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Norwegian University of
Science and Technology

Doctoral Thesis

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Convergence of Industrial Ecology Methods for the Analysis of our Socio-economic Metabolism

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May 7, 2015

To Monique

But one day I secretly overheard the spell —it was just three syllables— by taking my stand in a dark place. He went off to the square after telling the pestle what it had to do, and on the next day, while he was transacting some business in the square, I took the pestle, dressed it up in the same way, said the syllables over it, and told it to carry water.

When it had filled and brought in the jar, I said, "Stop! Don't carry any more water. Be a pestle again!"

But it would not obey me now; it kept straight on carrying until it filled the house with water for us by pouring it in! At my wit's end over the thing, [. . .] I took an axe and cut the pestle in two; but each part took a jar and began to carry water, with the result that instead of one servant I had now two.

Philopseudes, Lucian of Samosata, ca. AD 150

Preface

This work was carried out at the Industrial Ecology Programme (IndEcol) and the Department of Energy and Process Engineering (EPT) at the Norwegian University of Science and Technology (NTNU) in Trondheim, Norway, in the period from 2010- 2015. The thesis has been submitted to the Faculty of Engineering Science and Technology (IVT) in partial fulfilment of the requirements for the degree of philosophiae doctor.

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My very first thanks go to my family. Je vous dois toute ma joie.

I wish to thank my friends, colleagues, and classmates at IndEcol for being such an amazing group of people. It is a rare privilege to be part of this honest, smart and friendly team. I am particularly indebted to Symbiosis, and to my many flatmates over the years, for helping me feel at home in Norway and for salvaging some life outside of work.

I am grateful to NTNU, EPT, and the Industrial Ecology Programme for their technical and financial support over the past years.

The contribution from all my co-authors is beyond measure. For their critical insights, for stimulating discussions, for their hard work and camaraderie, and for both challenging and preserving my sanity, very special thanks are due to Stefan Pauliuk, Richard Wood, Konstantin Stadler, Thomas Dandres, Evert Bouman, Christopher Mutel, Bernhard Steubing, Daniel Müller, Troy Hawkins, Bhawna Singh, and Linda Ager-Wick Ellingsen.

For tactfully helping me improve my English, and for her comments on almost all my articles, I cannot thank Christine Hung enough.

The articles of this thesis would not be half as robust without the dedicated efforts of so many anonymous reviewers and editors. Thank you.

I am deeply honoured to have such a committee assess my thesis; and I am most grateful for their time and critical comments.

My very last thanks are due to my supervisor, Anders Hammer Strømman, and my co-supervisor, Edgar Hertwich, for their leadership and guidance, for their trust and the freedom they gave me, for their patience and constant support, and for all their teachings.

Contents

Chapter 1

Introduction

1.1 The riddle of sustainability

From its humble hunter-gatherer beginnings, humanity has thoroughly transformed itself through agrarian and industrial revolutions (Haberl et al., 2011), asserting ever more control over its direct environment and gaining unprecedented levels of material ease and opportunities. Today, humanity's *socioeconomic metabolism* (Ayres and Simonis, 1994; Fischer-Kowalski and Hüttler, 1999; Fischer-Kowalski and Haberl, 1998; Fischer-Kowalski and Weisz, 1999; Pauliuk and Müller, 2014) —the material and energy flows and stocks under human control— has reached such a magnitude that it significantly alters our planet's natural cycles. Our influence on land and ecosystems (Vitousek, 1997; Foley et al., 2005; Haberl et al., 2007), on the climate (IPCC, 2013; IPCC, 2014), and on the cycles of nutrients (Gruber and Galloway, 2008) and other chemicals (e.g., Gordon, Bertram, and Graedel, 2006) is of geological scale (Crutzen, 2006; Zalasiewicz et al., 2010).

Despite their sheer magnitude, however, these transformations are often the result of unintended side-effects, under-informed decisions, and market or governance failures (Hardin, 1968; Brown, 2001; Costanza et al., 1997; Moxnes, 2000), potentially to the long-term detriment of both humans and wildlife (e.g., Worlds Health Organization, 2014).

It is increasingly evident that the current model of economic development, with its ever growing metabolism, in untenable (Jackson 2009, and also Arrow et al. 1995). We may already be stretching some of the limits of our planet's "safe operating space" (Rockström et al., 2009), just as an important fraction of humanity is striving to partake in the material affluence of the developed world. The riddle of our time may well be how to depart from a "cowboy economy" (Boulding, 1966) —or, in the author's view, a Sorcerer's apprentice economy— to a sustainable way of life for all (see World Commission on Environment and Development, 1987; Steinberger and Roberts, 2010; Fischer-Kowalski et al., 2011a; Haberl et al., 2011).

The field of industrial ecology may be seen as one of the scientific responses to this riddle of sustainability (Frosch and Gallopoulos, 1989; Jelinski et al., 1992; Huppes and Ishikawa, 2010). It is "a multidisciplinary field that analyses material [...] and energy flows of industrial and consumer systems at a variety of spatial scales, drawing on environmental and social science, engineering, business and policy" (International Society for Industrial Ecology, 2014). It is based on the premise that a combination of research tools from different discipline can offer a holistic system perspective more apt to guide society toward a balance with its environment.

1.2 Research questions and thesis structure

Among the tools used to gain this system perspective, lifecycle assessment (LCA), environmentally extended input–output analysis (EEIO), and material flow analysis (MFA) are central to the industrial ecology literature. These data-intensive tools, which operate at different scales and relate differently to natural science and economic modeling paradigms, all offer insights into our socio-economic metabolism and relate environmental impacts to our production and consumption. However, despite a growing understanding of their partial compatibility and complementarity (Bouman et al., 2000; Duchin, 2009; Suh et al., 2004), and despite repeated calls for their further integration (e.g., Suh and Nakamura, 2007; Haes et al., 2004; Weidema, 2011), these tools are typically used in isolation. The hybridization of these methods remains rare, ad-hoc, and work intensive; a consistent integration remains elusive.

The present thesis then asks: *how can further integration of core industrial ecology data and tools add efficiency and consistency to research on sustainability?* This ambitious overarching research question may never be fully resolved, but this thesis strives nonetheless to yield a partial answer by addressing three sub-questions.

Q1: How can industrial ecology *data and databases* be integrated so as to bring greater research efficiency and consistency?

Q2: How can the integration of *models and software tools* contributed to greater research clarity and efficiency?

Q3: How can these integrations contribute to a more consistent match between research methods and objectives?

These sub-questions are not fully independent and partly overlap, but they nonetheless help focus and structure this thesis, as illustrated by figure 1.1.

The thesis comprises seven main articles (figure 1.1, full boxes) that motivate or build-upon each other (dashed and full arrows). On the vertical axis, figure 1.1 connects these articles to the overarching question and the three sub-questions of the thesis. On the horizontal axis, it arranges the articles based on the timescale of the integrations that they investigate, from assessments of current practice to guidance for long-term integration efforts. The articles in this thesis are ordered so as to follow the logical connection between them and to present increasingly important departures from the *status quo*. As further detailed in the conclusion and in appendix C, this thesis is motivating further research on a practical ontology and an accounting structure for the socio-economic metabolism (figure 1.1, dotted box).

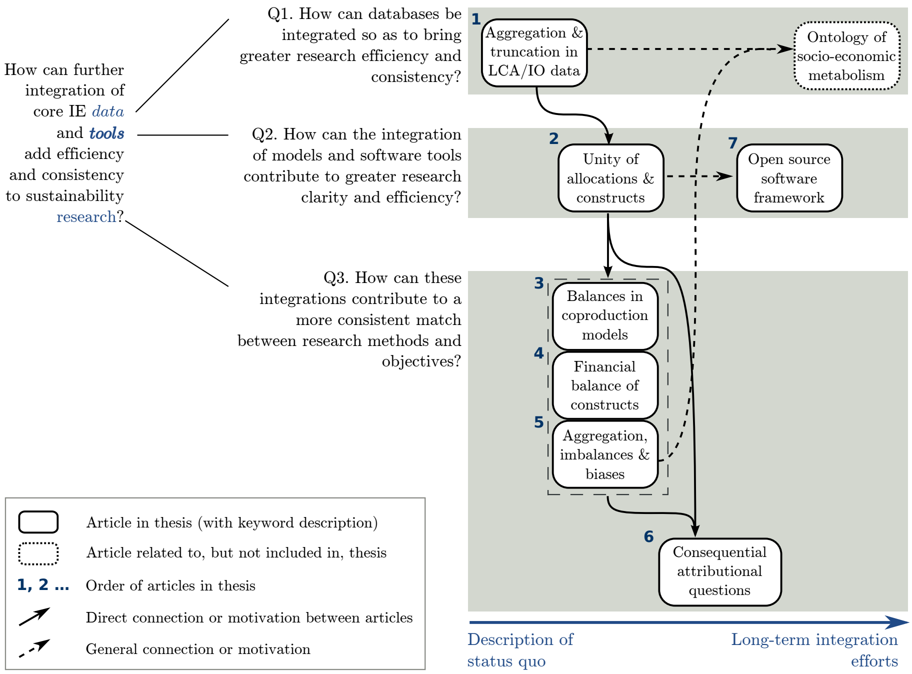

Figure 1.1: Structure of thesis

1.3 Overview of articles

A rich body of literature argues in favor of hybridization of LCA and EEIO, and multiple case studies compare the results of pure process-based LCA, pure EEIO, and hybrid analyses. Few studies, however, analyze the compatibility and complementarity of complete LCA and EEIO databases. The first article of this thesis strives to fill this gap.

Article 1 (chapter 2): Article 1 performs an empirical comparison of a process-LCA database with a national EEIO in terms of truncation and aggregation issues. Many economic sectors were found to be under-represented in the process-LCA database, which points to probable underestimations of the impacts arising from these sectors in current LCA studies. This article finds that LCA and EEIO data sets are complementary in their coverage of the economy. Their integrated development has the potential to lead to significant efficiency gains.

Such an integrated database development, however, is hindered by differing modeling assumptions in LCA and EEIO practice. Although LCA and EEIO calculations are equivalently based on the Leontief inverse, the two fields differ in their treatment of coproduction and in their construction of symmetric technical coefficient matrices. This motivates the second article of this thesis, which aims at harmonizing these modeling practices.

Article 2 (chapter 3): Article 2 proposes a unified framework for the treatment of coproducts in LCA and EEIO. From a single, generalized allocation equation, all typical LCA allocations and EEIO constructs are derived. The level of traceability of the data is central to explaining the differences between typical LCA and EEIO models; whereas supply and *traceable* use table (StUT) can be directly converted to symmetric coefficient matrices by allocation, supply and *untraceable* use table (SuUT) require an additional aggregation step. Typical EEIO constructs are then expressed as the combination of a allocation model and an aggregation model.

In addition to formally connecting allocation and construct models, this joint analysis also enabled the identification of new modeling options. The dominant EEIO constructs were found to be special cases of more broadly defined, more flexible, modeling families. Similarly, insights from EEIO helped distinguish between two different LCA models that had previously been collectively referred to under the umbrella concept of "system expansion". The integration of allocations and constructs then reveals that practitioners of both sub-fields have access to more diverse and more clearly defined coproduction models than had been previously realized (sub-question Q2).

This clarification of both inventory structures (StUT and SuUT) and coproduction modeling options forces a re-evaluation of the type of research questions that can be handled by LCA and EEIO models.

One of the core objectives of the study of the socioeconomic metabolism is to track the flows and accumulations of stocks. This type of analysis is typically performed with MFA tools, but extensions of Leontief-type models are also sometimes used for this a purpose (e.g., Nakamura and Nakajima, 2005; Nakamura et al., 2014). This use of LCA and EEIO is dependent, however, on their capacity to simultaneously conserve mass, energy, and value, which in turn is influenced by the choice of coproduction models (allocations and constructs) and the level of aggregation. Articles 3 to 5 then explore different methodological aspects pertaining to the further integration of LCA and EEIO with MFA.

Article 3 (chapter 4): Making use of the harmonized framework developed in article 2 , article 3 investigates the influence of coproduction models on the capacity of LCA and EEIO models to simultaneously respect mass, energy, elemental, and economic balances. None of the coproduction modeling families are balanced in general, but special cases can allow for fully balanced Leontief production functions. This is notably the case for ideal substitution (as assumed by the byproduct-technology construct (BTC)) and ideal alternate activity assumptions (as assumed by the commodity-technology construct (CTC)). These special cases, however, are partly dependent on the level of aggregation of the system description, which has some bearing on article 5 . In addition, this article evaluates the capacity of allocations and constructs to respect production balance, which has implications for article 6 .

Article 4 (chapter 5): The analysis in article 3 demonstrated that BTC always leads to balanced process descriptions across all unit layers (mass, energy content, value, etc.), and that the industry-technology construct (ITC) necessarily respects the balance of the unit layer to which it is applied (e.g., respect of mass balance when applied to mass layer). These proofs are in direct opposition with the proofs of Jansen and Raa (1990a), which find that BTC and ITC do not generally respect financial balance when applied to a monetary supply and use tables (SUTs). Article 4 resolves this contradiction in the literature, identifying two embedded assumptions in the proofs of Jansen and Raa (1990a) that overly restrict their financial balance test and cause false negatives. It further confirms the validity of the balance assessments in article 3 .

Article 5 (chapter 6): Imbalances may arise in LCA and EEIO descriptions due to the presence of inhomogeneous product groups, which in turn are caused by the level of aggregation of the description. These imbalances can be interpreted as violations of fundamental physical laws, such as the conservation of mass and energy. Merciai and Heijungs (2014) recently addressed this issue for situations of price inhomogeneities in EEIO analyses, which lead them to warn against possible biases and physical inconsistencies arising from the use of EEIO tables recorded in monetary units. Article 5 extends their analysis and demonstrates that inhomogeneous aggregation can lead to imbalances across unit layers in both LCA and EEIO, regardless of the choice of monetary or physical units. Leveraging insights from article 3 , chapter 6 then further clarifies the relation between inhomogeneous aggregation, physical and financial imbalances, coproduction modeling, and the presence or absence of a systematic bias in lifecycle results.

The tracking of material, energy and value flows is not the only research objective to which this thesis can bring greater consistency. The diverse set of coproduction models identified in article 2 , and the joint analysis of their balance properties (articles 3 and 4), can potentially help refine the distinction between attributional and consequential analyses (sub-question Q3).

