed by AAA that producing a certain amount of cow meat has the same requirements as producing an equivalent amount of steer meat, and the remainder of the requirement of the dairy cow farming would be ascribed to milk production. In other words, we assume that producing cow meat is technologically similar to producing steer meat, and we use this assumption to split the requirements between milk production and cow meat production. Contrary to PSA, which is based on the substitutability between two commodities, AAA is thus based on assumptions as to the technical similarity of productions. This allocation does not depend on a market analysis, as nothing is "avoided" (cf. equations (8) and (9)).

Formalizing AAA requires the identification of an alternate producer for each secondary product, and this choice may be recorded in the industry-by-product *alternate activity matrix*. Furthermore, with a multi-unit inventory, a choice must be made as to what unit will be used in the alternate technology assumption. For example, if cow meat and steer meat are not identical across all properties, we must choose relative to what property a technological equivalence will be assumed. Do we assume that the steer and cow have the same requirement per kilogram (kg) of meat? Per MJ of meat? Per $ of meat? Let us refer to this property as the *production equivalence property*.

Combining AAA equations (equations (SI-11) and (SI-12)) with the equation defining the balance of property m in allocated flows (equation (6)) yields an equation representing the balance of m in alternate-activity-allocated flows (equation (SI-33)). The solution set of this equation, which necessarily corresponds to the set of all situations where AAA leads to balanced recipes (section SI-3.4), is expressed in proposition 3.

Proposition 3 (AAA recipe balance). *Let the alternate technology descriptions ($\mathbf{A}^\Gamma$ and $\mathbf{F}^\Gamma$) be balanced with respect to property m. Then all recipes derived by the alternate activity allocation of a balanced activity J will themselves be balanced with respect to property m if and only if the amount of m in each secondary product of J is equal to the amount of m in the primary product of its associated alternate technolgy.*

In other words, AAA-based recipes will be balanced in terms of a property m if the assumed requirements for each secondary product are taken from the production of a "technological proxy" that contains an equal amount of m.

For the AAA of dairy cow raising, let us use steer meat production as the best technological proxy for cow meat growth. Furthermore, we assume that these animals' requirements for muscle growth are most similar per kg of muscle (rather than per energy content or protein content, for example). We therefore assume the same requirements to produce a certain mass of meat, regardless of whether it is steer or cow meat. We analyze which balances are upheld by such a coproduction model in table 6.

Because the splitting is based on the assumption of a technical equivalence per mass of meat, the mass balance is necessarily respected. On the other hand, as an equivalent mass of steer meat contains more value and more carbon than cow meat, proposition 3 is violated in these layers, giving rise to residuals.

AAA	Value Layer ($)			Mass Layer (kg)			Carbon Layer (kg)		
	milk	cow meat	steer meat	milk	cow meat	steer meat	milk	cow meat	steer meat
Supply	1.9	4.9	6.1	1.0	1.0	1.0	0.54	0.53	0.62
Product requirements:									
milk	0	0	0	0	0	0	0	0	0
cow meat	0	0	0	0	0	0	0	0	0
steer meat	0	0	0	0	0	0	0	0	0
feed	1.5	5.0	5.0	5.9	20	20	2.4	8.1	8.1
Factor requirements:									
manure	0	0	0	−3.9	−17	−17	−1.6	−6.8	−6.8
respiratory water	0	0	0	−0.37	−1.0	−1.0	0	0	0
CO_2	0	0	0	−0.92	−2.5	−2.5	−0.25	−0.68	−0.68
O_2	0	0	0	0.33	1.3	1.3	0	0	0
labor	0.38	1.1	1.1	0	0	0	0	0	0
Residual	−0.071	1.2	0	0	0	0	-5.2×10^{-3}	0.090	0

Table 6: Flows allocated with AAA and further split in terms of their monetary, mass, and carbon content layers. The presence of a residual indicates an imbalance.

Contrary to PSA, AAA explicitly describes the production of secondary products in the system; they do not leave the system or avoid anything. Thus, cow meat and steer meat are both present.

It is interesting to note that, although PSA and AAA both lead to imbalances in the carbon layer, these imbalances are of opposite signs. In PSA, the allocated

recipe for milk production showed an excess of carbon (positive residual), while the alternate-activity-allocated recipe presents a carbon deficit (negative coefficient). Relative to steer meat, cow meat contains more carbon per $, the property governing substitutability in PSA, but less carbon per kg, the property guiding technology assumption in AAA.

