

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

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## Abstract

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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.

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# Introduction

## 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; 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 lifecycle 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.

## 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 Huppel, 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 ecospold2 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). The 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 Raa, 1990; ten Raa and Rueda-Cantuche, 2007; European Commission, 2008).

LCA allocations and EEIO constructs bear little resemblance 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 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; Huppel, 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 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 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.

## 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 imbalances 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 *Exclusive secondary products and aggregation error* and *Sensitivity to inhomogeneity in product groups*).

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

This article first presents the defining characteristics and balances of a multilayered SUT. We then derive 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 the *Result synthesis* section. We then discuss practical implications for various research questions.

## SUT inventory

### Mixed-unit SUT

Both LCA and EEIO inventories describe the technosphere in terms of a set of activities ( $\star$ ) 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 ( $\mathbf{V}_{\bullet\star}$ ). The requirements of these activities are then recorded in two separate tables: a use table ( $\mathbf{U}_{\bullet\star}$ )<sup>1</sup> for product requirement and an extension table ( $\mathbf{G}_{\star\star}$ ) 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,  $\text{O}_2$ , 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).

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<sup>1</sup> 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 ( $\mathbf{U}_{\bullet\star}$ ), it becomes a SourceIndustry-per-commodity-per-industry table ( $\mathbf{U}_{\star\bullet\star}$ ).

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

## 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 ( $u_{fuel,CHP}^{carbon}$ ), whilst the economic value of this same fuel input would be found in the monetary layer ( $u_{fuel,CHP}^{monetary}$ ).<sup>2</sup>

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 ( $\Delta$ ) of products and factors of production in a property-per-product table ( $\Lambda_{\Delta\bullet}$ ) and a property-per-factor table ( $\Lambda_{\Delta\star}$ ), respectively, with each property normalized relative to the unit used in a mixed-unit SUT. Assuming homogeneous product groups (Weisz and Duchin, 2006),<sup>3</sup> 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

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<sup>2</sup> 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 ( $\mathbf{G}_{**}^{monetary}$ ) (Duchin, 2009).

<sup>3</sup> 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 7 of the SI.

service would be recorded in  $\mathbf{V}$  as a positive entry in the monetary layer and a negative entry in the mass layer (see SI, section 5).<sup>4</sup>

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.

## 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).

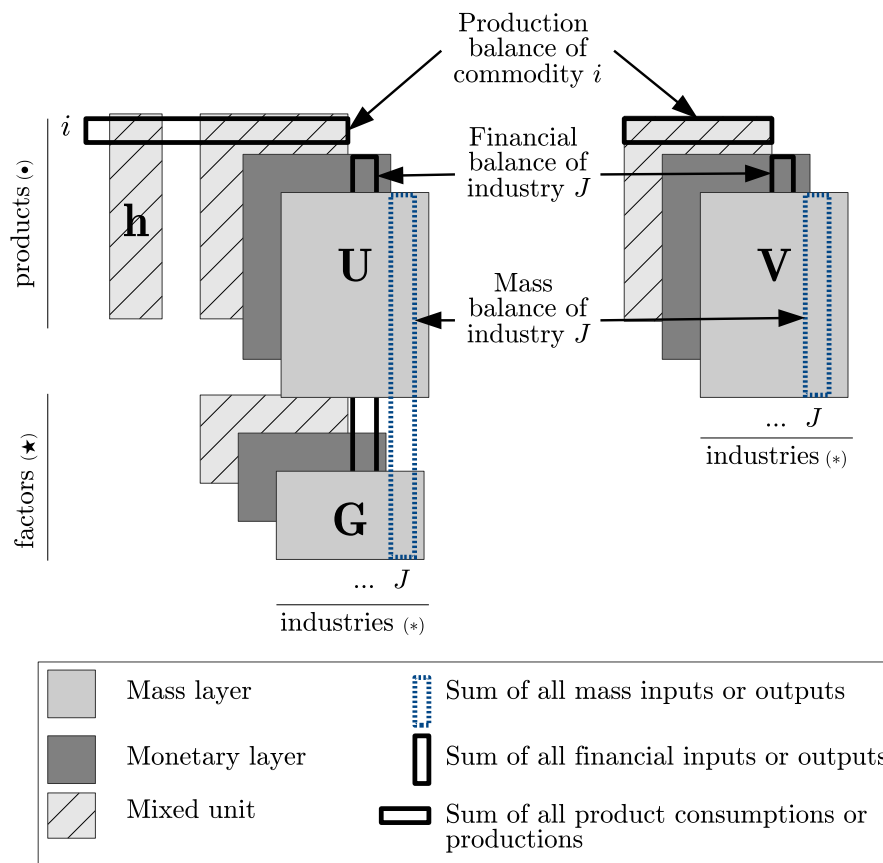


Figure 1: Multilayered supply ( $\mathbf{V}$ ) and use ( $\mathbf{U}$ ) inventory tables (SUT), with environmental extensions ( $\mathbf{G}$ ) and final consumption ( $\mathbf{h}$ ), derived from a mixed-unit layer (hatched). Column-sums in the different layers assess the financial and mass balances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

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

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

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

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

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  $(\mathbf{\Lambda}_{\Delta\bullet}, \mathbf{\Lambda}_{\Delta\star})$ .

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

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

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 from 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  $\left(\sum_{J \in \star} v_{iJ}\right)$  must be met by an equal total consumption, either intermediate  $\left(\sum_{J \in \star} u_{iJ}\right)$  or final ( $h_i$ ) (equation (3)).

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

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

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.



## 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.<sup>5</sup> 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 ( $i, j, k \dots \in \bullet$ ) by this specific activity, that is, allocated product flows  $\mathbf{Z}_{\bullet Ji}$ ,  $\mathbf{Z}_{\bullet Jj}$ , and  $\mathbf{Z}_{\bullet Jk}$ .<sup>6</sup>

$$\text{allocation} : \mathbf{U}_{\bullet J}, \mathbf{V}_{\bullet J} \rightarrow \mathbf{Z}_{\bullet J\bullet} \quad (4)$$

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<sup>7</sup> 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

<sup>5</sup> 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.

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

<sup>7</sup> 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.

coefficient matrix ( $\mathbf{A}$ ). Various aggregation constructs — notably the CTC, ITC, ESC, and BTC — thus produce product-by-product representations (equation (5)) based on different assumptions (United Nations, 1999; European Commission, 2008).<sup>8</sup>

$$\text{aggregation construct} : \mathbf{U}_{\bullet*}, \mathbf{V}_{\bullet*} \rightarrow \mathbf{Z}_{\bullet\bullet} \quad (5)$$

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?

## 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 before extending our analysis to IO constructs, making use of the fact that all constructs can be expressed either as multiple repeated or aggregated allocations (Majeau-Bettez et al., 2014) (see SI, section 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  $J$ :

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

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

## 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;<sup>9</sup> cow farming coproduces milk and cow meat, whereas steer farming solely produces steer meat.

<sup>8</sup> along with associated environmental extensions: *factor aggregation construct*  $\mathbf{G}_{**}, \mathbf{V}_{\bullet*} \rightarrow \mathbf{G}_{\bullet\bullet}$

<sup>9</sup> 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).

products/factors	units	Use flows	Supply flows	Factor requirements
		CHP	CHP	CHP
electricity	\$	0	23.6	
heat	\$	0	2.15	
coal	kg	105	0	
CO <sub>2</sub>	kg			-328
O <sub>2</sub>	kg			238
waste heat	kJ			-1.04 × 10 <sup>3</sup>
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

products/factors	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 <sub>2</sub>	kg					-4420	-754
O <sub>2</sub>	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.

products/factors	units	energy kJ	value \$	carbon kg	dry mass kg
electricity	$\text{\$}^{-1}$	51.4	1.00	0	
heat	$\text{\$}^{-1}$	566	1.00	0	
coal	$\text{kg}^{-1}$	33.0	0.0950	0.850	
CO <sub>2</sub>	$\text{kg}^{-1}$	0	0	0.273	
O <sub>2</sub>	$\text{kg}^{-1}$	0	0	0	
waste heat	$\text{kJ}^{-1}$	1.00	0	0	
labor	$\text{\$}^{-1}$	0	1.00	0	
milk	$\text{kg}^{-1}$		1.92	0.542	1
cow meat	$\text{kg}^{-1}$		4.85	0.533	1
steer meat	$\text{kg}^{-1}$		6.07	0.623	1
feed	$\text{kg}^{-1}$		0.250	0.402	1
manure	$\text{kg}^{-1}$		0	0.402	1
respiratory water	$\text{kg}^{-1}$		0	0	1
CO <sub>2</sub>	$\text{kg}^{-1}$		0	0.273	1
O <sub>2</sub>	$\text{kg}^{-1}$		0	0	1
labor	$\text{\$}^{-1}$		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  $\mathbf{A}$  matrices (Tables S2, S3, S7 and S8), 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 6 of the SI. As indicated by the absence of residuals, these examples are fully balanced in every property layer.

## 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 (S7) and (S8)) in the equation defining the balance of property  $m$  in allocated flows (equation (6)). The resulting equation (S24) 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 3.2 in the SI.

**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 ( $\alpha$ ). 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.<sup>10</sup> 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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<sup>10</sup> 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
<i>Product requirements:</i>						
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
<i>Factor requirements:</i>						
CO <sub>2</sub>	0	0	0	0	-3.5	-3.5
O <sub>2</sub>	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.

## 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.

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

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; Huppel, 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 the *Alternate activity allocation* section) (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  $j$  displaces 0.8 units of  $i$ , a substitution coefficient of 0.8 exists between these two products. We combine the equations that represent substitution-allocated flows (equations (S9) and (S10)) 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 (S30)), 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 3.3 of the SI).

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.<sup>11</sup> 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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<sup>11</sup> 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
<i>Product requirements:</i>						
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
<i>Factor requirements:</i>						
manure	0	0	-4.9	-17	-2.0	-6.8
respiratory water	0	0	-0.43	-1.0	0	0
CO <sub>2</sub>	0	0	-1.1	-2.5	-0.29	-0.68
O <sub>2</sub>	0	0	0.41	1.3	0	0
labor	0.44	1.1	0	0	0	0
Residual	0	0	0.012	0	$2.0 \times 10^{-3}$	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.

## 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.

$$\text{requirements of } j = \text{requirement of } J - \text{assumed requirements for coproducts} \quad (9)$$

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 (S11) and (S12)) 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 (S33)). The solution set of this equation, which necessarily corresponds to the set of all situations where AAA leads to balanced recipes (SI, section 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 technology.*

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
<i>Product requirements:</i>									
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
<i>Factor requirements:</i>									
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 <sub>2</sub>	0	0	0	-0.92	-2.5	-2.5	-0.25	-0.68	-0.68
O <sub>2</sub>	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	$-5.2 \times 10^{-3}$	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.

## 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 in their example produces a meat that is assumed identical to steer meat.

## 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 (SI, section 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 3.5 of the SI), 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 ( $\mathbf{U}_{**}$ ) (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.<sup>12</sup> 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 SI, section 2.2). As traceable constructs are simply repeated allocations, the insights from the analyses of PA, PSA, and AAA directly apply to traceable partitioning construct (tPC), traceable product substitution construct (tPSC), and traceable alternate activity construct (tAAC).