Article 6 (chapter 7): The LCA community increasingly distinguishes between an attributional perspective, which asks what environmental impact may be associated with a final consumption, and a consequential perspective, which typically asks how impacts may change as the result of a change in final consumption. A literature review of coproduction types is performed, and a list of defining characteristics for attributional and marginal consequential perspectives is compiled. Article 6 then evaluates the compatibility of the different allocation or construct models, when applied to various types coproduction, with attributional and marginal consequential research objectives. This concordance analysis yields clear practical recommendations.

The further integration of industrial ecology (IE) presents both opportunities and challenges for tool and software software development. On the one hand, it may be an occasion to pool development resources, avoid double work performed in parallel in the different sub-communities, and ensure that the enhanced flexibility of IE system representations is reflected in its software. On the other hand, it raises issues of interoperability of tools, may force the joint manipulation of large and dissimilar data sets. Article 7 argues that a more transparent and collaborative open-source software development framework is required for the further development and integration of IE.

Article 7 (chapter 8): Article 7 reviews software development activities in IE and identifies challenges with respect to transparency, re-usability, and interoperability. It investigates how best practice guidelines for scientific programming could be applied within the IE community, and it argues in favor of an open-source development framework for greater efficiency and scientific credibility. As a first effort in this direction, article 7 presents an open-source Python toolbox, which includes a SUT object class (pySUT.py) that can perform the allocation and construct calculations from chapter 3. It also proposes a module (ecospold2matrix.py) that can reorganize an LCA data set into a SUT matrix structure for easier integration with EEIO practice. These tools are then put in relation with other LCA, EEIO and MFA software.

Chapter 2

Evaluation of process- and input–output-based life cycle inventory data with regard to truncation and aggregation issues

Guillaume Majeau-Bettez, Anders Hammer Strømman, Edgar Hertwich

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2.1 Introduction

Top-down and Bottom-up Perspectives in Life Cycle Studies

Lifecycle assessment (LCA) and input–output analysis (IO) studies both strive to quantify the direct and indirect impacts of production and consumption activities. Since the late 1990s, many methods have been proposed to hybridize the two approaches, such as IO-based, integrated (Suh et al., 2004), tiered (Strømman, Peters, and Hertwich, 2009), waste IO (Nakamura and Kondo, 2002), separative (Williams, 2004), and path exchange (Lenzen and Crawford, 2009) hybrid life cycle assessments (HLCA). Although significant differences distinguish these inventories, all are based on the principle of a disaggregated and detailed process-based description of the most important activities (foreground) linked to an aggregated but complete model of the rest of the economy (background). Although, in theory, HLCAs are superior (Finnveden et al., 2009; Suh and Nakamura, 2007) to either LCA or environmentally extended input–output analysis (EEIO), notably in regard to system boundary definition (Suh et al., 2004), these hybrid assessments have yet to enter mainstream practice and become an explicit priority of the field's guidelines (European Commission, 2010) and standards (International Organization for Standardization, 1997; International Organization for Standardization, 2006). The lack of quantitative assessments of the presumed advantages of HLCA relative to LCA and EEIO (Williams, Weber, and Hawkins, 2009; Crawford, 2008) may partly explain its slow adoption. This manuscript presents quantitative evaluations of the limitations of both conventional LCA and EEIO. In this study, we linked data sets from both fields and compared them. We then used EEIO as a reference point to evaluate the extent to which the LCA database covers the different sectors of the economy. We also used the LCA data to assess uncertainty issues due to aggregation in EEIO.

Although EEIO and LCA have technical differences, they share a common mathematical framework (Weisz and Duchin, 2006). Distinctions between the two techniques arise largely because of the different levels of resolution at which they operate (Suh and Nakamura, 2007). Conventional LCAs typically describe activities in a bottom-up process-based manner, providing more detail and a deeper understanding of the nature of activities at the product level. On the other hand, conventional EEIO inventories are based on national or regional accounting tables, and thus describe economic activities in a top-down manner at a macro level (Suh and Huppes, 2005). The opposite perspectives of these two approaches and the different levels of data resolution lead to fundamentally different strengths and shortcomings.

Truncation Bias in LCA

As all economic activities are ultimately linked to each other, to accurately describe any value chain would require that the entire economy be inventoried. In practical terms, process-based LCAs necessarily fail to account for a fraction of the activities required to fulfill any given final demand (Suh and Huppes, 2005; Suh and Huppes, 2002). Consequently, process-LCAs systematically underestimate environmental impacts (Lenzen and Dey, 2000). The consequences of this truncation bias are expected to depend on the goal of the LCA study. If a comparative LCA strictly aims to rank processes whose value chains involve activities within a similar industry mix, it may be "hoped" that all inventories suffer from similar levels of incompleteness, in which case the ranking would be relatively insensitive to truncation error. However, in situations where processes fulfilling equivalent functions have value chains that involve different industry mixes, it has been demonstrated that their ranking in a comparative process-LCA may be determined strictly by the difference in the level of truncation of their background inventories (Lenzen, 2002b). If the goal of an LCA is not solely comparative, an underestimation bias is even more problematic. This is notably the case if a study is intended to provide a standalone life cycle inventory (LCI) in a database, or if results are expressed as absolute environmental footprints (Larsen and Hertwich, 2010) to guide sustainable consumption.

Suh and Huppes (2002) pointed to the use of EEIO data to estimate missing inventory elements and to direct inventory efforts. Junnila (2006), Williams (2004), and Ferrao and Nhambiu (2009) compared process-based LCA case studies with EEIO or HLCA equivalents and found the process-based results to be 30–60% lower. Another approach for assessing truncation is based on the comparison of the process-based foreground of an HLCA relative to the complete system description of the study. Using this approach, Williams (2004), Crawford (2008), Zhai and Williams (2010) and Acquaye et al. (2011) found that the process-based fraction of their inventories typically represented 20–50% of the total environmental impact. The two evaluation methods may not be equivalent because process-inventory efforts may differ between LCA and HLCA. The neglected elements of process-based LCIs may also be investigated via structural path analysis (Lenzen, 2002a; Treloar, 1997) and the price model (Strømman and Solli, 2008).

Another LCA truncation assessment technique involves modifying an EEIO data set to model an incomplete system description. Lenzen and Dey (2000), Lenzen (2002b) and Lenzen (2000), and Rowley, Lundie, and Peters (2009) used power series expansion of EEIO life cycle impacts to model LCAs that would fail to inventory value chains beyond a certain number of steps upstream. They estimated that process-LCA could typically suffer from upstream truncation of 30–50%. Their model represents process-inventory practice in a simplified manner by assuming that each tier of the value chain is either fully inventoried or not at all. Norris (2002) proposes a different model, which does not limit the number of tiers covered but rather the completeness with which elements are described. If each IO sector is truncated of its minor inputs such that 10% of the upstream impacts are lost, the median cumulative effect of this "pruning" is an underestimation by 35% of the total impact.

Aggregation and Uncertainty in EEIO

Contrary to LCA, IO inventories encompass the entire economy of a region to infinite order but necessarily operate at an aggregated level (Williams, Weber, and Hawkins, 2009). With all the activities of a national economy lumped into a few hundred sectors at best, IO data is blind to individual processes. Consequently, it cannot be used to guide technological or consumer choices at a product level (Suh and Huppes, 2002; Lenzen, 2000).

Two types of aggregation lead to increased uncertainty: the aggregation of data from multiple producers undertaking the same process (process-averaging) and the aggregation of different processes constituting an industry category (coarse-graining) (Williams, Weber, and Hawkins, 2009; Lenzen, 2000). By moving the system description away from a one-to-one correspondence between industry and commodity, coarse-grain aggregation also increases allocation uncertainty (Lenzen, 2000; Miller and Blair, 2009).

Aggregation is but one of the many sources of uncertainty related to IO data, along with price homogeneity considerations, variability in capital expenditures, and differing technology descriptions of imports (Suh et al., 2004; Williams, Weber, and Hawkins, 2009). Uncertainties in IO data have been estimated on the basis of the fluctuations in IO time-series (Yamakawa and Peters, 2009) and the standard deviations of industry surveys (Lenzen, 2000; Lenzen, Wood, and Wiedmann, 2010). The correspondence that occurs in HLCA when more detailed process data are substituted for more generic EEIO data can also be used to evaluate EEIO uncertainty (Crawford, 2008). Little work, however, has examined the specific contribution of data aggregation to the uncertainty of IO results. Lenzen (2000) correlated the standard deviation of industry surveys with the logarithm of the number of aggregated industries.

. . . and Vice Versa

This is not to say that LCA is devoid of aggregation and uncertainty issues or that EEIO is free from cutoff considerations. On the contrary, the quantitative treatment of uncertainty in LCA has received increased interest in literature (Williams, Weber, and Hawkins, 2009; Ross, Evans, and Webber, 2002; Lloyd and Ries, 2007). Also, it is not uncommon for LCA practitioners to work with aggregated data (Williams, Weber, and Hawkins, 2009; Hischier et al., 2005). With regard to system boundary issues in EEIO, studies may fail to account for nontransactional activities during the use and disposal phases of products (Williams, Weber, and Hawkins, 2009; Lenzen, 2000) or may exclude infrastructure requirements (Crawford, 2008; Lenzen and Dey, 2000; Lenzen, 2001), i.e., capital goods. Truncation errors may also arise in EEIO because of the insufficient number of environmental stressors systematically recorded (Suh and Huppes, 2005). Nevertheless, uncertainty in LCA and system boundary definitions in EEIO do not constitute the most pressing problems, but rather the reverse.

Priority Substructures

Efficiently focusing data collection efforts is a crucial aspect in the management of uncertainty and truncation bias (Williams, Weber, and Hawkins, 2009; Suh and Huppes, 2002), especially for database compilation. The fields of LCA and IO have developed a series of techniques to identify the most critical elements of production systems. The tolerable limit (Sherman and Morrison, 1950) and the elasticity-based (Tarancón et al., 2008) approaches to identifying important coefficients in IO are equivalent to the one-way sensitivity (Björklund, 2002) and the perturbation (Heijungs, 2010) analyses used in LCA, respectively. On the other hand, key sector and cluster linkage analyses, which assess the interactions between the substructures of production systems and are richly discussed in IO literature (Lahr, 2001), seem relatively absent from LCA literature. A more extensive review is provided in the Supporting Information (SI). This study makes use of Hirschmanian linkages (Jones, 1976; Hirschman, 1958) to identify key sectors.

Comparisons of Complete Databases

As demonstrated by Norris (2002), truncation issues are compounded in process-based data sets. The same logic applies to aggregation uncertainty in IO data sets. There is thus a need to go beyond case-study comparisons and contrast whole data sets. Very little work has been done in this direction. Mongelli, Suh, and Huppes (2005) compared the structures of the process-based ETH-96 and the IO-based MIET 2.0 data sets. Overall, the input structures were found to have similar shapes. Whereas most discrepancies between the input structures appeared stochastic, the share of CO_2 embedded in inputs of capital goods, transport, and services was found to be systematically underestimated in the process-based LCIs.

Objectives and Scope

The literature points to the need for more systematic and quantitative investigation of truncation error and aggregation uncertainty in life cycle disciplines, especially for complete data sets. It also highlights the fundamental complementarity between the LCA and EEIO techniques. As was stressed by Williams, Weber, and Hawkins (2009), one approach can be used to evaluate the strengths and weaknesses of the other. To build upon this concept, we propose simple yet novel evaluations of the truncation and aggregation issues in conventional LCA and EEIO data. This study aims to contribute quantitative insights to the broader discussion on the integration of LCA and EEIO in a common framework. Thus, we propose to explore some ways in which process-based and EEIO-based data sets can be useful to each other's development.

The implicit assumption lying behind the use of generic process-based data sets is that these data sets can adequately represent the background economic activities required to support the delivery of a functional unit (FU), relieving the practitioner from an unrealistic amount of data collection. We examine this assumption in terms of data truncation and aggregation. It would be partially invalidated if it were found that important and complex sectors of the economy are represented in the LCA data set by a disproportionately small fraction of the process descriptions. As some types of inputs are thought to be systematically underestimated in life cycle technology descriptions (Mongelli, Suh, and Huppes, 2005), there is a need to assess to what extent this translates into an underrepresentation of some sectors of the economy in LCA databases. This angle of investigation may be reformulated in terms of inventory efforts. Are the limited inventory resources allocated to the different sectors of the economy in a manner consistent with empirical indicators of their environmental, structural, and economic importance?

Aggregation and uncertainty issues in IO tables have been investigated using the dispersion of data from comparable industry surveys (Lenzen, 2000). To the best of our knowledge, such an assessment has never been undertaken using a complete LCA database as proxy for "survey data". We thus reverse the traditional order of comparisons, and quantify EEIO limitations relative to an LCA data set. With this approach, we also aim to identify variations in sensitivity to aggregation. Are some sectors more robust than others to aggregation uncertainty? What is the level of homogeneity of each sector of the economy at different aggregation levels?

2.2 Methods

Conceptual Framework

Indicators were necessary in order to quantify the more complex elements of this study. The number of LCA processes describing a given portion of the economy was assumed to be representative of the "inventory effort" it received. Similarly, the number of subsectors in each IO sector was used as a relative indicator of the sector's diversity and complexity. Global warming potential (GWP) and total value added were respectively used as indicators for environmental and economic importance. Finally, the structural importance of IO sectors was quantified by Hirschmanian key sector analysis (Jones, 1976) (see SI).

Data Selection and Preparation

This analysis is based on the ecoinvent 2.1 database (Centre, 2009) and the nonhybridized OpenIO (Applied Sustainability Center - University of Arkansas and Sylvatica, 2008) database. The latter, a 2002 EEIO of the United States, provided the necessary level of resolution to be effectively combined and contrasted with a process-based data set. Its 430 economic sectors are organized in a hierarchical manner defined by the U.S. Bureau of Economic Analysis (2010) (BEA), where the number of digits of a sector code indicates its level of specificity or disaggregation (in this case from 2 to 6 digits) (see SI). Final demand vectors for the U.S. economy were produced from the 2002 Detailed Use

Table of the BEA (Stewart et al., 2007). The ecoinvent data set, with approximately 4000 processes in multiple geographical settings, is the most complete and transparent process-LCA database. The two data sets were arranged as square requirement matrices: commodity-by-commodity at producer price for OpenIO and process-by-process with physical units for ecoinvent. CML 2000 characterization factors were used to express emissions as midpoint impact indicators (Guinée, 2002).

The total value added, life cycle GWP intensity, and total GWP emissions—from production and consumption perspectives—were calculated for each economic sector of the OpenIO table at 6-digit resolution (details and equations in SI). The ecoinvent processes were classified within the different economic sectors, for both the BEA and the International Standard Industry Classification (ISIC) (United Nations, 2008) systems (see SI). The total number of ecoinvent processes belonging to each economic sector was calculated at different levels of aggregation.