4.5 Balance of all properties in allocation

No allocation scheme can claim to always respect all balances. The assessment of the balance of property m requires that this property be put in relation to the partitioning property (in the case of PA), to the production equivalence property (in the case of AAA), or to the presence of this property in substituted products (for PSA).

What about the respect of *all* balances? Can an allocation systematically yield recipes that are fully consistent with all conservative properties of the product system? Extending the above rules for property m to all properties, and thus describing stricter balance criteria, leads to the following corollaries:

Corollary 1.1 (Balanced PA across all layers)**.** *Technical recipes modeled by partition allocation will respect all balances if and only if all coproducts are identical to each other in terms of all conservative properties.*

Corollary 2.2 (Balanced PSA across all layers)**.** *Technical recipes modelled by product substitution allocation will* systematically *respect all balances if and only if each secondary product perfectly substitutes (1:1 ratio) a product from primary production that is identical in terms of all conservative properties.*

Corollary 3.1 (Balanced AAA across all layers)**.** *Technical recipes modeled by alternate activity allocation will respect all balances if and only if the technology assumed for each secondary commodity is taken from an activity that primarily produces a commodity that is identical in terms of all conservative properties.*

An illustration of corollary 3.1 is provided by Weidema and Schmidt (2010). The reason why their AAA allocation of a dairy cow is balanced across all layers is that the cow produces a meat that is assumed identical to steer meat.

4.6 Balanced recipes from constructs

Constructs can always be expressed in terms of repeated allocations, either directly or with an additional aggregation step. We find that the rules governing the balances of the underlying allocations of a construct will necessarily also apply to the construct itself (section SI-2.2).

Proposition 4. *Each recipe in a traceable or aggregation construct will be balanced with respect to a property m if this construct is based on allocations that conserve this property m.*

We refer to all EEIO constructs applicable to a traditional SUT as *aggregation constructs*, as they can be split in two steps: an allocation of all industries, and then a summation step to describe an average recipe for each product (Majeau-Bettez et al., 2014). As the sum of any two balanced recipes will itself be balanced

(lemma 3, section SI-3.5), an aggregation construct that is based on balanced allocations will necessarily also be balanced. The rules devised for PA, PSA and AAA thus also apply to aggregation partitioning construct (aPC), aggregation product substitution construct (aPSC), and aggregation alternate activity construct (aAAC).

Since none of the different allocation families can be qualified as balanced in general, neither can the different aggregation construct families. However, BTC is a special case of the aPSC that requires exactly the conditions that lead to a balanced PSA across all layers (corollary 2.2): it is based on the assumption of a 1:1 substitution between identical products. Similarly, CTC is a special case of aAAC that respects corollary 3.1: it requires that each secondary production be resolved with the technology of an identical product from a (unique) primary production.

The ESC is a special case of the aPC based on the surplus method, and its balances then follow that of this special case of PA: only properties absent from secondary products will be balanced in the resulting ESC recipes.

It could be argued that the ITC is not, strictly speaking, appropriately defined for application to a multilayered SUT. If an aPC is applied using the same partitioning property for every industry, then the resulting flow matrix will respect the industry technology assumption in the layer of this partitioning property, but not in the other layers (Majeau-Bettez et al., 2014). Regardless, any property layer that does respect the ITC definition is also necessarily balanced, following proposition 1.

Beyond traditional SUT, some inventories contain additional data and record use flows that are traceable to a specific supplier, thus adding an extra dimension to the use table ($\mathbf{U}_{*\bullet*}$) (Majeau-Bettez et al., 2014). In this case, the coefficient u_{IiJ} denotes the use by activity J of product i sourced specifically from industry I, rather than from the average production mix.[12] From such a StUT, a symmetric system description is simply obtained by applying allocation to each industry in turn, without need for aggregation or any further modeling (see section SI-2.2). As traceable constructs are simply repeated allocations, the insights from sections 4.2 to 4.5 directly apply to traceable partitioning construct (tPC), traceable product substitution construct (tPSC), and traceable alternate activity construct (tAAC).

5 Production balances

In the previous section, we examined how different models generate balanced recipes across multiple property layers from initially balanced industry descriptions (figure 1, column sums). We now turn to assess whether these models respect or perturb the balance between production and consumption initially found in the SUT inventory (figure 1, row sums).