## 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 commodity

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<sup>12</sup>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).

(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:

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

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

$$\mathbf{AVe} = \mathbf{Ue} \quad (11)$$

is identical to the “material balance” test of Jansen and Raa (1990).<sup>13</sup>

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 6, in the SI).

$$\mathbf{A}_{\bullet J \bullet} \mathbf{V}_{\bullet J} = \mathbf{U}_{\bullet J} \quad (12)$$

As demonstrated in sections 4.2 and 4.3 of the SI, PA and AAA are always production-balanced. On the contrary, PSA necessarily perturbs the production balance (SI, section 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 (SI, section 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 Raa (1990).

## Result synthesis

### 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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<sup>13</sup> 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 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	✗ <sup>1</sup>	✓	✓
PSA/PSC	✗ <sup>2</sup>	✗	✓
- BTC	✓	✗	✗
AAA/AAC	✗ <sup>3</sup>	✓	✓
- CTC	✓	✓	✗

<sup>1</sup> : Balanced across all layers if and only if all coproducts are identical to each other within each industry.

<sup>2</sup> : Systematically balanced across all layers if and only if each secondary coproduction perfectly substitutes an identical commodity from primary production.

<sup>3</sup> : 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 the *Exclusive secondary products and*

*aggregation error* section.

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 the discussion section.

## 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 S1). 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 S1). 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  $\Lambda$  (see SI, section 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; Huppel, 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 other forms of coproduction (in agreement with Weidema, 2014).

## **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 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/metalloids”. Clearly, there are industries that primarily produce sweeteners, biomass, and 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<sub>2</sub> 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?

## 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 Ardenne 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.

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

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## **Abstract**

This supporting information defines terminology and notation, provides equations for the various allocations and constructs, presents the mathematical proofs, extends the discussion on the representation of waste treatment, compiles complementary tables from the two numerical examples, and discusses the sensitivity of our analysis to product group inhomogeneities.

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# 1 Terminology and notation

## 1.1 Term definitions

In this article, the terms *product* and *commodity* are considered synonymous and refer to a good or service that is supplied and used by the technological system (technosphere). This is to be contrasted with a *factor of production*, which designates an entity that cannot be produced by the technological system within a given time period (Duchin, 2009). In this article, factors of production include capital, labor, natural resources, and emissions of environmental stressors<sup>1</sup>.

The entities that produce products are referred to indiscriminately as *activities* or *industries*. The use of products and factors of production by industries are collectively designated as *requirements*. Let the *inventory* of an activity designate the survey of its use flows, supply flows, and flows of factors of production.

A *coproduct* is any of two or more commodities produced by the same industry (ISO, 1998). The coproduct that generates the maximum value for an industry is its *primary product* (Londero, 1999), and the others are considered *secondary*.

Secondary coproducts may be characterized as either *ordinary* or *exclusive* (United Nations, 1999). If a commodity is always produced as a secondary coproduct, and therefore no industry may be found for which this commodity is the primary coproduct, then this secondary product is said to be exclusive (e.g., molasses are exclusive secondary products of the sugar industry; no industry is dedicated to producing molasses as their main product).

Secondary coproducts are also classified based on the strength of their dependence and technological link to their primary product (European Commission, 2008). A *byproduct* is technologically linked to, and produced simultaneously with, a primary product. The demand level for a byproduct does not influence the production volume of the coproducing activity. On the contrary, a *subsidiary product* is technologically unrelated to the primary product, and its production volume is free to change independently from that of the primary production. *Joint products* present intermediate situations (United Nations, 1999).

## 1.2 Notation

Table S1 summarizes the notation and variables used in this article. Throughout this supporting information (SI), some equations are best expressed in coefficient notation, others follow a matrix notation, and others are presented with both notations in parallel for greater convenience to the reader.

Bold lowercase and uppercase characters denote vectors and matrices, respectively. Individual coefficients are represented by lowercase, italic letters. Braces  $\{ \}$  emphasize that an inner vector-product within its bounds is reduced to a 1x1 matrix, that is, a scalar.

The sets  $\bullet$ ,  $*$ , and  $\star$  respectively hold all commodities, all activities, and all factors of production. Indices  $i$ ,  $j$ , or  $k$  point to individual commodities (element of  $\bullet$ ). Indices  $I$ ,  $J$ , or  $K$  designate individual activities (element of  $*$ ). Indices  $c$  designates an individual factor, element of  $\star$ .

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<sup>1</sup> Indeed, the existence of large natural reservoir in which industries can dilute their emissions is a valuable asset that cannot be produced by the technosphere.

Symbol	Coefficients	Name	Definition
Sets and Indices:			
$\bullet$		Set of all commodities (also whole matrix commodity-dimension)	
$i, j, k$		indices representing specific commodities	$\in \bullet$
$*$		Set of all activities (also whole matrix activity-dimension)	
$I, J, K$		indices representing specific activities	$\in *$
$\mathcal{P}$		Set of all combinations of commodities and activities that are primary production	
$\mathcal{S}$		Set of all combinations of commodities and activities that are <i>not</i> primary production	
$*$		Set of all factors of production (also whole matrix factor-dimension)	
$c$		indice representing specific factor of production	$\in *$
$\Delta$		Set of all conservative properties (also whole matrix property-dimension)	
$m$		indice representing a specific property	$\in \Delta$
Operators:			
$\mathbf{e}$		vertical vector of ones (and zeros, depending on filters)	
$\mathbf{0}$		matrix of zeros	
$\mathbf{E}$		matrix of ones (and zeros, depending on filters)	
Modifiers and Filters:			
$\hat{\square}$		transpose	
$\square$		secondary products only	
$\bar{\square}$		primary products only	
$\hat{\square}$		diagonalization of vector OR filter-out off-diagonal elements of matrix	
$\bar{\square}$		single-output activities only	
Inventory Data			
$\mathbf{U}_{**}$	$u_{i,j}$	untraceable Use matrix	
$\mathbf{U}_{**}$	$u_{i,j}$	traceable Use matrix	
$\mathbf{V}$	$v_{i,j}$	supply matrix	
$\mathbf{h}$	$h_i$	inventoried final consumption	
$\mathbf{G}_{**}$	$g_{c,j}$	net use of factors of production	
$\Lambda_{\Delta*}$	$\lambda_{mj}$	conservative properties of products	
$\Lambda_{\Delta*}$	$\lambda_{mc}$	conservative properties of factors	
Intermediate, Calculated Variables			
$\mathbf{B}$	$b_{i,j}$	normalized product use by industries	$= \mathbf{U}(\widehat{\mathbf{e}_* \mathbf{V}})^{-1}$
$\mathbf{S}$	$s_{c,j}$	normalized factor use by industries	$= \mathbf{G}(\widehat{\mathbf{e}_* \mathbf{V}})^{-1}$
Intermediate Variables for Specific Models			
$\Psi$	$\psi_{i,j}$	partitioning (intensive) property	
$\Phi$	$\phi_{j,i}$	partitioning coefficient	
$\Gamma_{**}$	$\gamma_{ji}$	alternate activity matrix	mapping, 1 or 0
$\Gamma_{*\Delta}$	$\gamma_{jmi}$	alternate activity matrix (with explicit production equivalence property)	mapping, 1 or 0
$\mathbf{A}^f$	d.s.	alternate technology coefficient matrix	
$\Xi$	$\xi_{ji}$	substitution table	
Final Variables			
$\mathbf{y}$	$y_i$	exogenously defined final demand	
$\mathbf{Z}$	d.s.	modeled intermediate flows	
$\mathbf{A}$	d.s.	modeled technical coefficient	
$\mathbf{x}$	$x_i$	total calculated production	$= \mathbf{L}\mathbf{y}$
$\mathbf{G}_{**}$ or $\mathbf{G}_{**}$	d.s.	Modeled (allocated or constructed) factors of production	
$\mathbf{F}_{**}$ or $\mathbf{F}_{**}$	d.s.	Modeled and normalized factors of production	
d.s. = dimensions specified with subscripts ( $\bullet, *, 1$ ) depending on situation			

Table S1: Notation and variables

Whenever necessary, these symbols and indices are used to indicate dimensions of matrices and vectors. For example, it may be specified that a use table ( $\mathbf{U}$ ) has products-by-industry dimensions as  $\mathbf{U}_{**}$ . Furthermore, these indices can also be used to “slice” specific sections of matrices. For example,  $\mathbf{U}_{\bullet J}$  designates the  $J^{\text{th}}$  column of matrix  $\mathbf{U}$ , thus selecting the use of all products by industry  $J$ .

The set  $\mathcal{P}$  is the set of all primary production flows in the system, whereas the set  $\mathcal{S}$  refers to all secondary production flows. If a commodity  $j$  is the primary product of an industry  $J$  the pair  $(j, J)$  is an element of  $\mathcal{P}$ , otherwise it belongs to  $\mathcal{S}$ . The two sets are thus complementary.<sup>2</sup>

Matrix  $\mathbf{E}$  and vertical vector  $\mathbf{e}$  are filled with coefficients of value 1, but may also contain zeros depending on the filters applied. Some filters only keep diagonal elements ( $\hat{\square}$ ), secondary product entries ( $\square$ ), primary product entries ( $\bar{\square}$ ), or single-output industries ( $\bar{\square}$ ). The identity matrix is therefore denoted by  $\hat{\mathbf{E}}$ , that is, a matrix of ones with its off-diagonal elements set to zero. Similarly,  $\bar{\mathbf{E}}_{**}$  is the

<sup>2</sup> In this way,  $\mathcal{S}$  is defined as also including productions of magnitude zero. If  $k$  is not produced by  $J$ , the pair  $(k, J)$  is an element of  $\mathcal{S}$ .

primary production matrix; it is a correspondence matrix that maps each activity to its primary product.

Transposition is denoted by  $\square'$ . The accent  $\hat{\square}$  denotes diagonalization when applied to a vector (contrary to its use as a filter when applied to a matrix).

## 2 Mathematical representation of inventories and models

This section provides mathematical representations that will be used in the proofs of the different balances. It starts with a conversion of a *mixed-unit* supply and use table (SUT) to a *multilayered* SUT, and then proceeds to define the different allocation models and construct models.

### 2.1 Multilayered SUT

Given property matrices ( $\Lambda_{\Delta\bullet}$  and  $\Lambda_{\Delta\star}$ ) that are normalized relative to the dimensions of a mixed-unit SUT, the separation of this mixed-unit SUT into multiple property layers is performed as in equations (S1) to (S3).