Database Assessment

As an initial step, the levels of detail of the process-based and IO-based descriptions of each economic sector were directly contrasted at a 2-digit resolution (table 2.1). This allowed for a rapid overview of the state of the art with regard to inventory completeness and specificity. To investigate these inventory patterns, the number of LCA descriptions in the different economic sectors was tested for correlation against these sectors' GWP impacts, GWP intensities, levels of value added, and degrees of linkage (table 2.2). The correlation analyses were performed at a 6-digit resolution and only included economic sectors with at least one ecoinvent process description. As the EEIO table only describes a single nation, a "one-region world" subgroup of the ecoinvent processes was devised in order to allow for a better comparison. Each good or service is counted only once in this subgroup, even if it has been inventoried in multiple countries (see SI). To identify broad patterns underlying the correlation results, we graphically examined the link between environmental impacts and inventory efforts at a 2-digit aggregation level (figure 2.1).

We then used the LCA data set to shed some light on EEIO data aggregation issues. At a given aggregation level, all processes contributing to a given economic sector were grouped in a "sample pool". Within this pool, the most common physical FU was identified (see SI). All processes that had a different FU were removed from the pool. For the remaining processes, the relative standard deviation (RSD) of their life cycle GWP intensities was calculated. This procedure was carried out for all economic sectors at all available aggregation levels. Some economic sectors did not have enough processes to allow for a sample distribution analysis and were therefore excluded. The manner in which aggregation levels affected the dispersions of the impact intensities was taken as an indicator of sensitivity to aggregation uncertainty (figure 2.2).

2.3 Results

Database Completeness and Specificity

Though the LCA database has nearly 10 times more entries than the IO table, this added specificity is not uniform. In fact, some sectors of the economy are altogether absent from the LCA database (table 2.1, ratios of zero). This is a phenomenon we refer to as "sectoral background truncation". As a result, all upstream inputs from a given portion of the economy are impossible to capture in the background of a process-based LCA. It is worth noting that many employment benefits and activities carried out at the workplace belong to these truncated sectors, for example, healthcare, accommodation, and food services. For some industries, these inputs may be the cause for the majority of certain types of impacts (Suh et al., 2004). Some economic sectors, though not completely absent from the LCA database, are described by only few inventories relative to the number of EEIO subsectors (table 2.1, ratios between 0 and 5). This may potentially lead to situations of "aggregation by proxy" in LCA, i.e., the use of a specific inventory to represent a broader economic sector. For other economic sectors such as waste management and utilities, the LCA data dwarfs its EEIO counterpart. The direct comparison of the two data sets thus further emphasizes their complementarity.

Table 2.2 summarizes the different correlation tests relating the importance of economic sectors and the number of process inventories dedicated to them (scatter plots in SI). The coefficients of determination of nearly 0 indicate that neither the value added nor the levels of linkage seem to have had any influence on the extent of the process-based descriptions of the different economic sectors. This would indicate that economic and structural factors have not played an important role in the development of the process-LCA database. Similarly, only a weak correlation was observed between the life cycle GWP intensity of a sector and its share of the ecoinvent process descriptions ($R^2 < 0.2$).

A greater level of concordance was observed between the total GWP impact of a sector and its importance in the LCA database. This positive correlation is stronger from a production perspective ($R^2 = 0.61$) than from a consumption perspective ($R^2 = 0.52$). The difference between these levels of correlation would seem to indicate that activities with important total direct emissions receive more inventory effort than activities causing emissions indirectly in their life cycle. The roughly 600 ecoinvent processes related to Electric power generation, transmission, and distribution largely account for these correlation levels. The detailed coverage of this sector is largely due to the inventory of electricity mixes in multiple countries. For the "one-region world" subgroup, which eliminates international overlaps, the levels of correlation between GWP and the number of inventories plummet ($R^2 < 0.09$).

In figure 2.1, the aggregated sectors were sorted in order of increasing total life cycle GWP from the consumption perspective (black line).This profile may be compared to that of the GWP from the production perspective (dashed line), the shares of LCA descriptions (dark bars), and IO subsectors (light

BEA economic sector	Number of processes	Number of subsectors	ratio
Information	0	14	0
Government Industries	0	12	0
Arts, Entertainment, and Recreation	0	9	0
Health Care and Social Assistance	0	8	0
Real Estate and Rental and Leasing	0	7	0
Finance and Insurance	0	6	0
Accommodation and Food Services	0	3	0
Educational Services	0	3	0
Management of Companies[a]	0	1	0
Retail Trade	0	1	0
Wholesale Trade	0	1	0
Professional[b] Services	2	14	0.14
Other Services[c]	20	13	1.5
Manufacturing	1619	279	5.8
Agriculture, Forestry, Fishing[d]	232	19	12
Transportation and Warehousing	158	10	16
Mining	196	11	18
Construction	254	7	36
Waste Management[e] Services	451	9	50
Utilities	948	3	3.2×10^2

[a][...]and Enterprises; [b] [...], Scientific, and Technical[...]; [c] [...](except Public Administration); [d] [...]and Hunting; [e] [...] and Remediation [and] Administrative and Support[...]

Table 2.1: Comparison of the levels of detail of the descriptions by process-LCA and by EEIO of the different economic sectors, at 2-digit resolution, in order of increasing ratios

bars). To not overwhelm this figure, only ecoinvent processes belonging to the “one-region world” subset were included (see SI).

The striking feature of figure 2.1 is that the sectors prioritized in the process-LCA database generally correspond to sectors for which the producer allocation of GWP is greater than the consumer allocation. This trend is observed in the case of utilities, transportation, mining, agriculture, and waste management, though not in the case of manufacturing and construction. Apart from these two important exceptions, figure 2.1 suggests that the implicit preference of process-LCAs for activities with important direct emissions, a trend previously identified at the 6-digit resolution level in table 2.2, also holds true for broader aggregated economic sectors. This notion that inventory efforts “peak” for sectors where direct emissions prevail is reinforced by the fact that, in every case, the share of process descriptions in LCA is greater than the share of subsectors in EEIO. Among the “background sectoral truncations” identified in table 2.1,

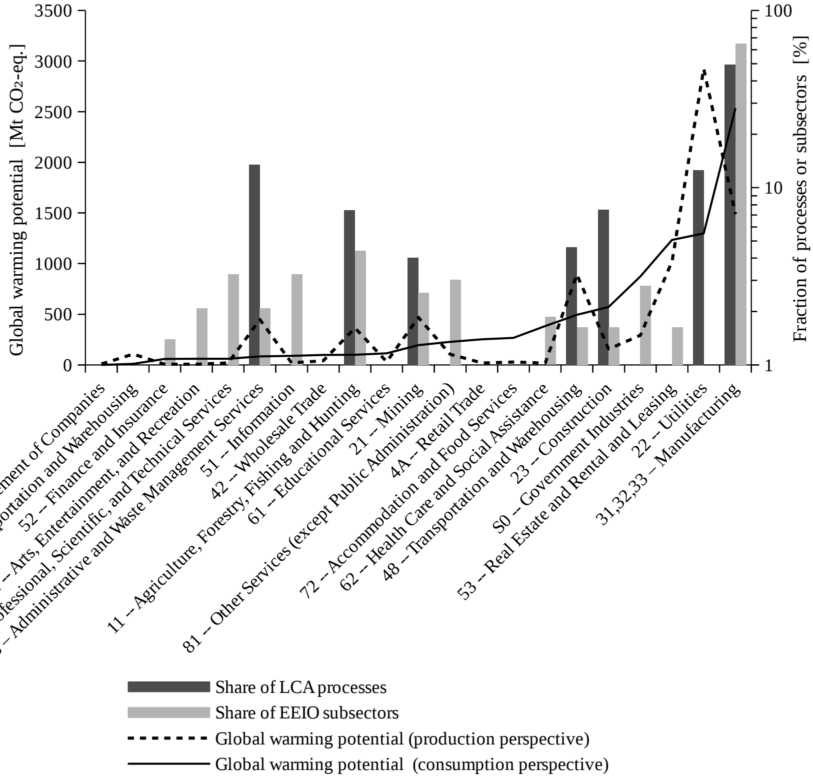

Figure 2.1: EEIO economic sectors (BEA, 2-digit resolution) in order of increasing life cycle global warming potential (consumer perspective), with the corresponding direct global warming potentials (producer perspective), shares of LCA processes, and 6-digit EEIO subsectors.

indicators of importance of economic sector[a]	coefficients of determination (R^2)	
	all countries[b]	one-region world[b]
Global warming potential		
producer perspective	0.61	6.9×10^{-2}
consumer perspective	0.52	5.5×10^{-2}
Global warming potential intensty	0.18	8.9×10^{-2}
Total value added	0.21	5.0×10^{-2}
Direct backward linkage	5.4×10^{-2}	2.2×10^{-2}
Indirect backward linkage	5.0×10^{-2}	2.6×10^{-2}
Direct forward linkage	5.9×10^{-4}	4.2×10^{-5}
Indirect forward linkage	3.4×10^{-4}	1.4×10^{-3}

[a] BEA, U.S. economy in 2002, 6-digit resolution; [b] 179 degrees of freedom

Table 2.2: Correlation between the Number of Process LCIs Belonging to Economic Sectors and Markers of the Environmental, Economic, or Structural Importance of These Sectors

figure 2.1 highlights healthcare and real estate as both environmentally important from a consumption perspective and relatively complex, i.e., with many IO subsectors.

Aggregation and Environmental Homogeneity

To provide some insight into the link between uncertainty and aggregation, we examined the dispersion of ecoinvent life cycle GWP intensities within each IO sector at different levels of aggregation. In figure 2.2, the RSD of the GWP intensities of the processes (y-axis) belonging to different economic sectors (x-axis) are plotted for different aggregation levels. As represented by the black bars, aggregating LCA processes in 4-digit resolution sectors caused a relative standard deviation less than 200% for approximately 85% of the sectors, and less than 100% for roughly half of them. A general increase in relative standard deviations is observed as economic sectors are aggregated from 4-digit to 1-digit, but the sensitivity to aggregation proves significantly inhomogeneous. For Manufacture, the RSD increases drastically with aggregation, going from less than 200% to 1000%. This is a vast sector with complex value chains. Water supply, sewage, and waste management also presents a strong sensitivity to aggregation. On the other hand, Electricity, gas, steam, and air conditioning, to which ecoinvent dedicates approximately 15% of its inventories, has dispersions of life cycle GWP intensities that are relatively low and invariant with respect to aggregation level (RSD $<$ 200%). The same is true for Transportation and storage. It seems reasonable that these energy- and emission-intensive sectors should be more robust under aggregation, as they are relatively homogeneous and have a large proportion of their emissions in the use phase.

An important general decrease in RSD is graphically observed when going from the 1- to 2-digit resolution, and somewhat less from 2- to 3-digit resolu-

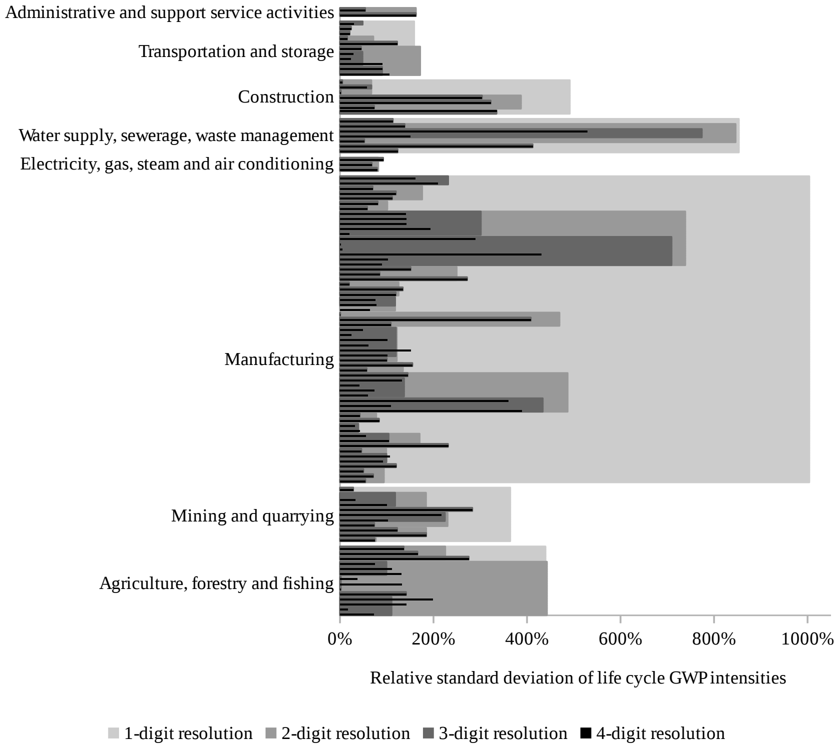

Figure 2.2: Relative standard deviations of life cycle global warming intensities of ecoinvent processes (for a common functional unit) belonging to a each economic sector (ISIC rev. 4), at different aggregation levels.

tion. With the exception of sectors in the manufacture of machinery, only a slight shift in dispersion is observed when going from 3- to 4-digit resolution. This may indicate diminishing marginal returns, in terms of precision gains, to disaggregation investments in EEIO.

2.4 Discussion

Assumptions and Challenges

Our study necessarily uses simple indicators to represent complex concepts, for example, research effort, inventory completeness, aggregation uncertainty, environmental impact, economic importance, and economic linkage. Using the number of process descriptions as an indicator for inventory effort implicitly assumes that process-based LCIs are equal in terms of difficulty and completeness. Although this assumption is certainly crude (Huele and Berg, 1998), it is expected that the great number of processes in the ecoinvent database allowed for an averaging out of extremes and a reliable "average inventory effort" indicator. For the sake of clarity and transparency, we restricted our environmental indicators to global warming. Although LCA and EEIO are concerned with a much broader range of impacts, climate change is one of the best understood and prevailing global environmental threats.

Some of the challenges and uncertainties of this study stem from its attempt to combine and contrast databases that model different types of systems. Some difficulties were encountered in classifying ecoinvent process descriptions within economic sectors, pointing to potential benefits from a harmonized classification framework. The OpenIO data is limited to the United States in 2002, whereas ecoinvent has an international approach, with a strong focus on Europe, over a broader time period. We foresee benefits in contrasting ecoinvent with a multiregion EEIO table rather than a country-specific one. More fundamentally, as our results indicate, the EEIO database strives to model a complete economy, while the LCA database does not, though it is often used as if it did.