The question is as follows: Can the model reproduce the total production and consumption flows of the inventory from which it was derived, or does it perturb the market balances in this system? More specifically, does the model calculate total production levels ($\mathbf{x}$) equal to the inventoried production levels for each

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[12]Product traceability in supply and traceable use table (StUT) inventories can be put in relation to the one-brand axiom in the LCA literature (Heijungs and Suh, 2002).

commodity (i.e., $\mathbf{Ve}$) when it is applied to a final demand ($\mathbf{y}$) equal to the original inventoried final demand ($\mathbf{h}$)? Thus, the criterion can be expressed as follows:

$$\mathbf{Ve} = \left(\hat{\mathbf{E}} - \mathbf{A}\right)^{-1}\mathbf{h} \tag{10}$$

This test, which can be simplified to equation (11) as shown in section SI-4.1,

$$\mathbf{AVe} = \mathbf{Ue} \tag{11}$$

is identical to the "material balance" test of Jansen and ten Raa (1990).[13]

The simplification to equation (11) offers the opportunity to evaluate how allocations fit in the overall production balance. If the technical coefficients resulting from the allocation of industry J (in $\mathbf{A}_{\bullet J\bullet}$) are scaled to fit the original production level of industry J (i.e., multiplied by $\mathbf{V}_{\bullet J}$), do they add up to the inventoried requirements of industry J (equation (12))? If yes, the allocation in question does not perturb the system's production balance, and vice versa otherwise (proposition 5).

$$\mathbf{A}_{\bullet J\bullet}\mathbf{V}_{\bullet J} = \mathbf{U}_{\bullet J} \tag{12}$$

As demonstrated in sections SI-4.2 and SI-4.3, PA and AAA are always production-balanced. On the contrary, PSA necessarily perturbs the production balance (section SI-4.4).

Constructs mirror the balances of their underlying allocations. Thus, partition-based constructs (tPC, aPC, ITC, ESC) and alternate activity constructs (tAAC, aAAC, CTC) are always production balanced, whilst product substitution constructs (tPSC, aPSC, BTC) are not (section SI-4.1). This broad assessment of production balance in the different allocation and construct families extends, and is in accordance with, the analysis of ITC, CTC and BTC by Jansen and ten Raa (1990).

6 Result synthesis

6.1 Overview of Balances in Allocations and Constructs

Table 7 summarizes the balances respected by the different model families. BTC and CTC are presented as special cases of product substitution construct (PSC) and alternate activity construct (AAC), respectively.

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[13] We preferred to instead designate this balance as the "production balance" because it relates to products rather than materials. Many products, especially services, do not have a clear material dimension, and yet their production and consumption must be balanced. Furthermore, it could have lead to confusion with mass and elemental balances, which are are assessed within industries (columns) rather than product markets (rows).

Model	balanced recipes across all layer	production balance	can represent exclusive secondary products
PA/PC/ITC/ESC	✗[1]	✓	✓
PSA/PSC	✗[2]	✗	✓
- BTC	✓	✗	✗
AAA/AAC	✗[3]	✓	✓
- CTC	✓	✓	✗

[1] : Balanced across all layers if and only if all coproducts are identical to each other within each industry.

[2] : Systematically balanced across all layers if and only if each secondary coproduction perfectly substitutes an identical commodity from primary production.

[3] : Balanced across all layers if and only if the technology assumed for each secondary coproduction is taken from an alternate activity that primarily produces an identical commodity.

Table 7: Overview of the different allocation and construct models in terms of [1] their capacity to generate balanced multilayered production functions, [2] their respect for production balance, and [3] their capacity to describe exclusive secondary products. The rows regroup different *partition models* — partition allocation (PA), partitioning construct (PC), industry technology construct (ITC), and European system construct (ESC) —, *substitution models* — product substitution allocation (PSA), product substitution construct (PSC) and byproduct technology construct (BTC) — and *alternate activity models* — alternate activity allocation (AAA), alternate activity construct (AAC) and commodity technology construct (CTC).

None of the model families investigated can be said to always yield balanced recipes (table 7, column 1). They all have the capacity to do so, however, depending on special characteristics of the SUT inventories (table 7, notes 1-3).

The special case that allows partition models to yield balanced recipes across all layers is perhaps the narrowest, as coproducts are not typically identical to each other across all properties of interest. Specific partitioned recipes may nonetheless be balanced across a number of layers, especially in situations where the coproducts have no or few physical dimensions.