The layer of property  $m$  in a multi-unit SUT, defined from the mixed-unit inventory:

$$u_{iJ}^m = \lambda_{mi} u_{iJ} \quad m \in \Delta, \forall (i, J) \in (\bullet, *) \quad (\text{S1})$$

$$v_{iJ}^m = \lambda_{mi} v_{iJ} \quad m \in \Delta, \forall (i, J) \in (\bullet, *) \quad (\text{S2})$$

$$g_{cJ}^m = \lambda_{mc} g_{cJ} \quad m \in \Delta, \forall (c, J) \in (\star, *) \quad (\text{S3})$$

This conversion assumes that the properties of a product or a factor are independent from its position in the system. In other words, the description of a product ( $\lambda_{mi}$ ) holds true regardless of which industry consumes it or produces it; this product group is homogeneous throughout the system. Upholding this common assumption of environmentally extended input-output (EEIO) and lifecycle assessment (LCA) (Duchin, 2009; European Commission, 2008; Merciai and Heijungs, 2014) ensures that coproduction modeling choices are the only source of imbalances (see section 7 for sensitivity analysis).

The above equations allow for the conversion between equation (1) and equation (2) in the main article.

### 2.2 Traceability in product allocations and constructs

We distinguish between two types of SUTs, depending on whether product use flows are traceable to their source or not. In a supply and traceable use table (StUT) the use table has three dimensions to describe each use flow: the source industry, the product that is being used, and the using industry. For example, in the traceable use matrix ( $\mathbf{U}_{\bullet\bullet\bullet}$ ), the coefficient  $u_{IiJ}$  would hold the amount of commodity  $i$  provided by industry  $I$  for use in industry  $J$ . Conversely, in

a supply and untraceable use table (SuUT), it would simply be recorded in a 2-dimensional product-by-industry table ( $\mathbf{U}_{\bullet\bullet}$ ) that industry  $J$  uses a certain amount of commodity  $i$  ( $u_{i,J}$ ) without recording any specific supplier.

Allocation can be applied individually to each industry, whether their requirement flows are traceably recorded or not. Regardless of the traceability of the requirements, these requirements are still split in the same way across coproducts (equations (S4) and (4), reproduced below).

$$\text{allocation} : \mathbf{U}_{\bullet J}, \mathbf{V}_{\bullet J} \rightarrow \mathbf{Z}_{\bullet J\bullet} \quad (\text{rep. 4})$$

$$\text{allocation} : \mathbf{U}_{*\bullet J}, \mathbf{V}_{\bullet J} \rightarrow \mathbf{Z}_{*\bullet J\bullet} \quad (\text{S4})$$

We define constructs as models yielding symmetric, self-consistent representations of intermediate flows. Such symmetric system representations can be achieved from traceable or untraceable inventories (equations (S5) and (5), reproduced below).

$$\text{aggregation construct} : \mathbf{U}_{\bullet\bullet}, \mathbf{V}_{\bullet\bullet} \rightarrow \mathbf{Z}_{\bullet\bullet} \quad (\text{rep. 5})$$

$$\text{traceable construct} : \mathbf{U}_{*\bullet\bullet}, \mathbf{V}_{\bullet\bullet} \rightarrow \mathbf{Z}_{*\bullet\bullet} \quad (\text{S5})$$

Thus, aggregation constructs describe the production of average products based on the use of average products ( $\mathbf{Z}_{\bullet\bullet}$ ), whilst a traceable construct will describe the production of traceable products based on traceable requirements ( $\mathbf{Z}_{*\bullet\bullet}$ ).

From these definitions, it is apparent that a traceable construct is equivalent to applying an allocation in turn to each activity of a StUT account (cf. equations (S4) and (S5)). On the other hand, an aggregation construct involves not only an allocation of each industry of an SuUT account but also a summation step to “aggregate away” the industries from the system descriptions (Majeau-Bettez et al., 2014).

The partition allocation (PA), product substitution allocation (PSA) or alternate activity allocation (AAA) of each industry in a StUT thus directly yields a traceable partitioning construct (tPC), a traceable product substitution construct (tPSC), or a traceable alternate activity construct (tAAC), respectively.

Alternatively, an aggregation partitioning construct (aPC), an aggregation product substitution construct (aPSC) or an aggregation alternate activity construct (aAAC) is respectively obtained by applying PA, PSA, or AAA to each industry of an SuUT inventory and then aggregating across the industry dimension. The industry technology construct (ITC), byproduct technology construct (BTC) and commodity technology construct (CTC) are respectively special cases of aPC, aPSC and aAAC (Majeau-Bettez et al., 2014).

As the traceability or untraceability of a product does not alter its composition or value, it has no bearing on the different balances. For simplicity, all demonstration and proofs are done with untraceable inventories — as these have one dimension less — without loss of generality. Traceability only potentially plays a role in situations where product groups are not assumed to be homogeneous, as explored in section 7.

## 2.3 Partition allocation equations

Partition allocation splits requirements across coproducts based on a common property that they share (equation (7)) (Guinée, 2002).

Let us describe all coproducts of industry  $J$  in terms of an intensive property that will be used to partition this industry. These descriptions are recorded in the  $J^{\text{th}}$  column of the product-by-industry *partitioning property matrix*  $\Psi$ . In other words, the descriptions of the coproducts are recorded in the column-vector  $\Psi_{\bullet J}$ .

These descriptions are then used to calculate the share of each coproduct flow (e.g.,  $v_{jJ}\psi_{jJ}$ ) relative to the total supply ( $\sum_{k \in \bullet} v_{kJ}\psi_{kJ}$ ) in terms of the selected partitioning property, which defines the so-called *partitioning coefficients* ( $\Phi$ ), as expressed in equation (S6) (Majeau-Bettez et al., 2014).

$$\phi_{Jj} = \frac{v_{jJ}\psi_{jJ}}{\sum_{k \in \bullet} v_{kJ}\psi_{kJ}} \quad \forall j \in \bullet \quad \Phi_{J\bullet} = \left( \widehat{\mathbf{V}'_{\bullet J} \Psi_{\bullet J}} \right)^{-1} \Psi'_{\bullet J} \widehat{\mathbf{V}_{\bullet J}} \quad (\text{S6})$$

Partitioning coefficients for industry  $J$  are then used to partition its use of products (equation (S7)) and of factors of production (equation (S8)). The outer vector-product of use flows ( $\mathbf{U}_{\bullet J}$ ) and partitioning coefficients ( $\Phi_{J\bullet}$ ) leads to a product-by-product representation of the allocated flows at industry  $J$  ( $\mathbf{Z}_{\bullet J\bullet}$ ).

$$\mathbf{Z}_{\bullet J\bullet} = \mathbf{A}_{\bullet J\bullet} \widehat{\mathbf{V}_{\bullet J}} = \mathbf{U}_{\bullet J} \Phi_{J\bullet} \quad (\text{S7})$$

$$\mathbf{G}_{*J\bullet} = \mathbf{F}_{*J\bullet} \widehat{\mathbf{V}_{\bullet J}} = \mathbf{G}_{*J} \Phi_{J\bullet} \quad (\text{S8})$$

**Definition 1.** Let equations (S6) to (S8) collectively define partition allocation.

## 2.4 Product substitution allocation equations

Product substitution allocation preserves a single production function per activity by assuming that secondary coproducts leave the system to avoid primary production outside the system boundaries (equation (8)) (Guinée, 2002).

Let the substitutability between products be recorded in a product-by-product *substitution matrix* ( $\Xi$ ). Coefficient  $\xi_{ij} = 0.8$  would indicate that one unit of secondary production of  $j$  avoids 0.8 units of primary production of  $i$ . This would typically be recorded in terms of the units that describe each product in the mixed-unit layer (figure 1). This substitution matrix then allows for the general representation of PSA by equations (S9) and (S10) (Majeau-Bettez et al., 2014).

$$\mathbf{A}_{\bullet J\bullet} \widehat{\mathbf{V}_{\bullet J}} = \mathbf{Z}_{\bullet J\bullet} = \mathbf{A}_{\bullet J\bullet} \widehat{\mathbf{V}_{\bullet J}} = \left( \mathbf{U}_{\bullet J} - \Xi \tilde{\mathbf{V}}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} \quad (\text{S9})$$

$$\mathbf{F}_{*J\bullet} \widehat{\mathbf{V}_{\bullet J}} = \mathbf{G}_{*J\bullet} = \mathbf{F}_{*J\bullet} \widehat{\mathbf{V}_{\bullet J}} = \mathbf{G}_{*J} \bar{\mathbf{E}}'_{\bullet J} \quad (\text{S10})$$

The allocated product flows of activity  $J$  ( $\mathbf{Z}_{\bullet J\bullet}$ ) equal the direct requirements associated with the primary production ( $\mathbf{A}_{\bullet J\bullet} \widehat{\mathbf{V}_{\bullet J}}$ ), which in turn equal the product requirements of the multi-functional activity ( $\mathbf{U}_{\bullet J}$ ) minus the products avoided by secondary productions ( $\Xi \tilde{\mathbf{V}}_{\bullet J}$ ).

**Definition 2.** Let equations (S9) and (S10) collectively define product substitution allocation. Consequently, let  $\Xi \tilde{\mathbf{V}}_{\bullet J}$  represent the product flows substituted by the secondary products of an activity  $J$ .



## 2.5 Alternate activity allocation equations

Alternate activity allocation split requirements across coproducts by assuming a technology of production for each secondary commodity and assigning the remainder of the requirements to the main product (equation (9)). Each technology assumption is based on the technology of an alternative production route for a similar or identical product (Majeau-Bettez et al., 2014).

Thus, in equation (S11), product requirements are assumed for all secondary productions of  $J$  ( $\mathbf{A}_{\bullet\bullet}^{\Gamma} \widehat{\mathbf{V}}_{\bullet J}$ ) based on an alternate technology description ( $\mathbf{A}_{\bullet\bullet}^{\Gamma}$ ), and the primary product is allocated the remainder of the joint requirements ( $\mathbf{U}_{\bullet J} - \mathbf{A}_{\bullet\bullet}^{\Gamma} \widehat{\mathbf{V}}_{\bullet J}$ ).

$$\mathbf{Z}_{\bullet J} = \left( \mathbf{U}_{\bullet J} - \mathbf{A}_{\bullet\bullet}^{\Gamma} \widehat{\mathbf{V}}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} + \mathbf{A}_{\bullet\bullet}^{\Gamma} \widehat{\mathbf{V}}_{\bullet J} \quad (\text{S11})$$

Equation (S12) applies the same allocation modeling to the use of factors of production.

$$\mathbf{F}_{\star J} = \left( \mathbf{G}_{\star J} - \mathbf{F}_{\star\bullet}^{\Gamma} \widehat{\mathbf{V}}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} + \mathbf{F}_{\star\bullet}^{\Gamma} \widehat{\mathbf{V}}_{\bullet J} \quad (\text{S12})$$

**Definition 3.** Let equations (S11) and (S12) collectively define all alternate activity allocations.

An alternative primary production must therefore be selected as best technological equivalent for each secondary product. In a mixed unit framework, this choice of alternate activity would be recorded directly in an industry-by-product table ( $\mathbf{\Gamma}$ ). If the technology of activity  $K$  is assumed for each secondary production of commodity  $k$ ,  $\gamma_{Kk} = 1$ ; otherwise  $\gamma_{Kk} = 0$ .