In the analysis of the effect of aggregation levels on the environmental homogeneity of EEIO, using the statistical dispersion of LCA data implicitly assumes that the LCA database "samples" the economy in a representative manner. Table 2.1 demonstrates that this is a weak assumption. Also, in the absence of prices for the nearly 4000 ecoinvent processes, the dispersions of life cycle GWP intensities had to be analyzed relative to physical units rather than monetary values. Although this certainly gives insights into the physical inhomogeneity of the different sectors of our production and consumption systems, it is of limited use for the estimation of EEIO result uncertainties.

Key Findings

The levels of detail with which LCA and EEIO data sets treat the different economic sectors were found to be complementary. We empirically observed that production and consumption systems are best represented by a combination of bottom-up and top-down perspectives, which leads us to argue in favor of a hybrid approach to modeling the background economy in life cycle studies. Even though the LCA data was more specific overall, many sectors of the economy were scarcely represented or even absent from the LCA data set, potentially leading to situations of "aggregation by proxy" and "sectoral background truncation" in process LCAs. This constitutes a warning against using the ecoinvent database as if it were a model of the economy.

From a hybrid perspective, process-based inventories can be seen as focused disaggregations of the overall EEIO description of the economy. Ideally, this disaggregation effort would be allotted to economic sectors proportionally to their life cycle importance. In current practice, however, our results indicate that this is not the case. Practically no correlation was found between the importance of economic sectors within the LCA database and the value added, the emission intensities, or the levels of linkage of these sectors. When international overlaps are excluded, climatic impacts do not correlate to inventory efforts either. This apparent absence of prioritization leads us to suspect a suboptimal allocation of LCA inventory resources, which a more hybrid perspective may be able to rectify in the future.

This research demonstrates a manner in which LCA data, taken as a set of “samples” of the economy, can help analyze EEIO tables. In spite of complications due to the use of physical units, we applied this approach to follow the effect of aggregation on the uncertainty related to life cycle GWP intensities (figure 2.2). The sensitivity to aggregation varied significantly, with special vulnerability for complex sectors. A trend of diminishing benefits of disaggregation was graphically observed. Beyond a certain level of complexity, it thus seems more efficient to turn to a bottom-up LCA approach than to compile ever more specific EEIO tables in a top-down manner.

As the challenges encountered in this study demonstrate, the ad hoc hybridization of individual LCAs is rendered difficult by the necessity to reconcile data sets that are developed independently for different purposes. Hurdles commonly encountered in HLCA include uncertainties related to prices, geography, time, and economic classification. It is expected that the successful merging of LCA and EEIO practices into a harmonized hybrid framework could greatly reduce these obstacles. We argue that the development of life cycle databases should move beyond a strictly process-based approach and fully embrace a hybrid perspective. As a first measure, it should become standard practice to record the prices and economic classifications of processes in the inventory phase of LCA. Then, life cycle databases should progressively allow for the compilation of hybrid inventories. It may also prove beneficial to estimate the missing inputs of existing process-based inventories and complement them with economic inputs in a parameterized manner (Strømman and Solli, 2008). Beyond this, insights from both EEIO and LCA should serve as a foundation for explicit database development strategies, thus directing research efforts toward sectors of the economy that are most critical, underrepresented, or complex. Ultimately, the field should strive for the complete integration of process- and IO-based data in a consistent, detailed, and balanced representation of the economy.

Our results bring quantitative confirmation to a growing but mostly qualitative understanding within industrial ecology: the presence of definite disadvantages in terms of precision, accuracy, and efficiency stemming from the lack of harmonization between LCA and EEIO in mainstream practice. The urgency of environmental problems is such that we cannot afford complacency on this issue; there is no excuse for carrying out research in a manner that does not make the best use of all available data. Furthermore, the development of generic life cycle data sets should be seen as something more than the mere compilation of individual inventories, but rather as an opportunity to model the metabolism of society. As demonstrated by this study, a hybrid approach is essential in this respect. A more vibrant and rigorous development of industrial ecology may be envisioned in the light of a shift of mainstream practice toward HLCAs and a successful merger of the LCA and EEIO frameworks.

Chapter 3

Unified theory of allocations and constructs in life cycle assessment and input–output analysis

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3.1 Introduction

Background

Lifecycle assessment (LCA) and environmentally extended input–output analysis (EEIO) share a common mathematical backbone (Leontief, 1936; Heijungs and Suh, 2002; Suh and Huppes, 2005; Weidema, 2011) and are often confronted with common methodological challenges. One of the most persistent of these is the treatment of coproducts (Finnveden et al., 2009) — situations where a single activity (e.g sugar farming) produces more than one product (e.g. molasses, crystal sugar and electricity). In such situations, models are used in both LCA and EEIO in order to "untangle" the inputs required to produce one coproduct from the inputs required to produce another coproduct. Whereas EEIO has traditionally tackled this problem with system-wide models, LCA practitioners usually resolve multi-output situations in a process-wise manner.

In EEIO, the treatment of coproducts has been investigated in the vast body of literature dedicated to *constructs*, i.e. the elaboration of symmetric system descriptions (represented as product-by-product or industry-by-industry tables) from rectangular, product-by-industry inventory tables. Jansen and Raa (1990b) and Rueda-Cantuche and Raa (2009) provide a review and an axiomatic evaluation of various constructs, notably the commodity-technology construct (CTC), the industry-technology construct (ITC), the byproduct-technology construct (BTC), the lump-sum construct (LSC), and the European-system construct (ESC). The interpretation of negative coefficients resulting from the CTC (Raa and Van der Ploeg, 1989; Almon, 2000) is indissociable from the treatment of byproducts, for which both Raa and Chakraborty (1984) and Londero (1999a) have proposed refinements. Lenzen and Rueda-Cantuche (2012a) demonstrated how various constructs may be calculated using block-arranged supply and use inventory tables, simultaneously yielding product-by-product and industry-by-industry representations. Hybrid constructs, which treat different industries with different modeling assumptions, have also been described (Jansen and Raa, 1990b; European Commission, 2008). For example, Bohlin and Widell (2006) proposed an optimization method, later extended by Smith and McDonald (2011), to guide the hybridization of ITC and CTC.

In LCA, the treatment of coproducts has taken the form of an ongoing debate on *allocation* issues (as reviewed by Guinée (2002) and Reap et al. (2008)). Some characteristics distinguish the LCA debate from the literature on constructs. First, LCA modeling choices are often made on a per-activity basis rather than system-wide. Second, LCA practitioners typically enjoy more freedom in defining their system's boundary and choosing the level of resolution of their study, which sometimes makes it possible to avoid coproduction issues altogether by means of disaggregation or classical system expansion (Guinée, 2002; International Organization for Standardization, 2006). Among the key divides that have framed the research frontier on allocation, we can single out the contrast between substitution modeling and partitioning (e.g. Heijungs and Guinée (2007), Weidema (2000), and Cherubini, Strømman, and Ulgiati

(2011)), and also the divide between economic partitioning and physical partitioning (reviewed by Ardente and Cellura (2012)).

Further important reference documents that define the current research frontier include European Commission (2008) and European Commission (2010). Heijungs (2001),and Suh (2009).

Because of the compatibility and the complementarity of LCA and input–output analysis (IO) (Majeau-Bettez, Strømman, and Hertwich, 2011; Mongelli, Suh, and Huppes, 2005; Norris, 2002), various hybrid EEIO-LCA methods have been devised (Suh et al., 2004): IO-based hybrid (Suh and Huppes, 2005), tiered hybrid (Lenzen, 2009; Strømman, Peters, and Hertwich, 2009; Strømman, 2009), path exchange hybrid (Lenzen and Crawford, 2009), integrated hybrid (Peters and Hertwich, 2006; Suh, 2004b; Suh, 2006), and waste input-output (Nakamura and Kondo, 2002; Nakamura et al., 2008; Nakamura et al., 2011). These hybridization techniques have all been described with, as their starting point, LCA and EEIO descriptions that are already symmetric, and therefore little attention has been paid to the harmonization of allocation and construct practices. The issue of coproduction is thus treated separately, and possibly inconsistently, for the LCA and the EEIO parts.[1]

An increasing number of material flow analyses use LCA or EEIO system descriptions as extensions, but precious few explicitly address allocation issues (e.g. supporting information of Milford et al. (2013)).

LCA and EEIO both have their history in attributional type analysis but are now increasingly being used to answer consequential type questions (Earles and Halog, 2011; Zamagni et al., 2012). Whilst some allocation and construct models seem better aligned with attributional questions, others seem more compatible with consequential analyses (Weidema and Schmidt, 2010; Suh et al., 2010). The debate concerning the treatment of coproducts therefore partly overlaps with the ongoing attributional-consequential divide.

Aim and Structure of the Study

Recently, Kagawa and Suh (2009) and Suh et al. (2010) have bridged the hitherto separate discussions on constructs and allocation. Their efforts to harmonize EEIO and LCA modeling have focused on the comparison of allocation and construct techniques in terms of their underlying assumptions. A formal description of a unified framework for the treatment of coproducts is still lacking, however.

The present article strives to fill this gap. We aim to reach a unified description of all modeling steps and assumptions necessary to go from an initial supply and use inventory (balanced accounting table) to a system description suitable for lifecycle calculations.

Our study furthers Raa and Rueda-Cantuche (2007), who described a generalized equation from which both CTC and ITC models can be derived. Ex-

[1] Hybridizing *unallocated* bottom-up and top-down inventories may bring greater consistency in hybrid analyses (for example Wood, 2011; Suh and Lippiatt, 2012).

tending their work, we propose a unique, generalized allocation equation, from which we derive all popular LCA allocation and EEIO construct models.

The first objective of this article is to provide a more formal description of the link between the different allocation and construct models: exactly which assumptions, properties, modeling choices or special cases mathematically distinguish these models? We therefore aim not only to describe the various models used in LCA and EEIO but to bind them in a common mathematical derivation. Based on this harmonized understanding, we then hope to bring useful insights and recommendations as to the most appropriate use of these modeling techniques.

After clarifying a common terminology, we classify the different types of inventories to which allocation and construct models are applied. We then describe specific situations where allocation is either not applicable or avoidable. For all other cases, we present in a generalized manner the relationship between allocation and construct models. Having clarified the path from allocations to constructs, we proceed to distinguish between two broad families of allocations: production-balanced and non-production-balanced models. Based on the combination of these two strategies, we obtain a single generalized allocation equation, from which we then derive a generalized construct equation. From these generalized representations, most popular practical allocations and constructs are derived by sequentially introducing the assumptions and simplifications inherent to each model. This approach arranges the different models in a "taxonomic tree" of modeling decisions and practical special cases. Based on this framework, we analyze the relation between LCA and EEIO models when applied to different types of inventories. This allows us to make recommendations concerning best inventory practice, separation of observation and modeling, and best use of allocations and constructs.

Throughout this article, mathematical demonstrations are made both in coefficient notation (left side) and in matrix notation (right side). All variables are defined in the last section.

3.2 Common Terminology

As this article strives to bridge LCA and EEIO practice, and as these two research communities have their distinct jargons and core concepts, it is crucial to briefly define some common terms. We also urge our readers to familiarize themselves with the notation of this article, presented in the *Terminology and notation* section.

In this article, the terms *product* and *commodity* are interchangeable and include both goods and services. The entities that produce these commodities are equivalently referred to as *industries* and *activities*.[2] A *coproduct* is any of two or more commodities produced by the same activity (ISO, 1998). The

[2] In other contexts, distinctions between activities and industries may be important, but not for this article; there is no need to distinguish between an activity and a "sub-activity".

coproduct that generates the maximum value for a given activity is considered its *primary product* (Londero, 1999a), and the others are considered *secondary*.

At the core of this article is the division between observation and modeling. We use the terms *inventorying* and *accounting* interchangeably to describe the observation of the inputs and outputs of industries. In this article, the term *modeling* then describes any departure from this initial representation. More specifically, we describe two general modeling approaches: allocations and constructs.

Both LCA and EEIO analyses are based on single-output Leontief production functions (Miller and Blair, 2009), i.e. technological "recipes" describing the production of each commodity in terms of a fixed ratio of inputs (Leontief, 1970; Dorfman, Samuelson, and Solow, 1958). The extraction of such recipes is the object of allocation.

Throughout this article, we use the term *allocation* to refer to any *modeling procedure that ascribes requirements specifically to the production of a commodity in spite of this commodity originating from a multi-output activity.* It should be noted that this definition of allocation is broader than that of the ISO 14044 standard (International Organization for Standardization, 2006) and includes substitution modeling.[3]

Lifecycle calculations require system descriptions that are not only based on single-output recipes, but also self-consistent and symmetric. The elaboration of such representation is precisely the object of *construct* models. By *self-consistent*, we mean that the production of each commodity is individually described by a recipe, and that each recipe is expressed strictly in terms of the commodities produced in the system (along with emissions and factors of production). A system description is *symmetric* if input and output flows are described with the same classification and level of detail (Smith and McDonald, 2011).

Constructs thus model system representations in terms of recipes that can be compiled in a square matrix of technical requirements, such as a commodity-by-commodity technical coefficient matrix ($\mathbf{A}$). Based on such constructed system descriptions, the total lifecycle production ($\mathbf{x}$) associated with an arbitrary final demand ($\mathbf{y}$) may then be calculated with the famous Leontief Inverse as in equation 3.1. [4]

$$\mathbf{x} = \mathbf{L}\mathbf{y} = \left(\hat{\mathbf{E}} - \mathbf{A}\right)^{-1}\mathbf{y} \tag{3.1}$$

[3]Heijungs and Guinée (2007) point to the confusion surrounding the term "allocation", which has been used in the narrow sense as a synonym of "partitioning", and in the broader sense to designate solutions to the multi-output problem.

[4]Lifecycle calculations have also been equivalently expressed in terms of un-normalized system descriptions (Heijungs and Suh, 2002). This very elegant approach skips the elaboration of a requirement matrix (Peters, 2006) and directly calculates a *scaling vector*, with which the different industries and their environmental impacts are re-scaled to match an arbitrary final demand. The explicit definition of a requirement matrix, however, simplifies other calculations such as structural path analysis. It will also simplify our demonstrations.

There is clearly a connection between the definitions of allocation and construct models. This connection, which we will soon clarify, serves as the foundation for this whole study.

3.3 Inventory Structure

We first classify and describe the starting point for allocation and construct models: the inventory.