The special cases that allow for fully balanced PSA and AAA are perhaps more common. Only in situations where a secondary product displaces and identical primary product (for PSA) or is allocated the same production requirements as those of an identical product (for AAA) will these allocations be balanced. These prerequisites overlap with the conditions that define BTC and CTC as special cases of these model families, and therefore BTC and CTC will always lead to balanced recipes across all layers. These special cases, however, come with an obvious restriction: for each secondary commodity, there must exist an industry that primarily produces an identical commodity. In other words, the inventory must be devoid of *exclusive secondary products* (table 7, third column). Alternate activity and product substitution models cannot be fully balanced if a secondary product is unique in terms of any of the conservative properties of interest.

The balance across multiple layers in modeled recipes is thus function of the similarity between products: similarity between coproducts in PA, between substituting products in PSA, and between technological proxies in AAA. In practice, however, the similarity between product groups is largely a question of classification and aggregation, as explored in section 6.3.

The question of market balances is more clear cut (table 7, second column): partition and alternate activity models are production-balanced, whereas substitution models are not. Contrary to mass or energy balance, however, the disruption of market balances can be intentional, depending on the question at hand, as explored in section 7.

6.2 Balances and waste treatment

The above results are articulated in terms of coproduction of commodities, but they are also directly applicable to the production and treatment of waste, as briefly discussed in this section.

Because of the many competing definitions of what constitutes a waste (cf. Frischknecht 1994; Weidema 2000; Heijungs and Suh 2002; ISO 2006; Schmidt et al. 2012), and because it may prove practically difficult to distinguish between a waste and a low-value byproduct (Nakamura and Kondo, 2002), there are two distinct methods for recording waste flows in an inventory. Before any allocation or construct is applied, it must be determined whether each waste flow should be considered a functional flow or not.

If a "waste" still has residual value, we may represent a waste-producing activity as *supplying* this waste to the technosphere, and a waste-treating industry as *using* this waste (see figure SI-1). The "waste" flow is thus treated exactly like a byproduct, and the waste-producing activity is then multifunctional. For example, the different allocations and constructs can be applied to a car manufacturer producing cars but also selling metal scrap. As a fraction of the requirements may then be allocated to the "waste" supply, the lifecycles of the products that derive from recycling may then include impacts generated in the initial waste production (Chen et al., 2010). This is notably the approach taken by methods that split environmental impacts of a first lifecycle across multiple recycling cycles (as reviewed by Ekvall and Tillman, 1997; Finnveden, 1999; European Commission, 2010). As this inventory choice simply treats waste like any other byproduct, our analysis of balances in allocations and constructs is directly applicable.

Conversely, a waste-producing activity may be recorded as *using* waste treatment services, and a waste-treating activity as *supplying* this service (see figure SI-1). This approach is more applicable to situations where the waste has a negative value, that is, the waste-treating activity provides a valuable service by accepting the waste and must be compensated for it (Heijungs and Suh, 2002). With this framework, it is the waste-treatment industry that is likely multifunctional, supplying both the treatment service and, for example, recycled materials or heat. Because this SUT representation does not record waste production as a functional supply flow, it automatically ensures that no requirement can be allocated to the waste, regardless of allocation or construct choices, and therefore products of the waste-treating activity cannot be held accountable for the lifecycle of the processed waste.

The original Leontief (1970) Pollution Abatement Model, the waste-IO models (Nakamura and Kondo, 2002), ecoinvent 2 (2010), ecoinvent 3.1 consequential or cut-off (2014), and FORWAST (Schmidt et al., 2010) all notably rely on the second inventorying strategy, representing waste treatment activities as supplying a service. That these models apply this strategy with different sign conventions

has no implication on lifecycle results or on our capacity to assess balances across multiple unit layers; equation (2) remains valid as long as signs are chosen correspondingly in the property table $\mathbf{\Lambda}$ (see section SI-5). Our analysis of the different allocations and constructs in table 7 is therefore directly applicable.

With substitution models (PSA/PSC/BTC), the byproducts of waste treatment industries displace products from primary production. This is notably the approach taken by the waste-IO model (Nakamura and Kondo, 2002), consequential studies in LCA (Weidema, 2000), and dynamic-MFAs of metals (e.g. Pauliuk et al., 2012). The so-called "value-corrected substitution" (Werner and Scholz, 2002; Huppes, 2000), "market-based" (Ekvall, 2000), and "end-of-life recycling" (Atherton, 2006) methods —reviewed by (Johnson et al., 2013)— also all apply substitution models to multifunctional waste treatment; they only differ in terms of how the substitution coefficients are determined. From table 7, all these substitution models will be fully balanced only if secondary products from waste treatment perfectly displace identical products from primary production.