However, a multi-unit framework offers the opportunity to select what we could call a *production equivalence property*. If the secondary product and its closest technological proxy are not perfectly identical, a choice must be made as to whether a technological equivalence is assumed per kilogram (kg) of product, or per kilojoule (kJ) of product, or per \$ of product, etc. This choice can be recorded in an extra dimension to  $\mathbf{\Gamma}$ , which becomes  $\mathbf{\Gamma}_{\star\Delta}$ . Taking the cattle farming example,  $\gamma_{STEER, mass, cow\_meat} = 1$  would indicate that the requirements of steer farming per kg of its primary product are assumed for each kg of cow meat. Reflecting this choice in a 2D  $\mathbf{\Gamma}$  (i.e., in terms of the reference unit of each product in the mixed-unit layer) is then a simple matter of unit conversion.

$$\gamma_{Jk} = \sum_{m \in \Delta} \frac{\gamma_{Jmk} \lambda_{mk}}{\lambda_{mj}} \quad \forall (j, J) \in \mathcal{P}, k \in \bullet \quad \mathbf{\Gamma}_{\star\bullet} = \sum_{m \in \Delta} \widehat{\mathbf{\Lambda}}_{m\bullet} \bar{\mathbf{E}}^{-1} \mathbf{\Gamma}_{\star m\bullet} \widehat{\mathbf{\Lambda}}_{m\bullet} \quad (\text{S13})$$

In the simplest case where each alternative technology is a single-output industry ( $\mathbf{\Gamma} = \dot{\mathbf{\Gamma}}$ ), the alternative technology coefficients ( $\mathbf{A}^{\Gamma}$ ) are simply compiled based on the normalized use coefficients ( $\mathbf{B}_{\bullet\star} = \mathbf{U}(\mathbf{e}'\mathbf{V})^{-1}$ ) of these industries,

$$\mathbf{A}^{\Gamma} = \mathbf{B}\dot{\mathbf{\Gamma}}_{\star\bullet} \quad (\text{S14})$$

and similarly with normalized factors of production ( $\mathbf{S}_{**} = \mathbf{G}_{**}(\widehat{\mathbf{e}'\mathbf{V}})^{-1}$ ).

$$\mathbf{F}^\Gamma = \mathbf{S}\dot{\Gamma}_{**} \quad (\text{S15})$$

In the more complicated cases where some of the selected alternative activities also have secondary products of their own, these must first be resolved by AAA before the technology of their primary product can be used in the allocation of other products (see Majeau-Bettez et al., 2014, for automation of this process).

### 3 Proofs of balanced recipes

In this section, we derive the inventory characteristics sufficient and necessary in order for the different allocations and constructs to yield recipes that are balanced in terms of a given conservative property.

#### 3.1 Formal representations of balanced allocated recipes

**Definition 4.** Let the inventory of an activity be balanced in terms of conservative property  $m$  if it respects equation (2). Furthermore, let equation (6) generally represents the balance of conservative property  $m$  in allocated flows.

The definition of a balanced allocation of industry  $J$  in terms of property  $m$  (equation (6)) is reproduced below.

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

It may be reformulated in matrix notation as in equation (S16).

Conservation of property  $m$  in the allocated flows of industry  $J$

$$\underbrace{\Lambda_{m\bullet} \mathbf{Z}_{\bullet Jj} + \Lambda_{m\star} \mathbf{G}_{\star Jj}}_{m \text{ in requirements allocated to } j} = \underbrace{\lambda_{mj} v_{jJ}}_{m \text{ in supply of } j} \quad \forall j \in \bullet \quad (\text{S16})$$

This balance can also be expressed in a normalized form, as in equation (S17). This equation applies to all non-null productions of  $j$  (i.e.,  $j \in \bullet | v_{jJ} \neq 0$ ), since it is not possible to calculate a normalized recipe ( $\mathbf{A}$  and  $\mathbf{F}$ ) for something that is not produced (division by zero).

Conservation of property  $m$  in normalized, allocated flows of industry  $J$

$$\Lambda_{m\bullet} \mathbf{A}_{\bullet Jj} + \Lambda_{m\star} \mathbf{F}_{\star Jj} = \lambda_{mj} \quad \forall j \in \bullet | v_{jJ} \neq 0 \quad (\text{S17})$$

These equations equivalently serve as the criterion for determining whether or not an allocation model generates recipes that are balanced in terms of a conservative property.

In the case of aggregation constructs, which result in symmetric system representations that do not explicitly describe industries, the balance equation (S16) is further simplified to equation (S18).

Conservation of property  $m$  in constructed flows

$$\underbrace{\Lambda_{m\bullet}\mathbf{A}_{\bullet j} + \Lambda_{m\star}\mathbf{F}_{\star j}}_{m \text{ in requirements to production of } j} = \underbrace{\lambda_{mj}}_{m \text{ in } j} \quad \forall j \in \bullet \quad (\text{S18})$$

### 3.2 Balanced recipes from partition allocation

**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  $J$ .*

*Proof.* Combining the equations that generally represent partition-allocated flows (equations (S7) and (S8)) with the definition of balanced allocated flows (equation (S17)) necessarily leads to an equation defining balanced partition-allocated flows (equation (S19)).

$$\Lambda_{m\bullet}\mathbf{U}_{\bullet J} \frac{\phi_{Jj}}{v_{jJ}} + \Lambda_{m\star}\mathbf{G}_{\star J} \frac{\phi_{Jj}}{v_{jJ}} = \lambda_{mj} \quad \forall j \in \bullet | v_{jJ} \neq 0 \quad (\text{S19})$$

This equation may be rearranged as in equation (S20).

$$(\Lambda_{m\bullet}\mathbf{U}_{\bullet J} + \Lambda_{m\star}\mathbf{G}_{\star J}) \frac{\phi_{Jj}}{v_{jJ}} = \lambda_{mj} \quad \forall j \in \bullet | v_{jJ} \neq 0 \quad (\text{S20})$$

Since it is given that the inventory of activity  $J$  is initially balanced with respect to  $m$ , from equation (2) the term in parenthesis is equal to the total amount of property  $m$  in the supply flows of industry  $J$  ( $\Lambda_{m\bullet}\mathbf{V}_{\bullet J}$ ).

$$\Lambda_{m\bullet}\mathbf{V}_{\bullet J} \frac{\phi_{Jj}}{v_{jJ}} = \lambda_{mj} \quad \forall j \in \bullet | v_{jJ} \neq 0 \quad (\text{S21})$$

From equation (S6), we reformulate the partition coefficient ( $\phi_{Jj}$ ) in terms of intensive properties ( $\Psi$ ), and we simplify. The braces  $\{\}$  indicate that the inner vector-product results in a scalar.

$$\{\Lambda_{m\bullet}\mathbf{V}_{\bullet J}\} \frac{\psi_{jJ}}{\{\Psi'_{\bullet J}\mathbf{V}_{\bullet J}\}} = \lambda_{mj} \quad \forall j \in \bullet | v_{jJ} \neq 0 \quad (\text{S22})$$

This equation may then be rearranged as in equation (S23).

$$\frac{\{\Lambda_{m\bullet}\mathbf{V}_{\bullet J}\}}{\{\Psi'_{\bullet J}\mathbf{V}_{\bullet J}\}} = \alpha = \frac{\lambda_{mj}}{\psi_{jJ}} \quad \forall j \in \bullet | v_{jJ} \neq 0 \quad (\text{S23})$$

As the left-hand side of this equation is independent of commodity  $j$ , its value is constant for all products of  $J$ . To highlight this fact, this term is simply denoted by a constant ( $\alpha$ ). This condition is equivalently expressed in coefficient notation.

Criterion for the conservation of  $m$  in the PA of industry  $J$ :

$$\frac{\lambda_{mj}}{\psi_{jJ}} = \alpha = \frac{\sum_{k \in \bullet} \lambda_{mk} v_{kJ}}{\sum_{k \in \bullet} \psi_{kJ} v_{kJ}} \quad \forall j \in \bullet | v_{jJ} \neq 0 \quad (\text{S24})$$

Equation (S24) thus expresses the necessary and sufficient condition for balanced PA. Equation (S24) will hold true, and consequently the allocated flows of  $J$  will satisfy both the criteria of PA and conservation of property  $m$ , if and only if the ratio between this property  $m$  and the partitioning property is constant  $\left(\frac{\lambda_{mj}}{\psi_{jJ}} = \alpha\right)$  for all coproducts (i.e.,  $\forall j \in \bullet | v_{jJ} \neq 0$ ).  $\square$

Let us extend this analysis to cover not only one property  $m$  but all conservative properties. Corollary 1.1 then describes a stricter special case that ensures fully balanced PA recipes.

**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.*

### 3.3 Balanced recipes from substitution allocation

**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.*

*Proof.* Let commodity  $j$  designate the primary product of an industry  $J$  (i.e.,  $(j, J) \in \mathcal{P}$ ). Combining the equations that generally represent substitution-allocated flows (equations (S9) and (S10)) with the definition of balanced allocated flows (equation (S16)) necessarily leads to the definition of balanced substitution-allocated flows (equation (S25)).

$$\Lambda_{m\bullet} \left( \mathbf{U}_{\bullet J} - \Xi \tilde{\mathbf{V}}_{\bullet J} \right) + \Lambda_{m\star} \mathbf{G}_{\star J} = \lambda_{mj} v_{jJ} \quad (\text{S25})$$

This equation may be rearranged as follows.

$$\left( \Lambda_{m\bullet} \mathbf{U}_{\bullet J} + \Lambda_{m\star} \mathbf{G}_{\star J} \right) - \Lambda_{m\bullet} \Xi \tilde{\mathbf{V}}_{\bullet J} - \lambda_{mj} v_{jJ} = 0 \quad (\text{S26})$$

Since it is given that the inventory of activity  $J$  is initially balanced, from equation (2) the term in parenthesis equals the total amount of property  $m$  in the supply flows of industry  $J$ .

$$\Lambda_{m\bullet} \mathbf{V}_{\bullet J} - \Lambda_{m\bullet} \Xi \tilde{\mathbf{V}}_{\bullet J} - \lambda_{mj} v_{jJ} = 0 \quad (\text{S27})$$

As  $j$  is the primary product of activity  $J$ , the difference between the first and the last term gives the total amount of property  $m$  contained in secondary productions of  $J$ .

$$\Lambda_{m\bullet} \tilde{\mathbf{V}}_{\bullet J} - \Lambda_{m\bullet} \Xi \tilde{\mathbf{V}}_{\bullet J} = 0 \quad (\text{S28})$$

Criterion for the conservation of  $m$  in the PSA of industry  $J$ :

$$\Lambda_{m\bullet}\tilde{\mathbf{V}}_{\bullet J} = \Lambda_{m\bullet}\Xi\tilde{\mathbf{V}}_{\bullet J} \quad (\text{S29})$$

Equation (S29) thus expresses the necessary and sufficient condition for balanced PSA with respect to property  $m$ . This equation will hold true, and therefore the allocated flows of activity  $J$  will satisfy both the definition of PSA and the conservation of property  $m$ , if and only if the sum total amount of  $m$  in the secondary products of  $J$  ( $\Lambda_{m\bullet}\tilde{\mathbf{V}}_{\bullet J}$ ) equal the sum total amount of  $m$  in the substituted products ( $\Lambda_{m\bullet}\Xi\tilde{\mathbf{V}}_{\bullet J}$ ).  $\square$

Equation (S29) may be reformulated in coefficient notation for greater convenience.