Prior to the introduction of the SNA-68 (United Nations, 1968; Lenzen and Rueda-Cantuche, 2012a), EEIO accounts directly recorded economic flows in symmetric tables, which could directly be normalized to technical requirement matrices (**A**). Similarly, it is still common practice in LCA to inventory systems directly in terms of normalized, pre-allocated "unit-processes", which collectively provide a symmetric system description. Multi-output activities are problematic for such symmetric inventorying strategies, since it becomes impossible to dissociate the observation (inventory) from the modeling (allocation, etc.). For example, while the inputs of the sugar industry may be observed and recorded without modeling, one cannot directly observe the requirements of "sugar production in the sugar industry", as these are not independent from the requirements of coproducts molasses and electricity.

This shortcoming is avoided by asymmetric accounts that explicitly inventory flows in terms of both commodities and activities. IO inventories are therefore routinely recorded in supply and use tables (SUTs) of dimensions commodity-by-activity. LCA inventories recorded in the ecoSpold2 format, for example, also follow this strategy (Ecoinvent Centre, 2013). The use of commodities by activities is recorded in a Use matrix (**U**), and the production of commodities by activities is recorded in a supply matrix (**V**). For example, the inputs to the sugar industry are recorded as observed in the use table, and the production volume of each coproduct is recorded as observed in the supply table. The modeling of Leontief production functions can then be performed separately from the observation and inventorying phase.

Henceforth, this article always assumes that activities are described as SUT inventories. The vector **h** represents the total inventoried final consumption. The vectors **q** and **g** respectively record the total observed production volume of each commodity and the total output volume of each activity.

In a supply table, it is always clear which activity produced which commodity (e.g. the matrix element v_{kJ} records the amount of k produced *by* activity J). In other words, the supply is always *traceable* to its source. However, this is not necessarily the case for the use table. We therefore distinguish between different types of SUT.

In a two-dimensional product-by-activity Use table ($\mathbf{U}_{\bullet *}$), it is not recorded where a product comes from; an average, *untraceable* product is used. The matrix element u_{iJ} only records the use of i by J and does not record where J sourced its input of i. The origin of the product can be recorded in an additional dimension, giving a traceable-Use table ($\mathbf{U}_{*\bullet *}$). For example, the use of electricity *from* the sugar-cane industry *by* industry J may be recorded in a three-dimensional traceable-Use table (with the coefficient $u_{SugarIndustry,\ electricity,\ J}$). We therefore distinguish between supply and *untraceable* use table (SuUT) and supply and *traceable* use table (StUT), as illustrated in figure 3.1 (top left and right).

Traceable inventories are more common in LCA studies (see "one brand axiom" in Heijungs and Suh (2002)), whereas EEIO is mostly based on untraceable inventories. This distinction between StUT and SuUT inventories will prove important for the harmonization of LCA and EEIO models.

3.4 From SUT to Single-Output Recipes

Simplest Case: a Single-Output Activity

In the case where an activity has only one output, it is trivial to obtain a Leontief production function from its supply and use description. Indeed, the inputs to the production of a sole product and the inputs recorded for its producing industry are one and the same.

For example, if activity J only produces commodity j, the use of i by this activity (u_{iJ}) is equal to the amount of i used for the production of commodity j in this activity (z_{iJj}) (Bohlin and Widell, 2006; Smith and McDonald, 2011). This in turn is equal to the product of the production volume (v_{jJ}) and the normalized technical requirement (a_{iJj}) for this production of j in industry J, i.e. $a_{iJj}v_{jJ}$ (equation 3.2).

In matrix notation, the transformation of inputs into outputs at activity J is represented in a product-by-product flow matrix $\mathbf{Z}_{\bullet J \bullet}$ (as later illustrated in hatched part of figure 3.1).[5] Because industry J is a single-output industry in this simplest case, every column but one in $\mathbf{Z}_{\bullet J \bullet}$ is filled with zeros, and the sole non-null column ($\mathbf{Z}_{\bullet Jj}$) is equal to the use of the activity ($\mathbf{U}_{\bullet J}$).

$$z_{iJj} = a_{iJj}v_{jJ} = u_{iJ} \quad \forall i, j \in \bullet, J \in \dot{*}$$
$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet}\widehat{\mathbf{V}_{\bullet J}} = \mathbf{U}_{\bullet J}\bar{\mathbf{E}}'_{\bullet J} \quad \forall J \in \dot{*} \quad (3.2)$$

In equation 3.2, $\bar{\mathbf{E}}$ is a correspondence matrix identifying the primary product (row) of each industry (column), and $\dot{*}$ is the set of all single-output activities. The outer product between $\mathbf{U}_{\bullet J}$ and $\bar{\mathbf{E}}'_{\bullet J}$ therefore assigns the inputs of industry J to the column describing the production of the sole product of industry J.

Of course, many commodities are produced in multi-output activities, and obtaining Leontief production functions for the lifecycle description of these commodities is more complex.

[5] The matrix $\mathbf{Z}_{\bullet J \bullet}$ is a 2-dimensional slice — representing product flows at only one industry, i.e. industry J — from the 3-dimensional, products-by-industries-by-products array $\mathbf{Z}_{\bullet * \bullet}$. Similarly, $\mathbf{V}_{\bullet J}$, $\mathbf{U}_{\bullet J}$, and $\bar{\mathbf{E}}_{\bullet J}$ are column vectors formed from the Jth columns of the 2-dimensional, products-by-industries matrices $\mathbf{V}$, $\mathbf{U}$, and $\bar{\mathbf{E}}$.

Avoiding Modeling

Supply and Use inventories allow for the description of multi-output activities. Such coproducing activities are usually problematic for lifecycle calculations and are typically handled with some form of modeling, i.e. allocation and constructs. In some circumstances, however, it may be possible to conduct a lifecycle analysis without introducing new assumptions.

Modeling may sometimes be avoided by *disaggregating* heavily aggregated multi-output activity descriptions. This requires the acquisition of additional data — i.e., opening the proverbial black box — and identifying separate production pathways for each coproduct (International Organization for Standardization, 2006). For example, eggs and milk may be coproducts of the agricultural industry, but disaggregation might reveal that this coproduction is the artificial result of the level of aggregation and that, in fact, eggs and milk are produced in distinct, independent sub-activities.

Alternatively, if it is not necessary to describe any of the coproducts individually, the multi-output inventory may be left untouched. The scope of the analysis is then expanded to assess not a single function but rather the basket of functions supplied by the multi-output activity. The analysis thus describes the lifecycle of the *bundle* of all coproducts in a fixed ratio (Heijungs and Frischknecht, 1998). This manner of expanding the scope of the analysis has been defined as *system expansion* (International Organization for Standardization, 2006). In other words, classical system expansion avoids allocation by performing a multi-functional comparison, thus broadening the scope of the study (Wardenaar et al., 2012; Guinée, 2002).

As disaggregation is not always possible, and as a multifunctional analysis is not always practical, LCA and EEIO practitioners typically require modeling to deal with coproduction, as detailed in the following section.

The Connection between Allocation and Construct

Most LCA and EEIO studies use two general modeling approaches — allocations and constructs — to deal with multi-output activities. Before describing the individual characteristics of the different practical models, let us first examine how allocation models and construct models relate at a general level.

We defined allocation as the modeling of recipes for the production of individual commodities even if they originate from multifunctional activities. A first implication of this definition is that the various allocation techniques model the requirements for the production of commodities based on the requirements of activities. In other words, rather than merely describing the use of products by an activity, we model the use of products in the production of a specific product via this activity. For example, when we perform allocation, we start from the observation that industry J uses a certain amount of commodity i (u_{iJ}) and we model that a certain amount of i is used specifically for the production of commodity j by activity J (z_{iJj}).

The hatched parts and dotted arrows in figure 3.1 illustrate the allocation of the inputs of a single industry (industry J) over all possible outputs. Starting from an untraceable inventory (pale gray, left), the allocation of a single activity leads to a product-by-product representation of the intermediate flows that occur via this activity. In other words, products are transformed into other products at this activity. In dark gray, the hatched part of the figure rather illustrates the allocation of the traceable inputs to activity J over all possible outputs, leading to a 3-dimensional flow matrix at industry J ($\mathbf{Z}_{*\bullet J\bullet}$).

How does this relate to constructs, which we defined as the modeling of a complete and symmetric representation of a production and consumption system? The allocation of a single activity certainly does not lead to a complete description of a system, as the other activities in its value chain are not described. If we perform an allocation in turn on *every* activity of the system (whole blue arrows), the whole production system is represented, but the symmetric and self-consistent character of the representation depends on the traceability of the initial inventory.

Starting from a StUT inventory (with a 3-dimensional use matrix, in dark gray), an allocation of the requirements of each activity over the different outputs leads directly to a 4-dimensional flow matrix with complete traceability. For example, if activity J sources its input i from activity I, the allocation of a share of u_{IiJ} to the output j gives the flow z_{IiJj}. The first two dimension reflect the nature and origin of the inputs, and the other two describe the nature and origin of the outputs. The inputs are thus described as precisely as the outputs, which constitutes a symmetric representation. The 4-dimensional matrix is best visualized by conveniently flattening two dimensions into one (Fig. 3.1, right). This description of the system is therefore both complete and symmetric, and it constitutes a valid construct with full traceability, a *traceable construct*.

On the contrary, starting from a SuUT inventory, the allocation of each activity's requirements over the different outputs does not generate a symmetric system description and does not constitute a valid construct. Rather, it generates a 3-dimensional flow table, with traceable outputs made from untraceable inputs (Fig. 3.1, left). For example, let us have activity J using commodity i in amount u_{iJ}. By any form of allocation, we assign a certain share of u_{iJ} specifically for the production of output j, i.e., a flow z_{iJj}. It is known where j was produced (activity J), but commodity i comes from "the market" and is not traceable to a specific producer of origin. This constitutes an asymmetric description of the commodities.

To obtain a symmetric flow matrix, the traceability of the outputs is sacrificed by summation across the activity dimension (Fig. 3.1, $\sum *$). For example, the use of i for the production of j by J (z_{iJj}) is summed with the requirements of i for the production of j by the other producers of j (z_{iIj}, z_{iKj}, etc.) to describe the total use of i in the production of j, i.e., z_{ij}. Both the inputs and outputs are now commodities of average character and without traceable spe-

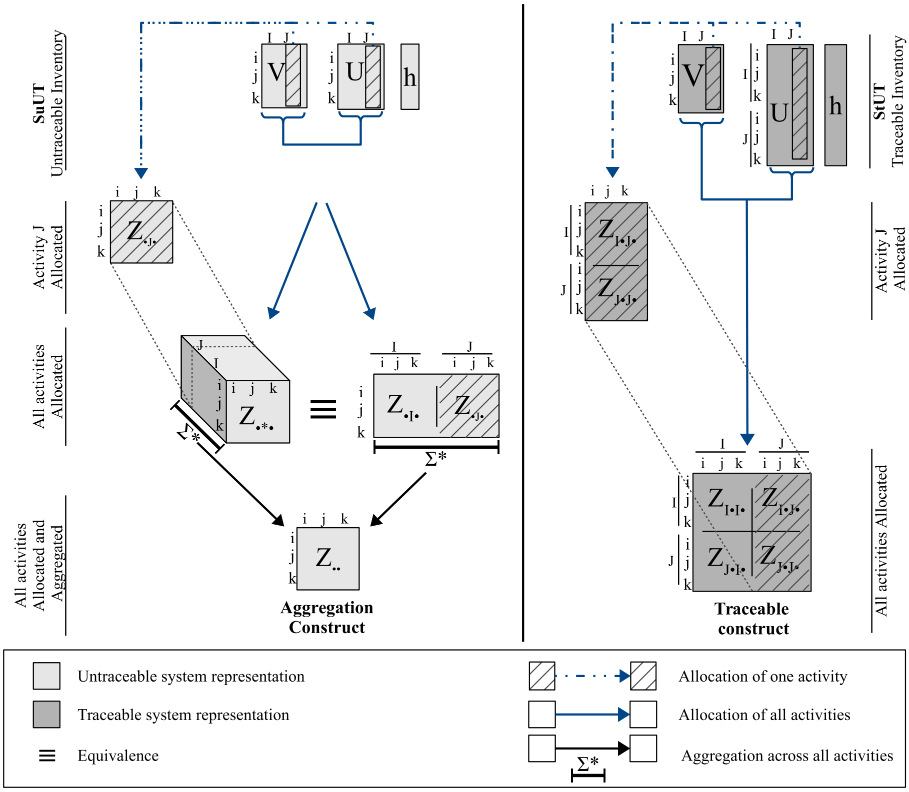

Figure 3.1: The relation between allocation and construct models, starting from untraceable data (SuUT, top left) or traceable data (StUT, top right) with balanced supply ($\mathbf{V}$), intermediate use ($\mathbf{U}$) and final consumption ($\mathbf{h}$). The allocation of a single activity (activity J, hatched) models the transformation of the different inputs into the various outputs (commodities i, j, k) at this activity, as represented by hatched matrices $\mathbf{Z}_{\bullet J \bullet}$ and $\mathbf{Z}_{*\bullet J \bullet}$. The allocation of each activity of a SuUT inventory leads to an asymmetric, 3-dimensional representation ($\mathbf{Z}_{\bullet * \bullet}$) that must be aggregated ($\sum *$) in order to obtain a symmetric system description (aggregation construct, $\mathbf{Z}_{\bullet\bullet}$). The allocation of every activity in a StUT leads directly to a symmetric, traceable representation (traceable construct, $\mathbf{Z}_{*\bullet*\bullet}$). SuUT = supply and untraceable use table; StuT = supply and traceable use table.

cific origins. We refer to such models as *aggregation constructs* (equation 3.3).

$$z_{ij} = \sum_{J \in *} z_{iJj} \quad \forall i, j \in \bullet \qquad\qquad \mathbf{Z}_{\bullet\bullet} = \sum_{J \in *} \mathbf{Z}_{\bullet J \bullet} \tag{3.3}$$

Our general treatment of allocation and construct models allows for a first important distinction. When applied to a traceable inventory (3-dimensional), a repeated, system-wide allocation is always equivalent to a construct, yielding a symmetric, traceable, 4-dimensional representation. However, when applied to a SuUT, a repeated allocation leads to an asymmetric system description (3-dimensional) and is therefore not equivalent to our definition of a construct; it is rather a first step that must be followed by an aggregation step in order to obtain a valid (aggregation, 2-dimensional) construct. This logically implies that aggregation constructs (e.g. ITC, CTC, BTC) can be described as the combination of an allocation model and an aggregation model, as we will do at some later point in this article.