Partition (PA/PC/ITC/ESC) models may split the requirements of a waste treatment activity based on any property of its treatment services and its coproducts (e.g., Heijungs and Guinée, 2007). From our analysis, such modeling will be balanced in terms of any property that scales proportionately to the partitioning property for all coproducts. For example, financial balance is guaranteed for value-based PA of waste-treatment activities.

The so-called "recycled content" or "cut-off" method to waste treatment — which [1] allocates no burden on waste entering a new recycling cycle (Finnveden, 1999; European Commission, 2010; Johnson et al., 2013), [2] allocates no burden on byproducts of waste-treatments, and [3] allocates all direct requirements of the waste-treating industry on its primary functional supply flow (Ecoinvent Centre, 2014)— is conceptually identical to the surplus method (Heijungs and Suh, 2002) or the ESC applied to a multifunctional waste treatment. Regardless of the name, they all apply PA based on the property of being a primary product or not. Such models will be balanced only for properties that scale proportionally to this partitioning property, that is, properties that are completely absent from any byproducts or waste supply flow.

For any given waste, the decision of whether to consider its production as a functional output or its consumption as a functional input has, of course, significant impacts on the inventory structure and, potentially, on the lifecycle results. Irrespective of this choice, however, the different allocations and constructs listed in table 7 remain applicable, and so is our analysis of their impact on the original inventory balances. We therefore find it counterproductive to discuss multifunctionality in waste production/treatment differently and separately —notably with a distinct jargon— from any other forms of coproduction.

6.3 Exclusive secondary products and aggregation error

In table 7, CTC is the only model that always yields balanced recipes and balanced markets. Although it might be tempting to disregard the problem of exclusive secondary products and declare a clear winner (cf. Jansen and ten Raa (1990)), the tradeoffs are more complex. First, Suh et al. (2010) demonstrated that CTC and BTC always lead to equal total lifecycle impact calculations. Second, and most

importantly, the inability of BTC and CTC to handle exclusive secondary products may force practitioners to aggregate their inventories in ways that introduce imbalances *before* the allocation/construct step.

The production of molasses, the harvest of straw, and the mining of tellurium are classic examples of exclusive secondary coproductions (United Nations, 1968); no industry primarily supplies these commodities, and their coproduction is always secondary to that of sugar, grain, and copper (Nassar et al., 2012), respectively. With enough resolution, even small differences can distinguish a secondary product as unique and therefore exclusive, as was the case for "cow meat" in our example. To enable the CTC or the BTC, such products must be removed from the SUT. In practice, this is done by reducing the resolution of the inventory. For example, molasses, sugar, and maple syrup could be aggregated as "sweeteners", straw and lumber as "biomass", tellurium and copper as "non-ferrous metals". Clearly, there are industries that primarily produce sweeteners, biomass, and non-ferrous metals; BTC and CTC are then applicable.

The problem with these aggregations of exclusive byproducts is that they coarsely combine products that are dissimilar and consumed in different ratios in different industries, creating inhomogeneous product mixes. This, in turn, destroys the initial column balances in the multilayered SUT and exacerbates aggregation error in lifecycle results (Weisz and Duchin, 2006). For example, let us have straw burned for local district heating and wood used for lumber. If we aggregate these two products, the district heating and the construction industry are described as requiring the same input: "biomass". Since straw and wood are not identical across all dimensions —e.g., they may differ in terms of sulfur content (cf. Knudsen et al., 2004; Nagel et al., 2009)— this aggregation will lead to a mismatch between the recorded fuel inputs to district heating and its observed outputs (e.g., SO_2 emissions). A similar mismatch would exist between the recorded inputs to construction and the actual composition of the building.

There is thus potential for problem shifting: in order for allocation and construct models to respect all balances of the inventory, practitioners must somehow work at a coarser resolution level, which in turn causes imbalances of its own in the inventory. Forcing the data collection in the straightjacket that is a "square SUT", where each commodity is the primary product of exactly one activity, seems counter-productive: in order to use a cleaner, balanced allocation or construct, we sacrifice the quality of the data compilation. This touches upon the boundary between observation and modeling. Where does the faithful observation of the world end? Where does modeling, gap filling, and projection start?