Criterion for the conservation of  $m$  in the PSA of industry  $J$ :

$$\sum_{k|(k,J)\in\mathcal{S}} \lambda_{mk}v_{kJ} = \sum_{k|(k,J)\in\mathcal{S}} \sum_{i\in\bullet} \lambda_{mi}\xi_{ik}v_{kJ} \quad (\text{S30})$$

Because the balance of the PSA recipe is function of the *sum* of the different substitutions, it is theoretically possible that multiple imbalanced substitutions add up to a balanced recipe by sheer coincidence.

As this is neither likely nor practical, we identify the more restricted condition for the *systematic* balance of PSA.

**Definition 5.** Given that a globally balanced modeling procedure can be broken down into multiple substeps, then the balance of this model is considered *systematic* if every substep of this model is also balanced.

**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.*

Let us extend this analysis to cover not only one property  $m$  but all conservative properties. Corollary 2.2 then describes a stricter special case that ensures fully balanced PSA recipes.

**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.*

### 3.4 Balanced recipes from alternate activity allocation

Since AAA treats primary and secondary products differently but presents recipes for both, the proof of its balance is split in two lemmas.

**Lemma 1** (AAA recipe balance for secondary products). *Given that all alternate technology descriptions ( $\mathbf{A}^\Gamma$  and  $\mathbf{F}^\Gamma$ ) are balanced with respect to property  $m$ , the recipe derived by AAA for a given secondary product of a balanced industry  $J$  will in turn conserve property  $m$  if and only if the primary product of the selected alternate technology contains an equal amount of  $m$ .*

*Proof.* Let  $k$  be a secondary product of industry  $J$ . Then, from equation (S11), the requirements that will be allocated to its production will equal those of the assumed equivalent technology.

$$\mathbf{A}_{\bullet Jk} = \mathbf{A}_{\bullet k}^\Gamma \quad (\text{S31})$$

$$\mathbf{F}_{*Jk} = \mathbf{F}_{*k}^\Gamma \quad (\text{S32})$$

This allows for the reformulation of the balanced allocation equation (equation (S17)) as equation (S33). Since the resulting equation combines a generic representation of secondary production recipes in AAA and the definition of balanced allocated flows, it constitutes the criterion for a balanced AAA recipe for secondary productions.

$$\Lambda_{m\bullet} \mathbf{A}_{\bullet k}^\Gamma + \Lambda_{m*} \mathbf{F}_{*k}^\Gamma = \lambda_{mk} \quad (\text{S33})$$

Since the alternative technology is given to be balanced, the term on the left of the equation then necessarily represents the  $m$ -content of the primary product of the alternative technology. This primary product may be identified by combining the primary production matrix ( $\bar{\mathbf{E}}$ ) of the alternate activity matrix ( $\mathbf{\Gamma}$ ), which simplifies equation (S33) to equation (S34).

$$\Lambda_{m\bullet} \bar{\mathbf{E}} \mathbf{\Gamma}_{*k} = \lambda_{mk} \quad (\text{S34})$$

Thus, in order for the AAA-modeled recipe of a given secondary product to be balanced, the amount of  $m$  in this secondary product ( $\lambda_{mk}$ ) must equal the amount of  $m$  ( $\Lambda_{m\bullet}$ ) in the primary product ( $\bar{\mathbf{E}}$ ) of the selected alternate technology ( $\mathbf{\Gamma}_{*k}$ ), that is,  $\Lambda_{m\bullet} \bar{\mathbf{E}} \mathbf{\Gamma}_{*k}$ .  $\square$

**Lemma 2** (AAA recipe balance for primary products). *Let the alternate technology descriptions ( $\mathbf{A}^\Gamma$  and  $\mathbf{F}^\Gamma$ ) be balanced with respect to property  $m$ . If the recipe allocated to each secondary product conserves property  $m$ , then the recipe modeled by AAA for the primary product of a balanced industry  $J$  will also conserve property  $m$ .*

*Proof.* Let  $j$  be the primary product of balanced industry  $J$ . From equations (S11) and (S12), this product flow is allocated the remainder of the requirements of  $J$  after technologies have been assumed for each secondary product.

$$\mathbf{Z}_{\bullet Jj} = \mathbf{U}_{\bullet J} - \mathbf{A}^\Gamma \tilde{\mathbf{V}}_{\bullet J} \quad (\text{S35})$$

$$\mathbf{G}_{*Jj} = \mathbf{G}_{*J} - \mathbf{F}^\Gamma \tilde{\mathbf{V}}_{\bullet J} \quad (\text{S36})$$

Combining equations (S35) and (S36) with the equation for balanced allocation (equation (S16)) then defines the criterion for the balance of the AAA-based recipe of a primary product (equation (S37)).

$$\Lambda_{m\bullet} \left( \mathbf{U}_{\bullet J} - \mathbf{A}^\Gamma \tilde{\mathbf{V}}_{\bullet J} \right) + \Lambda_{m*} \left( \mathbf{G}_{*J} - \mathbf{F}^\Gamma \tilde{\mathbf{V}}_{\bullet J} \right) = \lambda_{mj} v_{jJ} \quad (\text{S37})$$

It is simply rearranged as follows.

$$(\Lambda_{m\bullet}\mathbf{U}_{\bullet J} + \Lambda_{m\star}\mathbf{G}_{\star J}) - (\Lambda_{m\bullet}\mathbf{A}^\Gamma + \Lambda_{m\star}\mathbf{F}^\Gamma) \tilde{\mathbf{V}}_{\bullet J} = \lambda_{mj}v_{jJ} \quad (\text{S38})$$

By virtue of the balance of industry  $J$ , the first term in parenthesis equals the total amount of  $m$  in the supply flows of that industry (i.e.,  $\Lambda_{m\bullet}\mathbf{V}_{\bullet J}$ ).

$$\Lambda_{m\bullet}\mathbf{V}_{\bullet J} - (\Lambda_{m\bullet}\mathbf{A}^\Gamma + \Lambda_{m\star}\mathbf{F}^\Gamma) \tilde{\mathbf{V}}_{\bullet J} = \lambda_{mj}v_{jJ} \quad (\text{S39})$$

Since alternate technologies are given as balanced, the remaining term in parenthesis must equal the  $m$ -content of the primary product of each alternate technology, which may be reformulated as follows.

$$\Lambda_{m\bullet}\mathbf{V}_{\bullet J} - (\Lambda_{m\bullet}\bar{\mathbf{E}}\Gamma) \tilde{\mathbf{V}}_{\bullet J} = \lambda_{mj}v_{jJ} \quad (\text{S40})$$

As it is given that all secondary product allocations are balanced, equation (S40) is further simplified based on equation (S34),

$$\Lambda_{m\bullet}\mathbf{V}_{\bullet J} - \Lambda_{m\bullet}\tilde{\mathbf{V}} = \lambda_{mj}v_{jJ} \quad (\text{S41})$$

which simplifies in turn to

$$\lambda_{mj}v_{jJ} = \lambda_{mj}v_{jJ} \quad (\text{S42})$$

□

Thus, if the AAA-recipes of secondary products are balanced, the criterion for a balanced AAA-recipe is also automatically upheld for the primary product.

**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 technology.*

*Proof.* The conditions of proposition 3 are the same as the necessary and sufficient condition for the conservation of  $m$  in the recipes of secondary products (lemma 1). They also comply with the sufficient conditions for the conservation of  $m$  in the AAA recipe of the primary product (lemma 2). For the balance of property  $m$  in *all* AAA-recipes (primary and secondary), it therefore constitutes the necessary and sufficient condition. □

Let us extend this analysis to cover not only one property  $m$  but all conservative properties. Corollary 3.1 then describes a stricter special case that ensures fully balanced AAA recipes.

**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.*

### 3.5 From balanced allocations to balanced constructs

**Lemma 3** (Sum of balanced recipes). *The sum of any two recipes will conserve a property  $m$  if both recipes are balanced with respect to this property  $m$ .*

*Proof.* Let the column vector  $\mathbf{a}$  represent the sum of the product requirements of two unrelated recipes  $\mathbf{Z}_{\bullet Jj}$  and  $\mathbf{Z}_{\bullet Ki}$ .

$$\mathbf{a} = \mathbf{Z}_{\bullet Jj} + \mathbf{Z}_{\bullet Ki} \quad (\text{S43})$$

Similarly, let the column-vector  $\mathbf{b}$  hold the sum of the factors of production used in the production of  $j$  by  $J$  ( $\mathbf{G}_{\star Jj}$ ) and in the production of  $i$  by  $K$  ( $\mathbf{G}_{\star Ki}$ ).

$$\mathbf{b} = \mathbf{G}_{\star Jj} + \mathbf{G}_{\star Ki} \quad (\text{S44})$$

From equation (S16), the criterion for the conservation of property  $m$  in this aggregation may be represented as follows.

$$\lambda_{mj}v_{jJ} + \lambda_{mi}v_{iK} = \Lambda_{m\bullet}\mathbf{a} + \Lambda_{m\star}\mathbf{b} \quad (\text{S45})$$

It may be reformulated based on equations (S43) and (S44),

$$\lambda_{mj}v_{jJ} + \lambda_{mi}v_{iK} = \Lambda_{m\bullet}(\mathbf{Z}_{\bullet Jj} + \mathbf{Z}_{\bullet Ki}) + \Lambda_{m\star}(\mathbf{G}_{\star Jj} + \mathbf{G}_{\star Ki}) \quad (\text{S46})$$

and further rearranged.

$$\lambda_{mj}v_{jJ} + \lambda_{mi}v_{iK} = (\Lambda_{m\bullet}\mathbf{Z}_{\bullet Jj} + \Lambda_{m\star}\mathbf{G}_{\star Jj}) + (\Lambda_{m\bullet}\mathbf{Z}_{\bullet Ki} + \Lambda_{m\star}\mathbf{G}_{\star Ki}) \quad (\text{S47})$$

As it is given that each allocated recipe individually conserves  $m$ , equation (S16) allows for further simplification.

$$\lambda_{mj}v_{jJ} + \lambda_{mi}v_{iK} = \lambda_{mj}v_{jJ} + \lambda_{mi}v_{iK} \quad (\text{S48})$$

As equation (S48) necessarily always holds,  $m$  is always conserved in the sum of two balance recipes.  $\square$

Thus, the sum of any number of balanced recipes will necessarily lead in to a balanced aggregate.

**Proposition 4** (Balanced recipes in constructs). *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  $m$ .*

*Proof.* In a traceable construct, an individual recipe is defined as the allocation of traceable requirements to a product (equation (S5)), without any further modeling or assumption, and therefore the rules that govern balanced allocations directly apply. In an aggregation construct, each recipe equals the sum of multiple allocated recipes, and from lemma 3 this sum will respect the same balances as the recipes that are summed. Therefore, regardless of their traceable or aggregation character, constructs present the same balances as their underlying allocations.  $\square$



It should be noted that lemma 3 and proposition 4 are not biconditional statements. They constitute sufficient conditions, not necessary and sufficient conditions, as the sum of two imbalanced recipes may lead to a balanced total by sheer coincidence. Thus, the summation term in an aggregation construct may just happen to be balanced in spite of the individual allocations being imbalanced. As such occurrences will most likely be rare and of little practical importance, we focus rather of the predictable relation: balanced allocations are sufficient to guarantee a balanced construct.