Industry-by-industry constructs, which do not explicitly represent products (Rueda-Cantuche and Raa, 2009), are beyond the scope of this article as they are too far removed from the problem of LCA allocation.[6]

Having effectively described system-wide constructs in terms of repeated allocations, we now turn to describe two broad categories of allocation.

Two General Allocation Strategies

The previous section put in relation allocation and construct models. This section presents two broad strategies for allocation modeling.

A first general strategy to model individual production recipes is to somehow *artificially split* the joint requirements of an activity over its different coproducts (Figure 3.2, center). This strategy models an individual recipe for each of the different coproducts (e.g. $\mathbf{Z}_{\bullet Jj}$ and $\mathbf{Z}_{\bullet Jk}$). Different allocation techniques perform this splitting differently.

Another broad strategy for modeling individual production recipes is to alter the supply flows so as to *artificially remove* all but one coproduct, thus recasting the multi-output activity as a single-output activity. In the example of Figure 3.2 (right), artificially abolishing the supply of k necessarily leads to the description of the individual production of the remaining product j, i.e. $\mathbf{Z}_{\bullet Jj}$. The inputs may or may not be rescaled to account for the alteration in the supply. Various practical allocation models apply this strategy in different ways.

[6] We argue that LCA practice is equivalent to a product-by-product representation, rather than an industry-by-industry representation, because LCA unit processes are typically defined following a product classification. For example, it would be quite typical to describe the unit process for the production of 1 kilogram of milk, which corresponds to a product classification (product = milk). On the contrary, precious few LCA studies would attempt to describe the production of 1 kilogram of agricultural output, which would correspond to an industry classification (industry = agricultural sector).

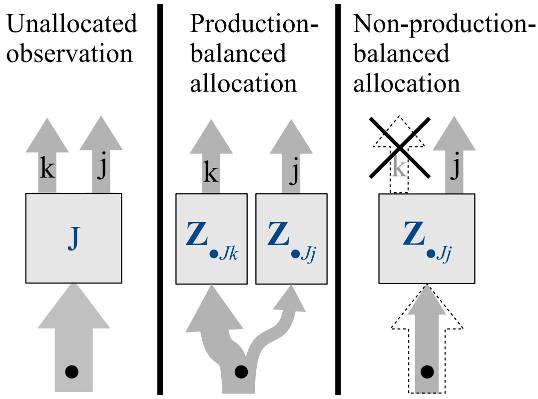

Figure 3.2: Two generalized allocation modeling options: The use of a set of products (•) by industry J in the coproduction of j and k [left] can be artificially split so as to produce independent recipes for each coproduct ($\mathbf{Z}_{\bullet Jk}$ and $\mathbf{Z}_{\bullet Jj}$) [center]. Alternatively [right], all coproducts but one can be artificially removed (dotted arrow for k removed) to isolate a recipe for the remaining output ($\mathbf{Z}_{\bullet Jj}$), with possible adjustments to the magnitude of the remaining flows (e.g. resized input • arrow).

One important distinction between these two modeling techniques pertains to the respect of *production balance*. A model is considered production-balanced if the production level that it calculates if applied to the originally inventoried final demand ($\mathbf{h}$) (i.e. $\mathbf{Lh}$) equals the originally inventoried production level for the different commodities ($\mathbf{q}$) (Jansen and Raa, 1990b). In other words, can the constructed model reproduce the total production and consumption flows from which it was derived, or does it perturb the initial ratio between these flows?

<u>System-wide Production balance:</u>

$$\mathbf{q} = \mathbf{Lh} = \left(\hat{\mathbf{E}} - \mathbf{A}\right)^{-1} \mathbf{h} \tag{3.4}$$

$$\mathbf{y} = \mathbf{h} \rightarrow \mathbf{x} = \mathbf{q}$$

The first allocation approach merely splits requirements and does not alter their total magnitude. The sum of the allocated flows adds up to the total observed flows, and therefore this modeling approach leads to system representations that respect production-balance. On the contrary, the second allocation method perturbs the original production balance by removing some supply flows and rescaling others. The different practical allocations and constructs that derive from this modeling approach therefore violate equation 3.4 and are not production-balanced.

As we will demonstrate, the various models familiar to LCA and EEIO practitioners — partitioning, substitution, CTC, ITC, BTC, etc. — are mere variations on these two basic modeling approaches. We therefore believe that Figure 3.2 represent two fundamental options in allocation: either requirements are split to generate multiple independent recipes, or coproducts are removed such that there remains only one independent recipe.

3.5 Formal Description of Generalized Allocations and Constructs

Generalized Allocation Equations

Figure 3.2 presents two allocation strategies: either artificially splitting joint requirements over all coproducts, or artificially recasting the multi-output activity as a single-output one. In this section, we wish to present these two approaches in mathematical terms.

At this point, we wish to represent allocation as generally as possible. We therefore stay clear of *how* the splitting or the output removal is done, and therefore we will express our equations simply in terms of use ($\mathbf{U}$), supply ($\mathbf{V}$), intermediate flows ($\mathbf{Z}$) and technical coefficients ($\mathbf{A}$).

For the production-balanced strategy, the splitting of joint requirements will be mathematically described in terms of technical coefficients exogenously assigned to secondary coproducts ($\underline{\tilde{\mathbf{A}}}$). This way of representing a splitting of inputs across coproducts may not seem very intuitive at first, but it is fully consistent with our general description.

Indeed, there is an infinity of ways in which a total amount may be divided between N parts, and such a splitting process has N-1 degrees of freedom. Therefore, if a modeler exogenously decides the manner of the splitting, this means that the splitting can be represented as the process of exogenously fixing the size of N-1 parts, leaving the remainder to the "last" part. In other words, the modeler has complete freedom to assign any value to N-1 parts, and the value assigned to the "last" part is fixed so that the splitting adds up to the total.

Similarly, there exists an infinity of ways in which joint inputs can be split across coproducts. This exogenous decision can be represented as the process of exogenously fixing the recipes of all but one of the coproducts. The modeler has complete freedom to assign any input structure to all coproducts except one, as long as the remaining coproduct is assigned the difference between these inputs and the inventoried total inputs to the joint production.

We need just one more distinction to express figure 3.2 in mathematical terms. We need the capacity to select "all but one one" outputs and the "remaining" output for a given activity. For the sake of simplicity and familiarity, we will refer to these as the set of *secondary products* and the *primary product*, respectively.[7]

[7] This nomenclature might make it seem as though this limits our framework to allocation

Therefore, any splitting of joint requirements may be conveniently represented as exogenously fixing the inputs to all secondary coproducts ($\underline{\tilde{\mathbf{A}}}_{\bullet J \bullet}\tilde{\mathbf{V}}_{\bullet J}$), the remaining (primary) coproduct being assigned the remainder of the activity's inputs ($\mathbf{U}_{\bullet J} - \underline{\tilde{\mathbf{A}}}_{\bullet J \bullet}\tilde{\mathbf{V}}_{\bullet J}$).

Any production-balanced allocation that splits requirements across coproducts is therefore represented in a generalized manner by equation 3.5. Depending on the values assigned to $\underline{\tilde{\mathbf{A}}}$ — i.e. depending the the rationale behind the splitting process — all the different practical, production-balanced allocation techniques may be derived from equation 3.5.

Production-balanced allocation of activity J:

$$z_{iJj} = a_{iJj} v_{jJ} = \begin{cases} u_{iJ} - \sum_{k|(k,J)\in\mathscr{S}} \underline{a}_{iJk} v_{kJ} & \forall\,(j,J) \in \mathscr{P}, i \in \bullet \\ \underline{a}_{iJk} v_{kJ} & \forall\,(k,J) \in \mathscr{S} | k = j, i \in \bullet \end{cases}$$

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet}\widehat{\mathbf{V}_{\bullet J}} = \underbrace{\left(\mathbf{U}_{\bullet J} - \underline{\tilde{\mathbf{A}}}_{\bullet J \bullet}\tilde{\mathbf{V}}_{\bullet J}\right)}_{\text{Requirements of primary product}} \bar{\mathbf{E}}'_{\bullet J} + \underbrace{\underline{\tilde{\mathbf{A}}}_{\bullet J \bullet}\widehat{\tilde{\mathbf{V}}_{\bullet J}}}_{\text{Requirements exogenously assigned to secondary products}} \quad \forall\, J \in * \qquad (3.5)$$

As for the non-production-balanced allocation, the equation representing this modeling approach (equation 3.6) is rather close to the equation for extracting Leontief production functions of single-output activities (equation 3.2). This is hardly surprising, as this modeling strategy artificially recasts multi-output activities as a single-output activities. It does so by introducing a $\underline{\mathbf{\Delta V}}$ term to artificially remove secondary outputs and a $\underline{\mathbf{\Delta U}}$ term to compensate for this perturbation in terms of the required inputs.

Non-production-balanced allocation of activity J:

$$z_{iJj} = a_{iJj}(v_{jJ} - \underline{\delta v}_{jJ}) = \begin{cases} u_{iJ} - \underline{\delta u}_{iJ} & \forall\,(j,J) \in \mathscr{P},\ i \in \bullet \\ a_{iJj} 0 = 0 & \forall\,(j,J) \in \mathscr{S},\ i \in \bullet \end{cases}$$

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet}(\widehat{\mathbf{V}_{\bullet J} - \underline{\mathbf{\Delta V}}_{\bullet J}}) = (\mathbf{U}_{\bullet J} - \underline{\mathbf{\Delta U}}_{\bullet J})\, \bar{\mathbf{E}}'_{\bullet J}\ \forall J \in * \qquad (3.6)$$

Equation 3.6 generally represents any modeling of a Leontief production function based on the alteration of the inventoried use and supply. Depending on the nature of $\underline{\mathbf{\Delta U}}$ and $\underline{\mathbf{\Delta V}}$, this equation can be reduced to different practical, non-production-balanced allocation techniques.

Thus, we find that three exogenous decisions underpin the two broad allocation strategies of figure 3.2: assumed production functions for secondary products ($\underline{\tilde{\mathbf{A}}}$), alterations to the original supply ($\underline{\mathbf{\Delta V}}$), and alterations to the original use ($\underline{\mathbf{\Delta U}}$). We refer to these three variables as the *decision variables*,

of activities with a clearly identifiable primary product, but it is not the case. At this level of generality, it merely means that our description of allocation is expressed in terms of one product selected among its coproducts. For many allocation techniques, this selection can be completely arbitrary.

as they reflect the different "levers" that a modeler can use to extract Leontief production functions. In other words, the distinction between the different allocation models can be fully explained by the choice of values assigned to these three, decisive variables. Whereas the first decision variable determines how requirements are split across coproducts (production-balanced allocations, figure 3.2, center), the last two decision variables determine how the activity is recast as a single-output one (non-production-balanced allocation, figure 3.2, right).

As equations 3.6 and 3.5 collectively describe production-balanced and non-production-balanced allocation strategies, their combination leads to a generalized allocation equation (equation 3.7) that should be reducible to any allocation method, depending on the values assigned to its three decision variables.

Equation 3.7 describes the generation of allocated flows and normalized recipes ($\mathbf{Z}$ and $\mathbf{A}$, respectively) based on inventory data ($\mathbf{U}$ and $\mathbf{V}$) and the three decision variables ($\underline{\tilde{\mathbf{A}}}$, $\underline{\mathbf{\Delta V}}$, $\underline{\mathbf{\Delta U}}$). The first term of the summation of the summation represents the requirement associated with the primary product of J, whereas the second describes the requirements allocated to secondary products, if any are preserved by the model.[8]

Setting variables $\underline{\mathbf{\Delta U}}$ and $\underline{\mathbf{\Delta V}}$ to null matrices simplifies the generalized allocation equation back to the production-balanced equation. Thus, in terms of $\underline{\mathbf{\Delta U}}$ and $\underline{\mathbf{\Delta V}}$, the production balance assumption is simply described by equation 3.8.

Production balance Assumptions:

$$\underline{\delta u}_{iJ} = \underline{\delta v}_{iJ} = 0 \;\; \forall\, i \in \bullet, J \in * \qquad\qquad \underline{\mathbf{\Delta U}} = \underline{\mathbf{\Delta V}} = \mathbf{0} \tag{3.8}$$

In the case of traceable inventories (StUT), some variables simply gain an extra dimension (see equations 3.32 and 3.33).

Generalized Aggregation Construct Equations

Starting from a SuUT, the allocation step must be followed by an aggregation step in order to construct a self-consistent, symmetric description. Therefore, simply adding an aggregation step to the generalized allocation equation yields a generalized aggregation construct. Thus, combining equations 3.7 and 3.3:

The summation in equation 3.3 completely removes activities from the resulting system description and produces a uniformly untraceable description of commodities (Fig. 3.1: left).

Given the connection between allocation and construct identified in figure 3.1 and the generalized nature of equation 3.7, equation 3.9 should be reducible to any aggregation construct depending on the values selected for the three decision variables ($\underline{\tilde{\mathbf{A}}}$, $\underline{\mathbf{\Delta V}}$, and $\underline{\mathbf{\Delta U}}$).