7   Discussion: What balance for what question?

In response to the title question of this article, we found that none of the allocation or construct model families are unconditionally balanced; only special cases can guarantee the simultaneous respect of all balances (table 7). Furthermore, these special cases depend partly on the level of aggregation, which can have negative implications of its own. These findings lead to the follow-up question of when these balances matter. What balances are required for what purpose?

If a study aims to track the flow and accumulation of materials, energy and value through the economy, balanced recipes are required, by definition. The use of

the Waste-IO model to track stocks and flows of various metals (Nakamura et al., 2008, 2011) constitutes a good example of such an analysis. More generally, any study at the frontier between MFA and LCA/EEIO must be particularly mindful of these balances. A computer manufacturer claiming that its products do not *contain* more than x% conflict metals, for example, is making a statement about the *accumulation* of materials through the lifecycle value chain of their product, and this certainly requires mass balances.

Footprinting and burden attribution studies split a total impact inside a closed system amongst all its different product flows. This implies that these product flows must be balanced within the system, and therefore production-balanced models (partition or alternate activity) seem required for this type of lifecycle question. The role of the other balances, however, is less clear. Attributional studies assign responsibility for a share of an impact, and the link between responsibility and physical balances is perhaps more subjective. For those arguing that industries exist for profitability and that responsibility follows the money (e.g., Weinzettel, 2012), physical balances should not be strictly required to connect a consumption to an impact. This logic would best fit a partition-allocation approach, where a single property (e.g., economic value) determines the split of all other layers (as reviewed by Ardente and Cellura, 2012).

For studies that rather model changes in open product systems, such as marginal consequential LCAs (Ekvall and Weidema, 2004; Zamagni et al., 2012), the production balance would actually be expected to *not* hold. If activities are understood as exchanging products directly with other activities outside the system boundary, then production and consumption do not need to be matched inside the system. This is well aligned with substitution models, in which products can leave the system under investigation to avoid production elsewhere. In terms of balanced recipes across property layers, it should be noted that a consequential "recipe" models not the whole production of a product but rather the changes caused by an additional production. As such changes include market-mediated flows, a match between the contents of inputs and output seems to not be required by this type of question.

Thus, just as our analysis cautions against general statements about the balanced character of a model without taking the underlying data into account, we also warn against overstating the universal necessity of these balances in allocated flows without considering the research question at hand.

8   Conclusion

This article identified the data characteristics required in order for the different allocation and construct models to simultaneously respect material, energy, financial and production balances. We found that previous assessments did not do justice to the complexity of the situation. None of the modeling families examined can be qualified as balanced in general, as their ability to respect balances across multiple layers depends on special characteristics of the inventories to which they are applied.

Furthermore, we found that such special cases are partly determined by the level of data aggregation. Notably, although CTC has been promoted for its ability to respect all balances, this ability depends on the pre-aggregation of the

SUT data to remove exclusive secondary products, which in turn necessarily leads to inhomogeneous product mixes and... imbalances.

Our assessment of the different allocations also illustrated how two models that have historically been collectively referred to as "system expansion" can behave very differently. In our allocation of a dairy cow's requirements, PSA and AAA differed in their allocation logic, their respect for production balances, the number of products within the system boundary, the layers that presented residuals (imbalances), and the signs that these residuals had. In the light of the ongoing attributional-consequential divide and the convergence of LCA and EEIO, it appears clearly that the opposition of "partition"-versus-"system expansion" is insufficient. Three modeling families, not two, dominate the LCA and EEIO literature.

In terms of research implications, we found that some questions are deeply affected by the respect of multiple balances, while others are not. The material and energy balances loom large over the integration of lifecycle analyses with MFA. The respect or perturbation of market balances partly distinguishes attributional and consequential assessments. The link between burden attribution and physical balances is more debatable however, and the bearing of these balances on consequential questions seems even more tenuous. Further research is required in this domain, and care should therefore be taken to not raise these balances as universal imperatives for modeled product systems.

Regardless of modeling choices and research questions, however, the credibility of the initial data is crucial to any system's analysis. Material, energy, financial and production balances remain essential quality checks for industrial ecology inventories. We therefore recommend that data collection steps be divided from modeling as much as possible. The practice of forcing observations in an aggregated "square" SUT to facilitate the application of certain models is counterproductive. Practitioners should make no compromise in publishing multilayered SUT inventories that are as detailed and balanced as possible, ensuring the physical and economic credibility of the initial survey data and a broader range of potential uses. It then falls upon the modeler to decide which allocations and constructs will best fit the question at hand, taking into account the additional aggregation that these models may require and the imbalances that they may introduce.

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