## 4 Proofs of production balances

This section determines whether an allocation or construct respects production balance or perturbs it.

### 4.1 General

**Definition 6.** Let equation (10), reproduced below, define production balance in constructs: a construct leads to a production balanced model if and only if it calculates the original total production volume of the inventory for each commodity ( $\mathbf{Ve}$ ) when applied to the original final consumption of the inventory ( $\mathbf{h}$ ).

**Proposition 5** (Production balance test of constructs). *An A-matrix and the original supply and use tables from which it was constructed will respect equation (10) and will thereby be production balanced if and only if equation (11) holds true when applied to the same data.*

*Proof.* Equation (11) is a direct simplification of equation (10). Indeed, the criterion for production balance,

$$\mathbf{Ve} = \left( \hat{\mathbf{E}} - \mathbf{A} \right)^{-1} \mathbf{h} \quad (\text{rep. 10})$$

may be rearranged as follows.

$$\left( \hat{\mathbf{E}} - \mathbf{A} \right) \mathbf{Ve} = \mathbf{h} \quad (\text{S49})$$

$$-\mathbf{A}\mathbf{Ve} = -\mathbf{Ve} + \mathbf{h} \quad (\text{S50})$$

$$\mathbf{A}\mathbf{Ve} = \mathbf{Ve} - \mathbf{h} \quad (\text{S51})$$

By definition, the difference between total production ( $\mathbf{Ve}$ ) and final consumption ( $\mathbf{h}$ ) must equal total intermediate consumption, which may be expressed in terms of the use table ( $\mathbf{Ue}$ ). This simplifies equation (S51) to equation (11), reproduced below.

$$\mathbf{A}\mathbf{Ve} = \mathbf{Ue} \quad (\text{rep. 11})$$

□

Equation (11) is identical to the test presented by Jansen and Raa (1990) for this same purpose. Let us now extend this to also assess production balance of allocation models.

**Proposition 6** (Production balance of allocations). *Let an aggregation construct be divided in two steps, an allocation step applied to all industries and an aggregation step summing over all industries. If each industry allocation respects equation (12) ( $\mathbf{A}_{\bullet J} \mathbf{V}_{\bullet J} = \mathbf{U}_{\bullet J}$ ), then the resulting aggregation construct will respect equation (11) and will be production balanced.*

*Proof.* We reformulate equation (11), based on the fact that a column vector ( $\mathbf{V}\mathbf{e}$ ) is necessarily equal to the row-sum of its diagonalization ( $\widehat{\mathbf{V}}\mathbf{e}\mathbf{e}$ ).

$$\mathbf{A}\mathbf{V}\mathbf{e} = \mathbf{U}\mathbf{e} \quad (\text{rep. 11})$$

$$\mathbf{A}_{\bullet\bullet} \widehat{\mathbf{V}}\mathbf{e}\mathbf{e} = \mathbf{U}\mathbf{e} \quad (\text{S52})$$

The product  $\mathbf{A}_{\bullet\bullet} \widehat{\mathbf{V}}\mathbf{e}$  is equal to the unnormalized flow matrix resulting from the construct.

$$\mathbf{Z}_{\bullet\bullet}\mathbf{e} = \mathbf{U}\mathbf{e} \quad (\text{S53})$$

Because this is an aggregation construct, it can be expressed as the sum, across all industries, of allocated flows.

$$\sum_{J \in \ast} \mathbf{Z}_{\bullet J} \mathbf{e} = \mathbf{U}\mathbf{e} \quad (\text{S54})$$

The right-hand side of this equation may also be expressed with a summation term.

$$\sum_{J \in \ast} \mathbf{Z}_{\bullet J} \mathbf{e} = \sum_{J \in \ast} \mathbf{U}_{\bullet J} \quad (\text{S55})$$

Expressing the different allocations in terms of normalized coefficients and supply flows,

$$\sum_{J \in \ast} \mathbf{A}_{\bullet J} \widehat{\mathbf{V}}_{\bullet J} \mathbf{e} = \sum_{J \in \ast} \mathbf{U}_{\bullet J} \quad (\text{S56})$$

and simplifying,

$$\sum_{J \in \ast} \mathbf{A}_{\bullet J} \mathbf{V}_{\bullet J} = \sum_{J \in \ast} \mathbf{U}_{\bullet J} \quad (\text{S57})$$

leads to an equation that must be true if equation (12) ( $\mathbf{A}_{\bullet J} \mathbf{V}_{\bullet J} = \mathbf{U}_{\bullet J}$ ) is true.

$$\sum_{J \in \ast} \mathbf{U}_{\bullet J} = \sum_{J \in \ast} \mathbf{U}_{\bullet J} \quad (\text{S58})$$

□

Thus, if each allocation respects equation (12), none of these allocations perturb production balance, and an aggregation construct based on these allocations must be production balanced as well. We therefore define equation (12) as the criterion for production-balance in individual allocations.

**Definition 7.** The allocated flows of a given industry will be considered production balanced if they comply with equation (12).

## 4.2 Production balance of partition allocation

**Proposition 7** (Production balance of PA). *Partition allocation always respects production balance.*

*Proof.* Combining equations (S6) and (S7), which collectively define PA of product flows (definition 1), yields a representation of partition-allocated flows ( $\mathbf{A}_{\bullet J} \widehat{\mathbf{V}}_{\bullet J}$ ) in terms of SUT and intensive partitioning properties ( $\Psi$ ).

$$\mathbf{A}_{\bullet J} \widehat{\mathbf{V}}_{\bullet J} = \mathbf{U}_{\bullet J} \left( \widehat{\mathbf{V}}'_{\bullet J} \Psi_{\bullet J} \right)^{-1} \Psi'_{\bullet J} \widehat{\mathbf{V}}_{\bullet J} \quad (\text{S59})$$

The left-hand side of this equation may be rendered identical to that of equation (12) by multiplying both sides of the equation by the summation vector  $\mathbf{e}$ ,

$$\mathbf{A}_{\bullet J} \widehat{\mathbf{V}}_{\bullet J} \mathbf{e} = \mathbf{U}_{\bullet J} \left( \widehat{\mathbf{V}}'_{\bullet J} \Psi_{\bullet J} \right)^{-1} \Psi'_{\bullet J} \widehat{\mathbf{V}}_{\bullet J} \mathbf{e} \quad (\text{S60})$$

and by simplifying based on the fact that the row-sum of the diagonalization of a column-vector equals the original column-vector.

$$\mathbf{A}_{\bullet J} \mathbf{V}_{\bullet J} = \mathbf{U}_{\bullet J} \left( \widehat{\mathbf{V}}'_{\bullet J} \Psi_{\bullet J} \right)^{-1} \Psi'_{\bullet J} \mathbf{V}_{\bullet J} \quad (\text{S61})$$

The diagonalization may be dropped for matrices of dimensions 1x1 (effectively scalars).

$$= \mathbf{U}_{\bullet J} (\Psi'_{\bullet J} \mathbf{V}_{\bullet J})^{-1} (\Psi'_{\bullet J} \mathbf{V}_{\bullet J}) \quad (\text{S62})$$

This simplifies the right-hand side of the equation to that of equation (12)

$$= \mathbf{U}_{\bullet J} \quad (\text{S63})$$

Equation (S63) is equal to equation (12) □

Thus, with PA, the allocated product flows always add up to the total use of original industry ( $\mathbf{U}_{\bullet J}$ ), which ensures that PA is always production-balanced, regardless of the choice of partitioning property.

## 4.3 Production balance of alternate activity allocation

**Proposition 8** (Production balance of AAA). *Alternate activity allocation always respects production balance.*

*Proof.* Multiplying both sides of equation (S11), which defines the AAA of product flows (definition 3), by a vertical summation vector  $\mathbf{e}$ ,

$$\mathbf{A}_{\bullet J} \widehat{\mathbf{V}}_{\bullet J} \mathbf{e} = \left( \mathbf{U}_{\bullet J} - \mathbf{A}^{\Gamma} \tilde{\mathbf{V}}_{\bullet J} \right) \tilde{\mathbf{E}}'_{\bullet J} \mathbf{e} + \mathbf{A}^{\Gamma} \tilde{\mathbf{V}}_{\bullet J} \mathbf{e} \quad (\text{S64})$$

$$(\text{S65})$$

renders the left-hand side of this equation equal to that of the equation defining production-balanced allocation (equation (12)).

$$\mathbf{A}_{\bullet J} \mathbf{V}_{\bullet J} = \left( \mathbf{U}_{\bullet J} - \mathbf{A}^\Gamma \tilde{\mathbf{V}}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} \mathbf{e} + \mathbf{A}^\Gamma \tilde{\mathbf{V}}_{\bullet J} \quad (\text{S66})$$

As the sum of vector  $\bar{\mathbf{E}}'_{\bullet J}$  is, by definition, a scalar of value 1,

$$= \left( \mathbf{U}_{\bullet J} - \mathbf{A}^\Gamma \tilde{\mathbf{V}}_{\bullet J} \right) \{1\} + \mathbf{A}^\Gamma \tilde{\mathbf{V}}_{\bullet J} \quad (\text{S67})$$

the right-hand side of the equation then also simplifies to that of equation (12).

$$= \mathbf{U}_{\bullet J} - \mathbf{A}^\Gamma \tilde{\mathbf{V}}_{\bullet J} + \mathbf{A}^\Gamma \tilde{\mathbf{V}}_{\bullet J} \quad (\text{S68})$$

$$= \mathbf{U}_{\bullet J} \quad (\text{S69})$$

Equation (S69) is equal to equation (12) □

AAA therefore always respects equation (12), and it is always necessarily production balanced. It should be noted that the proof holds regardless of the value of  $\mathbf{A}^\Gamma$ .