[8] In other words, if $(\tilde{\mathbf{V}} - \underline{\tilde{\mathbf{\Delta V}}}) \neq \mathbf{0}$.

$$
z_{iJj} = a_{iJj}(v_{jJ} - \underline{\delta v}_{jJ}) =
\begin{cases}
u_{iJ} - \underline{\delta u}_{iJ} - \sum\limits_{k|(k,J)\in\mathscr{S}} \underline{a}_{iJk}(v_{kJ} - \underline{\delta v}_{kJ}) & \forall\,(j,J)\in\mathscr{P},\ i\in\bullet \\
\underline{a}_{iJk}(v_{kJ} - \underline{\delta v}_{kJ}) & \forall\,(k,J)\in\mathscr{S}|k=j,\ i\in\bullet
\end{cases}
$$

$$
\mathbf{Z}_{\bullet J\bullet} = \mathbf{A}_{\bullet J\bullet}(\widehat{\mathbf{V}_{\bullet J} - \underline{\mathbf{\Delta V}}_{\bullet J}}) = \underbrace{\Big((\mathbf{U}_{\bullet J} - \underline{\mathbf{\Delta U}}_{\bullet J}) - \underline{\tilde{\mathbf{A}}}_{\bullet J\bullet}(\tilde{\mathbf{V}}_{\bullet J} - \underline{\mathbf{\Delta}\tilde{\mathbf{V}}}_{\bullet J})\Big)}_{\text{Requirements of primary product}} \bar{\mathbf{E}}'_{\bullet J} + \underbrace{\underline{\tilde{\mathbf{A}}}_{\bullet J\bullet}(\widehat{\tilde{\mathbf{V}}_{\bullet J} - \underline{\mathbf{\Delta}\tilde{\mathbf{V}}}_{\bullet J}})}_{\substack{\text{Requirements of}\\ \text{secondary products}\\ \text{(if any)}}} \ \forall J\in * \quad (3.7)
$$

Generalized aggregation construct:

$$z_{ij} = a_{ij} \sum_{J \in *} (v_{jJ} - \underline{\delta v}_{jJ}) = \sum_{J|(j,J) \in \mathscr{P}} \left(u_{iJ} - \underline{\delta u}_{iJ} - \sum_{k|(k,J) \in \mathscr{S}} \underline{a}_{iJk} (v_{kJ} - \underline{\delta v}_{kJ}) \right) + \sum_{K|(j,K) \in \mathscr{S}} \underline{a}_{iKj} (v_{jK} - \underline{\delta v}_{jK}) \;\; \forall \, i, j \in \bullet$$

$$\mathbf{Z}_{\bullet\bullet} = \mathbf{A}_{\bullet\bullet} (\widehat{\mathbf{Ve} - \underline{\boldsymbol{\Delta}\mathbf{V}}\mathbf{e}}) = \sum_{J \in *} \left(\underbrace{\left((\mathbf{U}_{\bullet J} - \underline{\boldsymbol{\Delta}\mathbf{U}}_{\bullet J}) - \underline{\tilde{\mathbf{A}}}_{\bullet J \bullet} (\tilde{\mathbf{V}}_{\bullet J} - \underline{\boldsymbol{\Delta}\tilde{\mathbf{V}}}_{\bullet J}) \right)}_{\text{Requirements of primary production}} \bar{\mathbf{E}}'_{\bullet J} + \underbrace{\underline{\tilde{\mathbf{A}}}_{\bullet J \bullet} (\widehat{\tilde{\mathbf{V}}_{\bullet J} - \underline{\boldsymbol{\Delta}\tilde{\mathbf{V}}}_{\bullet J}})}_{\substack{\text{Requirements of} \\ \text{secondary production}}} \right) \quad (3.9)$$

If decision variables $\underline{\mathbf{\Delta V}}$ and $\underline{\mathbf{\Delta U}}$ are null (equation 3.8), the inventoried use and supply are unaltered and the aggregation construct is production-balanced.

Generalized production-balanced aggregation construct:

$$z_{ij} = \sum_{J|(j,J)\in\mathscr{P}} \left(u_{iJ} - \sum_{k|(k,J)\in\mathscr{S}} \underline{a}_{iJk} v_{kJ} \right) + \sum_{K|(j,K)\in\mathscr{S}} \underline{a}_{iKj} v_{jK} \;\; \forall\, i, j \in \bullet$$

$$\mathbf{Z}_{\bullet\bullet} = \sum_{J\in *} \left((\mathbf{U}_{\bullet J} - \underline{\tilde{\mathbf{A}}}_{\bullet J \bullet} \tilde{\mathbf{V}}_{\bullet J}) \bar{\mathbf{E}}'_{\bullet J} + \underline{\tilde{\mathbf{A}}}_{\bullet J \bullet} \widehat{\tilde{\mathbf{V}}_{\bullet J}} \right) \quad (3.10)$$

Except for minor differences in notation, equation 3.10 is equivalent to the generalized construct put forth by Raa and Rueda-Cantuche (2007). As they demonstrate, both the ITC and the CTC may be derived from this general equation (Fig. 3.3: RRC), depending on the simplifying economic assumption applied to replace the three-dimensional $\underline{a}_{iJk}$ and $\underline{a}_{iKj}$ coefficients.

3.6 A Taxonomic Tree of Models

We have so far presented allocations and constructs in a completely generic manner. Let us now sequentially introduce simplifying assumptions to derive, from our generalized representations, the different allocations and constructs familiar to practitioners: partitioning allocation, substitution allocation, CTC, ITC, BTC, etc.

Figure 3.3 summarizes our efforts to formally link the different allocation and construct models in a consistent framework. It highlights the assumptions and modeling choices that distinguish or relate the different models.

At the top of the figure, we start with either a SuUT (left) or a StUT (right) inventory. The boxes in black represent the generalized equations that we have already covered (eqs. 3.5, 3.6, 3.7, 3.9, 3.10). The extreme left and right of the figure show conceptually what steps a SuUT or a StUT inventory undergoes with an aggregation or a traceable construct, respectively. The center of the figure, between the vertical dashed lines, presents the derivation of the different practical allocations and constructs. The simplifying assumptions introduced in the derivation of each model are presented as numbered, italic text along the arrows. The derivation of traceable constructs is presented in dark gray and stops midway through the figure, whereas the derivation of aggregation constructs is in pale gray and extends to the bottom of the figure. Four constructs used in EEIO are shown to be special cases of more broadly defined aggregation constructs (geometric symbols, in blue).

There is a general perception that LCA practitioners are restricted to a choice between partitioning and "system expansion". On the contrary, we identified four mathematically distinct allocation models, two of which resolve the multifunctionality problem based on the existence of alternative or competing producers (figure 3.3: dashed box). To distinguish these two allocation techniques —as they have both been designated simply as "system expansion"

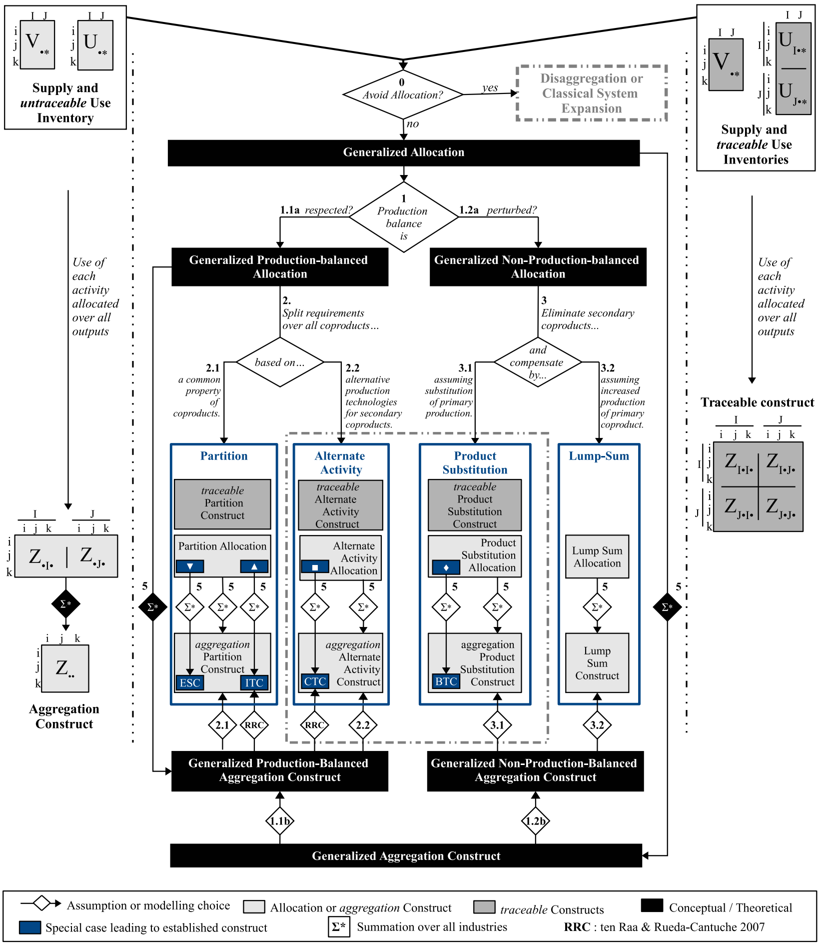

Figure 3.3: The coproduction taxonomic tree: Derivation of practical allocation techniques and aggregation constructs (pale gray), along with traceable constructs (dark gray), from generalized equations (black) by sequential introduction of simplifying assumptions (numbered, italic text), with pure economic constructs as special cases of more broadly defined constructs (dark blue, geometric symbols). Traceable inventories end as traceable constructs mid-height in the figure, as no further modeling is required, whereas untraceable inventories are aggregated post-allocation in order to give symmetric tables at the bottom of the figure. Abbreviations: European-system construct (ESC), industry-technology construct (ITC), commodity-technology construct (CTC), byproduct-technology construct (BTC). Special cases: binary partitioning (▽), equal intensive partitioning property for all outputs within each industry (△), exactly one primary producer per commodity (□), substitution only possible between identical products and always with 1:1 ratio (◊). Other symbols: summation across all industries ($\sum *$).

in the literature (e.g. Schmidt and Weidema (2007), Weidema and Schmidt (2010), and Cherubini, Strømman, and Ulgiati (2011))— we have taken the liberty to give them specific names: *alternate-activity allocation (AAA)* and *product-substitution allocation (PSA)*. It can already be noted from figure 3.3 that the former is in the production-balanced modeling family, whereas the other follows a non-production-balanced strategy.

In the following sections, we formally present the different connecting branches of the taxonomic tree. Figure 3.3 can be used as a sort of "road map" for the coming section, and we will repeatedly refer to it. We start by deriving all allocations. From these, we then derive all associated constructs, and finally we derive the models used in EEIO as special cases of these more broadly defined constructs.

From Generalized to Practical Allocation Models

We here derive the different allocation methods as applicable to untraceable inventories (SuUT). Their application to traceable inventories adds an extra dimension, and these slight reformulations are presented in the *Traceable Allocations and Constructs* section to not overburden the main text.

Partition Allocation

Partition allocation (PA) is a production-balanced model that artificially splits the requirements of an activity across its different outputs based on a common intensive property of these products, for example, energy density or price (Fig. 3.3:2.1).[9]

Let the product-by-activity matrix $\mathbf{\Psi}$ store the intensive properties used for PA. For example, if the coproducing activity J is partitioned based on energy content, the column $\mathbf{\Psi}_{\bullet J}$ will hold the energy density of its various outputs. Conversely, if J is partitioned based on economic value, $\mathbf{\Psi}_{\bullet J}$ will hold the prices of the various outputs.

The assumptions of PA may be formalized in terms of our three decision variables as follows: First, neither use nor supply are altered (equation 3.8: $\underline{\mathbf{\Delta U}} = \underline{\mathbf{\Delta V}} = \mathbf{0}$). Second, the requirements are split ($\underline{\tilde{\mathbf{A}}}$) such that each coproduct is ascribed requirements [1] proportionally to its share of the total output in terms of a given property and [2] following the same input structure as that of the coproducing industry. These assumptions reduce the generalized allocation equation to a practical PA equation (see intermediate steps in the

[9] intensive properties, such as energy density or price, are independent from the production volume, in contrast to extensive properties like mass, volume, or value.

Derivation of PA section, with $\underline{\tilde{\mathbf{A}}}$ detailed at equation 3.38):

$$z_{iJj} = a_{iJj} v_{jJ} = u_{iJ} \underbrace{\frac{v_{jJ}\psi_{jJ}}{\sum\limits_{k\in\bullet} v_{kJ}\psi_{kJ}}}_{\phi_{Jj}} \quad \forall\, i,j \in \bullet, J \in *$$

$$\mathbf{Z}_{\bullet J\bullet} = \mathbf{A}_{\bullet J\bullet}\widehat{\mathbf{V}_{\bullet J}} = \mathbf{U}_{\bullet J} \underbrace{\left(\widehat{\mathbf{V}'_{\bullet J}\mathbf{\Psi}_{\bullet J}}\right)^{-1} \mathbf{\Psi}'_{\bullet J}\widehat{\mathbf{V}_{\bullet J}}}_{\mathbf{\Phi}_{J\bullet}} \quad \forall\, J \in * \tag{3.11}$$

PA is typically expressed more simply using partitioning coefficients ($\mathbf{\Phi}$), as defined in the underbrace of equation 3.11.

$$z_{iJj} = u_{iJ}\phi_{Jj} \quad \forall\, i,j \in \bullet, J \in * \qquad \mathbf{Z}_{\bullet J\bullet} = \mathbf{U}_{\bullet J}\mathbf{\Phi}_{J\bullet} \quad \forall\, J \in * \tag{3.12}$$

Partitioning allocation is thus a member of the production-balanced modeling family that bases its splitting of requirements on the input structure of the coproducing industry and a property of the coproducts.

Alternate-Activity Allocation

Partitioning Allocation splits requirements proportionately to a property of the coproducts, but this is of course not the only way in which joint requirements can be split. For example, one option is to ascribe to secondary coproducts the inputs that they would have required had they been produced as the primary product of some alternate activity (Fig. 3.3:2.2) and ascribe the remainder of the joint requirements to the primary product.

We refer to this modeling technique as *alternate-activity allocation (AAA)*. A technology is assumed for the secondary productions of a given commodity based on the requirements of an alternative, primary production route for this same commodity. Studies such as Cherubini, Strømman, and Ulgiati (2011) and Weidema and Schmidt (2010) are good examples of such modeling, although they have been referred to as "system expansion".

This allocation model may be contrasted with the *disaggregation* method of avoiding modeling (*Avoiding Modeling* section, above). Whilst disaggregation identifies an independent input structure for secondary products by collecting additional information, AAA *assumes* an independent input structure for secondary products based on an alternate production technology description. AAA could therefore be considered a sort of "proxy-based disaggregation".

AAA also bears similarities to substitution allocation (see next section), as both rely on the existence of other production pathways to resolve a coproduction. AAA differs from substitution, however, by virtue of its respect of production balance; the requirements are still split between the coproducts. The total inputs and outputs of each activity remain identical to that recorded in the inventory (equation 3.8, decision variables $\underline{\mathbf{\Delta U}} = \underline{\mathbf{\Delta V}} = \mathbf{0}$). Thus, both primary and secondary productions remain available for intermediate or final use, i.e. no observed flow is substituted, nothing is "avoided".