#### 4.4 Non-production balance of substitution allocation

**Proposition 9** (Non-production balance of PSA). *Any non-trivial product substitution allocation does not respect production balance.*

*Proof.* Equation (S9), which defines PSA of product flows (definition 2), is first multiplied on both sides by the summation vector  $\mathbf{e}$  to transform the left-hand side of this equation to that of equation (12).

$$\mathbf{Z}_{\bullet J} = \mathbf{A}_{\bullet J} \widehat{\mathbf{V}}_{\bullet J} = \left( \mathbf{U}_{\bullet J} - \Xi \tilde{\mathbf{V}}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} \quad (\text{S70})$$

$$\mathbf{A}_{\bullet J} \widehat{\mathbf{V}}_{\bullet J} \mathbf{e} = \left( \mathbf{U}_{\bullet J} - \Xi \tilde{\mathbf{V}}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} \mathbf{e} \quad (\text{S71})$$

$$\mathbf{A}_{\bullet J} \mathbf{V}_{\bullet J} = \left( \mathbf{U}_{\bullet J} - \Xi \tilde{\mathbf{V}}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} \mathbf{e} \quad (\text{S72})$$

By definition, the sum of  $\bar{\mathbf{E}}'_{\bullet J}$  is a scalar of value 1.

$$= \left( \mathbf{U}_{\bullet J} - \Xi \tilde{\mathbf{V}}_{\bullet J} \right) \{1\} \quad (\text{S73})$$

$$= \mathbf{U}_{\bullet J} - \Xi \tilde{\mathbf{V}}_{\bullet J} \quad (\text{S74})$$

Except in the trivial case where secondary products displace nothing ( $\Xi \tilde{\mathbf{V}}_{\bullet J} = \mathbf{0}$ ), equation (S74) will always differ from equation (12), and PSA is therefore never production balanced. □

## 5 Balanced SUT with waste treatment

Many different, contradicting definitions of what constitutes a waste can be found in the literature (Frischknecht, 1994; Weidema, 2000; Heijungs and Suh, 2002; International Organization for Standardization, 2006; Schmidt et al., 2012). Even with a clear-cut theoretical definition, it may prove practically difficult to distinguish between a low-inconvenience waste and a low-value byproduct (Nakamura and Kondo, 2002). For these reasons, waste flows have been inventoried with two significantly different perspectives: either waste production as a supplied functional flow, or waste treatment as a supplied functional flow.

If a “waste” still has residual economic value and is purchased by the waste-treating activity, it makes sense to consider this purchase as a *use flow of the waste-treating activity*. For example, in figure S1-left, the waste-treating activity  $W$  purchases the waste  $w$  in order to recycle it into product  $j$ , and  $w$  may therefore be considered a requirement of  $W$  and a byproduct of activity  $I$ , coproduced along with its primary product  $i$  (figure S1-left). This, in turn, implies that part of the emissions and requirements of  $I$  may be allocated to  $w$  and then passed on to the lifecycle account of  $j$ . In open-loop recycling, this perspective may thus lead to the allocation of impacts across recycling cycles (e.g., Chen et al., 2010).

Conversely, if a treating activity provides a valuable service by handling an inconvenient waste, it is reasonable to consider that the acceptance of this waste constitutes a provision of service, that is, a *supply flow of the waste-treating activity*. In figure S1-right, if  $I$  has to pay  $W$  in order to obtain its treatment of waste, then activity  $W$  may be considered a multifunctional activity, supplying both commodity  $j$  and waste treatment. In this case, none of the upstream burdens of the waste’s lifecycle could be passed on to the lifecycle of  $j$ .

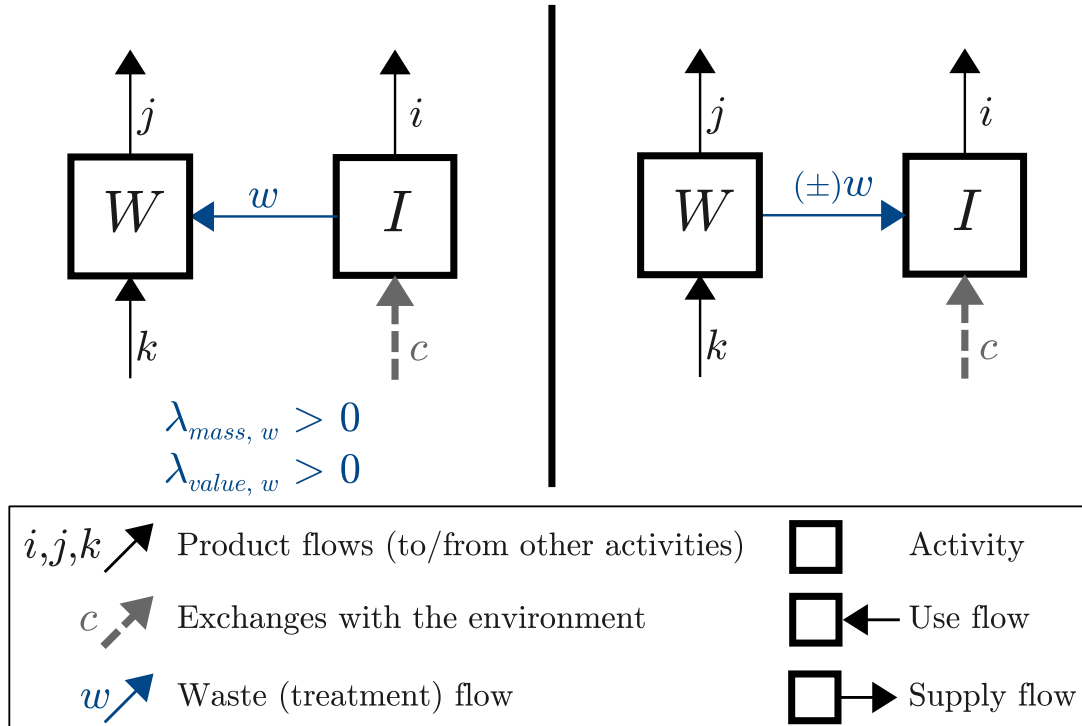


Figure S1: Two different system representations of waste treatment. Left: waste as byproduct supplied by activity  $I$  and used as input by the waste-treating activity  $W$ . Right: waste treatment as a useful service supplied by the waste-treating activity  $W$  and used by activity  $I$ .

Many models follow the logic of figure S1-right and record waste treatment in the supply table ( $\mathbf{V}$ ), but they do so with differing sign conventions. The Leontief (1970) pollution abatement model, waste-IO (Nakamura and Kondo, 2002), and Ecoinvent 2 (Ecoinvent Centre, 2010) all record the supply of waste treatment with a positive coefficient. Following their logic, figure S2-left could be read as “activity  $W$  supplies the treatment of 5 kg of waste to  $I$ ”. This defines  $w$  not as the waste but as the treatment service, measured in kilograms of waste removed and treated. Therefore, each unit of  $w$  is associated with a positive value ( $\lambda_{value, w} > 0$ ) and a negative mass ( $\lambda_{mass, w} < 0$ ), signifying removal from the client activity or the waste market).

On the contrary, ecoinvent 3 (Ecoinvent Centre, 2014) records this same supply of treatment service with a negative coefficient. Following this convention, figure S2-right can be read as “activity  $W$  supplies a service to  $I$  by providing it with  $-5$  kg of waste”, or more fluidly as “activity  $W$  supplies a service to  $I$  by taking in its 5 kg of waste”. This sign convention then defines  $w$  as the actual waste, which necessarily has a positive mass ( $\lambda_{mass, w} > 0$ ) and, in this example, a negative value ( $\lambda_{value, w} < 0$ ).

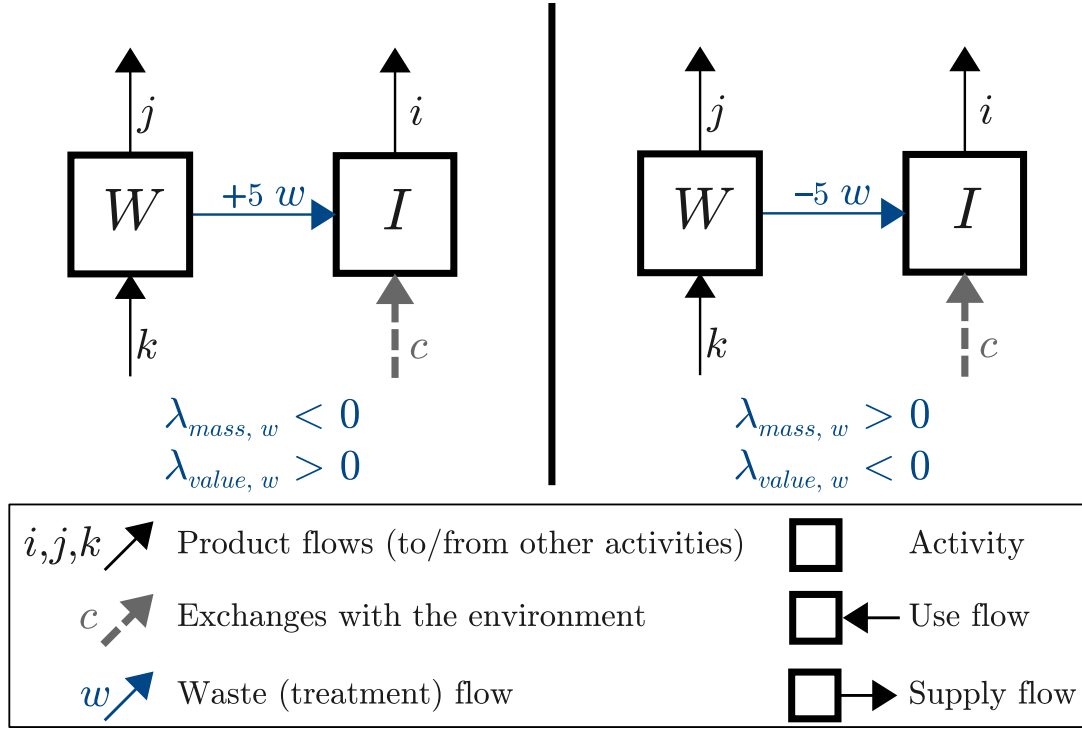


Figure S2: Two different sign conventions for representing waste treatment as a supply flow from the waste-treating industry, with the corresponding sign change in the property table ( $\Lambda$ ). Left: a positive supply of waste treatment service. Right: a negative supply of waste material.

The opposing signs in the property tables ( $\Lambda$ ) under the two conventions of figure S2 ensures that equation (2) (reproduced below) is always directly applicable, regardless of sign conventions, to assess activity balances across all layers.

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

## 6 Numerical examples: Balanced layers of SUT inventories

### 6.1 Combined heat and power example

Tables S2 and S3 respectively record conservative properties of products and factors of production from the combined heat and power (CHP) example. The value, energy and carbon contents of these flows are normalized relative to the units used in the mixed-unit SUT (table 1).

		electricity	heat	coal		
		$\$^{-1}$	$\$^{-1}$	$\text{kg}^{-1}$		
$\Lambda_{\Delta\bullet}$	=	value	\$	1.00	1.00	0.0950
		energy	kJ	51.4	566	33.0
		carbon	kg	0	0	0.850

Table S2: Value, energy and carbon contents per unit of the different products of the CHP system.

		CO <sub>2</sub>	O <sub>2</sub>	waste heat	labor		
		$\text{kg}^{-1}$	$\text{kg}^{-1}$	$\text{kJ}^{-1}$	$\$^{-1}$		
$\Lambda_{\Delta\star}$	=	value	\$	0	0	0	1.00
		energy	kJ	0	0	1.00	0
		carbon	kg	0.273	0	0	0

Table S3: Value, energy and carbon contents per unit of the different factors of production of the CHP system.

Based on these properties, and following equations (S1) to (S3), we separate the mixed-unit flows of the CHP plant (table 1) in monetary, energy, and mass layers in tables S4 to S6.

value (\$)	Use flows	Supply flows	Factor requirements	Residual
	CHP	CHP	CHP	
electricity	0	24		
heat	0	2.1		
coal	10	0		
CO <sub>2</sub>			0	
O <sub>2</sub>			0	
waste heat			0	
labor			16	
total	10	26	16	0

Table S4: Use flows, supply flows and use of factors of production by a fictional CHP plant, expressed in terms of their financial value (\$)



energy (kJ)	Use flows CHP	Supply flows CHP	Factor requirements CHP	Residual
electricity	0	1216		
heat	0	1216		
coal	3474	0		
CO <sub>2</sub>			0	
O <sub>2</sub>			0	
waste heat			-1042	
labor			0	
total	3474	2432	-1042	0

Table S5: Use flows, supply flows and use of factors of production by a fictional CHP plant, expressed in terms of their energy content (kJ)

carbon (kg)	Use flows CHP	Supply flows CHP	Factor requirements CHP	Residual
electricity	0	0		
heat	0	0		
coal	89	0		
CO <sub>2</sub>			-89	
O <sub>2</sub>			0	
waste heat			0	
labor			0	
total	89	0	-89	0

Table S6: Use flows, supply flows and use of factors of production by a fictional CHP plant, expressed in terms of their carbon content (kg)

None of the layers present residuals, and this fictional CHP plant is therefore fully balanced in terms of its financial, energy and carbon dimensions.

## 6.2 Cattle example

Tables S7 and S8 respectively record conservative properties of products and factors of production from the cattle example. The value, mass, and carbon contents are normalized relative to the units used in the mixed-unit SUT representation (table 2).

			milk kg <sup>-1</sup>	cow meat kg <sup>-1</sup>	steer meat kg <sup>-1</sup>	feed kg <sup>-1</sup>
$\Lambda_{\Delta\bullet}$	=	value	\$ 1.92	4.85	6.07	0.250
		dry mass	kg 1.00	1.00	1.00	1.00
		carbon	kg 0.542	0.533	0.623	0.402

Table S7: Value, dry mass, and carbon contents per unit of the different products of the cattle example.

		manure kg <sup>-1</sup>	respiratory water kg <sup>-1</sup>	CO <sub>2</sub> kg <sup>-1</sup>	O <sub>2</sub> kg <sup>-1</sup>	labor \$ <sup>-1</sup>	
$\Lambda_{\Delta^*}$	=	value \$	0	0	0	0	1.00
		dry mass kg	1.00	1.00	1.00	1.00	0
		carbon kg	0.402	0	0.273	0	0

Table S8: Value, dry mass and carbon contents per unit of the different factors of production of the cattle example.

Based on these properties, and following equations (S1) to (S3), we separate the mixed-unit flows of the cattle farming activities (table 2) in monetary, mass and carbon layers (tables S9 to S11).

Value (\$)	Use flows		Supply flows		Factor requirements		Residual
	Raising Cow	Raising Steer	Raising Cow	Raising Steer	Raising Cow	Raising Steer	
milk	0	0	7990	0			
cow meat	0	0	1180	0			
steer meat	0	0	0	1840			
feed	7350	1520	0	0			
manure					0	0	
respiratory water					0	0	
CO <sub>2</sub>					0	0	
O <sub>2</sub>					0	0	
labor					1820	320	
total	7350		9170		1820		0
total		1520		1840		320	0

Table S9: Use flows, supply flows and net use of factors of production throughout the fictional lives of a dairy cow and a steer for slaughter, expressed in terms of their monetary value (\$)

Mass (kg)	Use flows		Supply flows		Factor requirements		Residual
	Raising Cow	Raising Steer	Raising Cow	Raising Steer	Raising Cow	Raising Steer	
milk	0	0	4170	0			
cow meat	0	0	243	0			
steer meat	0	0	0	304			
feed	29389	6090	0	0			
manure					-20440	-5110	
respiratory water					-1810	-309	
CO <sub>2</sub>					-4420	-754	
O <sub>2</sub>					1690	385	
labor					0	0	
total	29389		4410		-24978		0
total		6090		304		-5790	0

Table S10: Use flows, supply flows and net use of factors of production throughout the fictional lives of a dairy cow and a steer for slaughter, expressed in terms of their mass composition (kg dry mass)

Carbon (kg)	Use flows		Supply flows		Factor requirements		Residual
	Raising Cow	Raising Steer	Raising Cow	Raising Steer	Raising Cow	Raising Steer	
milk	0	0	2260	0			
cow meat	0	0	130	0			
steer meat	0	0	0	189			
feed	11807	2450	0	0			
manure					-8210	-2050	
respiratory water					0	0	
CO <sub>2</sub>					-1210	-206	
O <sub>2</sub>					0	0	
labor					0	0	
total	11807		2390		-9420		0
total		2450		189		-2260	0

Table S11: Use flows, supply flows and net use of factors of production throughout the fictional lives of a dairy cow and a steer for slaughter, expressed in terms of their carbon content (kg carbon)

None of the layers present residuals, and the fictional dairy cow and steer farming activities are therefore fully balanced in terms of their financial, mass and carbon dimensions.

## 7 Sensitivity to inhomogeneity in product groups

In this section, we briefly revisit the different proofs of this article and discuss to what extent their validity depends on the homogeneity of product group property descriptions. It therefore maps out in greater detail the scope of applicability of this analysis.

A product group is considered homogeneous if its properties —such as price, energy density, or carbon content— are constant throughout the system description. Inhomogeneity in product group descriptions is a known source of imbalances across property layers in EEIO and LCA (Weisz and Duchin, 2006), even in the absence of any coproduction modeling (e.g., Merciai and Heijungs, 2014). As this study strives to single-out the specific consequences of coproduction model choices, it excludes all other sources of imbalances and assumes a “clean” starting point: a fully balanced, multilayered SUT inventory, with product groups that are homogeneous in terms of all conservative properties.

In the present framework, the assumption of product group homogeneity is made explicit in the product property table ( $\Lambda_{\Delta\bullet}$ ) and is involved in the conversion between the mixed-unit system description and the different property layers of the multi-unit representation.

First, it must be noted that production balance (preserving row-sum balance) is assessed directly in the mixed-unit layer, with each product described in terms of whatever unit proves most convenient. The assessment of this balance therefore does not depend on unit conversions and homogeneous product group descriptions. In other words, it is not necessary to have a homogeneous description of a product across multiple layers to assess that an allocation or construct does not perturb the balance between supply and demand. Propositions 7 to 9 are therefore robust to inhomogeneity in product group descriptions.

Second, it is clearly impossible to assess whether a model preserves the initial balances of an inventory if this inventory is, in fact, not initially balanced. Consequently, our assessments of balanced recipes are not applicable to situations where inhomogeneous product groups lead to imbalances directly in the SUT inventory. Such SUT imbalances would arise, for example, if *average* product properties were used to derive the different property layers of the SUT (equations (S1) and (S2)) despite the presence of inhomogeneous product mixes. The analyses of balances in allocated recipes are clearly inapplicable to such pre-disturbed inventories.

The presence of inhomogeneous product groups does not, however, preclude the possibility of a balanced multilayered SUT inventory. A mixed-unit layer can be split into balanced property layers even in the presence of inhomogeneities, as long as the conversion is performed using product descriptions that reflect this inhomogeneity. This requires that properties be described for every product *in each activity*, which adds a new dimension to the product-property table ( $\Lambda_{\Delta*\bullet}$ ), and transforms equations (S1) and (S2) to equations (S75) and (S76).

Layer of property  $m$  in a multi-unit SUT with inhomogeneous product groups:

$$u_{iJ}^m = \lambda_{mJi} u_{iJ} \quad m \in \Delta, \forall (i, J) \in (\bullet, *) \quad (\text{S75})$$

$$v_{iJ}^m = \lambda_{mJi} v_{iJ} \quad m \in \Delta, \forall (i, J) \in (\bullet, *) \quad (\text{S76})$$

For example, instead of using average product prices to derive a monetary layer from a mixed-unit layer, per-industry product prices would be used in situations of price inhomogeneity (Merciai and Heijungs, 2014). The balance of each layer of the inventory can then be expressed in terms of these per-industry properties as in equation (S77) (instead of equation (2)).

$$\sum_{i \in \bullet} \lambda_{mJi} u_{iJ} + \sum_{c \in \star} \lambda_{mc} g_{cJ} = \sum_{j \in \bullet} \lambda_{mJj} v_{jJ} \quad m \in \Delta, J \in \ast \quad (\text{S77})$$

The applicability of propositions 1 to 3 to such a balanced but inhomogeneous SUT then depends on whether or not their proofs can be reformulated in terms of the 3-dimensional product-property matrix and equation (S78) (instead of equation (6)).

$$\sum_{i \in \bullet} \lambda_{mJi} z_{iJj} + \sum_{c \in \star} \lambda_{mc} g_{cJj} = \lambda_{mJj} v_{jJ} \quad m \in \Delta, J \in \ast, \forall j \in \bullet \quad (\text{S78})$$

The proof of proposition 1, which describes the criterion for balanced PA, depends only on the properties of products within the allocated industry. As it never requires the description of products elsewhere in the system, it is not affected by product inhomogeneities between industries, and its proof is easily reformulated in terms of equation (S78) and  $\mathbf{\Lambda}_{\Delta \ast \bullet}$ . Our assessment of PA will therefore hold even in case of product group inhomogeneity, as long as the initial inventory is balanced.

The assessment of PSA does put in relation the properties of products inside and outside of the multifunctional activity; proposition 2 and corollary 2.1 are expressed in terms of an equality between secondary products and the products that they substitute. When applied to an SuUT, PSA automatically models the substitution of products from average primary production mix (Majeau-Bettez et al., 2014). If product descriptions are inhomogeneous in terms of property  $m$ , the amount of  $m$  in substituted products will then depend on the primary producers' market shares, which are lost in the normalization process. Consequently, we find that proposition 2 is not applicable to situations where an untraceable SUT presents product group inhomogeneities.

Conversely, if PSA is applied to a balanced StUT inventory, proposition 2 remains valid in spite of inhomogeneous product mixes. In a traceable substitution, an explicit choice must be made as to the specific primary producer of the displaced commodity. This traceability of each substituted flow to its source activity ensures that the  $m$ -content of substituted product flows is unambiguous, even in the case of inhomogeneous product mixes.

In contrast, the balance of AAA (proposition 3) depends on the assumption that the alternate technology descriptions ( $\mathbf{A}^\Gamma$  and  $\mathbf{F}^\Gamma$ ) are balanced throughout the system. In other words, a balanced recipe is expected stay balanced regardless of which industry applies it. This, however, will not hold true if product groups are not homogeneous. We therefore find that our assessment of AAA models is not robust to product group inhomogeneities.

In summary, the propositions of this study present different levels of sensitivity to inhomogeneity in product group descriptions. The assessment of production balance only requires a balanced mixed-unit layer and is therefore least affected. Given an initially balanced SUT in spite of inhomogeneous product groups, our assessment of PA remains fully valid, and our assessment of PSA depends on traceability, but our general rule for the balance of AAA becomes inapplicable. The balanced character of each untraceable PSA or each AAA assumption would then need to be assessed on a case-by-case basis.

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