With AAA, the practitioner must first explicitly select the alternative primary producer whose technology will be assumed for every secondary production of each commodity. Let us record this choice in an *alternate-activity matrix* $\mathbf{\Gamma}$, with activity-by-commodity dimensions, where γ_{Jj} equals 1 if activity J is the chosen alternate primary producer of commodity j and equals 0 otherwise.[10]

Having selected alternate producers, the requirements of their primary products must be isolated and recorded in a commodity-by-commodity matrix of *alternate technology* coefficients ($\mathbf{A}^{\Gamma}_{\bullet\bullet} = function(\mathbf{\Gamma}, \mathbf{U}, \mathbf{V})$), as detailed in the *Compilation of Alternate Technology Matrix* section. AAA modeling then assumes these recipes for all secondary productions. This may be formalized in terms of our decision variables as $\underline{\tilde{\mathbf{A}}} = \mathbf{A}^{\Gamma}$, which directly simplifies the generalized production-balanced allocation (equation 3.5) to the Alternate-Activity Allocation equation.

$$z_{iJj} = a_{iJj}v_{jJ} = \begin{cases} u_{iJ} - \sum\limits_{k|(k,J)\in\mathscr{S}} a^{\Gamma}_{ik}v_{kJ} & \forall\,(j,J) \in \mathscr{P}, i \in \bullet \\ a^{\Gamma}_{ik}v_{kJ} & \forall\,(k,J) \in \mathscr{S}|k = j, i \in \bullet \end{cases}$$

$$\mathbf{Z}_{\bullet J\bullet} = \left(\mathbf{U}_{\bullet J} - \mathbf{A}^{\Gamma}_{\bullet\bullet}\tilde{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J} + \mathbf{A}^{\Gamma}_{\bullet\bullet}\widehat{\tilde{\mathbf{V}}_{\bullet J}} \;\; \forall\, J \in * \tag{3.13}$$

Equation 3.13 is practical only if $\mathbf{A}^{\Gamma}_{\bullet\bullet}$ can be compiled, which is not guaranteed. In other words, AAA depends on our ability to [1] robustly distinguish between primary and secondary products and [2] describe an alternative production technology for each of these secondary products. If the alternate activities selected are all single-output activities, the compilation of $\mathbf{A}^{\Gamma}$ is straightforward, as the requirements of these alternate activities and the requirements of their primary product are one and the same.

AAA modeling is thus a member of the production-balanced allocation family in which the requirements are split based on assumed technologies for secondary products.

Example of AAA As an example of AAA modeling, let us have it that a grain farm (GRAIN) produces both wheat and coproduct straw, which is sold and burned as biomass. Thus, by alternate-activity allocation:

$$\mathbf{Z}_{\bullet,GRAIN,wheat} = \mathbf{U}_{\bullet,GRAIN} - \mathbf{A}^{\Gamma}_{\bullet,biomass}v_{biomass,GRAIN} \tag{3.14a}$$

$$\mathbf{Z}_{\bullet,GRAIN,biomass} = \mathbf{A}^{\Gamma}_{\bullet,biomass}v_{biomass,GRAIN} \tag{3.14b}$$

[10] For the sake of simplicity, equation 3.51 assumes that the same activity is always selected as the alternate primary producer for all secondary productions of a given commodity, regardless of the activity in which this secondary production occurs. Should different primary productions be selected as alternate technologies for different secondary productions, this would simply add a dimension to the alternate-activity matrix: $\mathbf{\Gamma}_{**\bullet}$, in which $\gamma_{JKj} = 1$ would indicate that activity J is selected as the alternate producer of j for assessing the secondary production of j in industry K.

Let us have multiple industries producing biomass as their primary output. Based on its technological similarity, a switchgrass farm named *GRASS* is chosen as the alternate primary producer of biomass whose technology will be assumed for the secondary coproduction of biomass (straw). Therefore, the alternate technology coefficients used for the allocation may be represented as in equation 3.15.

$$\mathbf{A}^{\Gamma}_{\bullet,biomass} = \mathbf{A}_{\bullet,GRASS,biomass} \tag{3.15}$$

Furthermore, if *GRASS* is a single-output activity, then $\mathbf{A}_{\bullet,GRASS,biomass}$ is known and equal to the normalized inputs to the activity *GRASS*, i.e. $\mathbf{B}_{\bullet,GRASS}$. In other words, if an activity has only one output, the technology of this activity and the technology of its output are one and the same:

$$\mathbf{A}^{\Gamma}_{\bullet,biomass} = \mathbf{A}_{\bullet,GRASS,biomass} = \mathbf{B}_{\bullet,GRASS} = \mathbf{U}_{\bullet,GRASS}\hat{\mathbf{g}}^{-1}_{GRASS} \tag{3.16}$$

Which finally allows for the Alternate-Activity Allocation of multi-output activity *GRAIN*.

$$\mathbf{Z}_{\bullet,GRAIN,wheat} = \mathbf{U}_{\bullet,GRAIN} - \mathbf{B}_{\bullet,GRASS}v_{biomass,GRAIN} \tag{3.17a}$$
$$\mathbf{Z}_{\bullet,GRAIN,biomass} = \mathbf{B}_{\bullet,GRASS}v_{biomass,GRAIN} \tag{3.17b}$$

However, if *GRASS* is also a multi-output activity (supplying, for example, grazing for cattle, game cover services, agrotourism, etc.), then $A_{\bullet,GRASS,biomass}$ must first be resolved by further “upstream” allocation before it can be used in the allocation of *GRAIN*. This process can be automated even for large SUT inventories, as described by equation 3.53.

Product-Substitution Allocation

Instead of splitting requirements across coproducts, substitution allocation isolates a standalone recipe for a primary product by recasting its multi-output producer as a single-output activity, effectively *deleting* its secondary coproducts ($\underline{\mathbf{\Delta V}} = \tilde{\mathbf{V}}$) (fig. 3.2, right, equation 3.43).

In the LCA community, this is usually understood with a *substitution logic*: the activity’s secondary coproducts have been taken to substitute primary production outside the original system boundary of the inventory. As these secondary products substitute production outside of the study’s system boundary, they do not add to the net supply within the system of interest, hence their removal from the system description.

The activity is credited for the removal of its secondary products and for preventing production in other activities by recasting the displaced commodities as negative inputs. A choice must therefore be made as to which commodity is displaced by secondary production and in what proportion. This choice is recorded in the product-by-product substitution coefficient matrix $\mathbf{\Xi}$; in which $\xi_{ij} = 0.9$ would indicate that each unit of j from secondary production displaces 0.9 units of i from primary production. Thus, decision variable $\underline{\mathbf{\Delta U}}$

accounts for this credit ($\underline{\boldsymbol{\Delta}\mathbf{U}} = \boldsymbol{\Xi}\tilde{\mathbf{V}}$).[11] These assumptions for decision variables $\underline{\boldsymbol{\Delta}\mathbf{V}}$ and $\underline{\boldsymbol{\Delta}\mathbf{U}}$ directly reduce the generalized non-production-balanced equation (equation 3.6) to a practical substitution allocation model (Figure 3.3:3.1; intermediate steps in the *Derivation of PSA* section):

$$z_{iJj} = \begin{cases} a_{iJj} v_{jJ} = u_{iJ} - \sum_{k|(k,J)\in\mathscr{S}} \xi_{ik} v_{kJ} & \forall\,(j,J)\in\mathscr{P}, i\in\bullet \\ 0 & \forall (k,J)\in\mathscr{S}|k=j, i\in\bullet \end{cases}$$
$$\mathbf{Z}_{\bullet J\bullet} = \mathbf{A}_{\bullet J\bullet}\widehat{\bar{\mathbf{V}}_{\bullet J}} = \left(\mathbf{U}_{\bullet J} - \boldsymbol{\Xi}\tilde{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J}\ \ \forall\, J\in * \quad (3.18)$$

For example, if the secondary production of straw by a grain farming activity displaces switchgrass in the biomass market, then PSA would recast this activity as supplying only grain (not straw) but also requiring negative inputs of switchgrass. Conversely, if it is judged that secondary straw production does not displace switchgrass but rather firewood, then the grain farm would require negative inputs of firewood instead of negative inputs of switchgrass.

The study by Schmidt and Weidema (2007) exemplifies well our definition of product-substitution allocation, though it has been described as “system expansion”. Contrary to AAA analyses, it explicitly describes secondary coproducts as monopolized by the displacement of primary productions, which in turn are clearly removed from the market.

If PSA is applied to a SuUT inventory (as in equation 3.18), no specific activity is avoided since the displaced commodities are not traceable to their source; rather, a weighted average of the different primary producers is displaced for each secondary coproduct. Thus, contrary to AAA, PSA does not model the secondary production of straw based on a specific provider of switchgrass if the inventory is recorded as SuUT. A traceable StUT allows for PSA modeling in which products traceable to specific suppliers are substituted (see the *Traceable Allocations and Constructs* section).

PSA is thus a member of the non-production-balanced allocation family, in which secondary products are removed from the system description (and the production mix) based on their capacity to substitute other products.

Lump-Sum allocation

Instead of completely removing secondary coproducts from $\mathbf{V}$ as in substitution allocation (equation 3.43), some models artificially *convert* these coproducts into the primary product by lumping them all together. A field producing 5 tonnes of grain and 2 tonnes of straw, for example, would be modeled as

[11] One could think of other ways to reduce an activity’s requirements to compensate for the removal of its secondary products and give credit for substituting primary production (equation 3.44). For example, similarly to AAA, the technical requirements of an avoided activity could be subtracted ($\underline{\boldsymbol{\Delta}\mathbf{U}}_{\bullet J} = \mathbf{A}^{\Gamma}_{\bullet\bullet}\tilde{\mathbf{V}}_{\bullet J}$). Such an “activity substitution” does not seem to have been applied in LCA or EEIO, however.

producing 7 tonnes of grain as its single output. Differences between a primary product and its secondary product are assumed to be negligible.

As the lumping process adds all the outputs together (see $\underline{\mathbf{\Delta V}}$ of LSA defined in equation 3.46), it is a requirement of this model that all the coproducts of a multi-output industry be measured in terms of a common unit. Though the output mix of each activity is altered, the total production volume of each activity is unchanged. As LSA assumes that coproducts are indistinguishable, the Use Table is unaffected by the change in production mix and requires no adjustment ($\underline{\mathbf{\Delta U}} = \mathbf{0}$).

These simplifying assumptions reduce the non-production-balanced allocation equation (equation 3.6) to the Lump-Sum Allocation (LSA) (Fig. 3.3:3.2; intermediate steps in the *Derivation of LSA* section).

$$z_{iJj} = \begin{cases} a_{iJj} g_J = u_{iJ} & \forall\ (j, J) \in \mathscr{P}, i \in \bullet \\ 0 & \forall\ (j, J) \in \mathscr{S}, i \in \bullet \end{cases}$$

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet} \big(\widehat{\bar{\mathbf{E}}_{\bullet J} g_J}\big) = \mathbf{U}_{\bullet J} (\bar{\mathbf{E}}_{\bullet J})' \ \forall\ J \in * \quad (3.19)$$

LSA modeling is thus a member of the non-production-balanced allocation family, in which secondary products are removed by assuming that they are identical to the primary product.

From Allocation to Aggregation and Traceable Construct Models

As presented in figure 3.1, applying any allocation model to each activity of a StUT inventory automatically results in a traceable, symmetric system description. Thus, applying equations 3.34, 3.35, or 3.37 to each activity of a system directly yields partition, alternate-activity, or substitution *traceable* constructs, respectively (Fig 3.3, dark gray).

Alternatively, an untraceable, symmetric system description can be obtained by first allocation each activity in a SuUT inventory and then summing across the industry-dimension of the resulting 3-dimensional matrix (figure 3.3:5, pale gray). «««< HEAD Thus, equations 3.11, 3.13, 3.18, or 3.19 are substeps of partition, alternate-activity, substitution, or lump-sum *aggregation* constructs, respectively (equation 3.20-3.23) (derivation in supporting information (SI) on the Journal website).
aggregation partition construct (PC):

$$z_{ij} = \sum_{J \in *} u_{iJ} \phi_{Jj} = \sum_{J \in *} \frac{u_{iJ} v_{jJ} \psi_{jJ}}{\sum\limits_{k \in \bullet} v_{kJ} \psi_{kJ}} \ \ \forall\ i, j \in \bullet$$

$$\mathbf{Z} = \mathbf{U\Phi} = \mathbf{U} \underbrace{\left(\widehat{\mathbf{V}'\mathbf{\Psi}}\right)^{-1} \mathbf{\Psi}' \circ \mathbf{V}'}_{\mathbf{\Phi}} \quad (3.20)$$

aggregation alternate-activity construct (AAC):

$$z_{ij} = \sum_{J|(j,J)\in\mathscr{P}} \left(u_{iJ} - \sum_{k|(k,J)\in\mathscr{S}} a^{\Gamma}_{ik} v_{kJ} \right) + \sum_{K|(j,K)\in\mathscr{S}} a^{\Gamma}_{ij} v_{jK} \;\; \forall\, i,j \in \bullet$$

$$\mathbf{Z}_{\bullet\bullet} = \left(\mathbf{U} - \mathbf{A}^{\Gamma}_{\bullet\bullet}\tilde{\mathbf{V}}\right)\bar{\mathbf{E}}'_{\bullet *} + \mathbf{A}^{\Gamma}_{\bullet\bullet}\widehat{(\tilde{\mathbf{V}}\mathbf{e})} \quad (3.21)$$

aggregation product-substitution construct (PSC):

$$z_{ij} = a_{ij} \sum_{J|(j,J)\in\mathscr{P}} v_{jJ} = \sum_{J|(j,J)\in\mathscr{P}} \left(u_{iJ} - \sum_{k|(k,J)\in\mathscr{S}} \xi_{ik} v_{kJ} \right) \;\; \forall\, i,j \in \bullet$$

$$\mathbf{Z}_{\bullet\bullet} = \mathbf{A}_{\bullet\bullet}\widehat{\bar{\mathbf{V}}\mathbf{e}_{*}} = \left(\mathbf{U} - \boldsymbol{\Xi}\tilde{\mathbf{V}}\right)\bar{\mathbf{E}}'_{\bullet *} \quad (3.22)$$

aggregation lump-sum construct (LSC):

$$z_{ij} = a_{ij} \sum_{J|(j,J)\in\mathscr{P}} g_J = \sum_{J|(j,J)\in\mathscr{P}} u_{iJ} \;\; \forall\, i,j \in \bullet$$

$$\mathbf{Z}_{\bullet\bullet} = \mathbf{A}_{\bullet\bullet}\left(\widehat{(\bar{\mathbf{E}}\hat{\mathbf{g}})\mathbf{e}}\right) = \mathbf{U}\bar{\mathbf{E}}' \quad (3.23)$$

Special Cases of Aggregation Constructs

The previous section presented a traceable and an aggregation construct for each allocation model. These constructs are as broadly defined as their underlying allocation; all partitioning properties, all substitution relations, all choices of alternate activity are covered. As we will demonstrate in the next section, the typical constructs employed in EEIO are more strictly defined, and therefore constitute special cases of aggregation constructs.

Industry Technology as Special Case of the Aggregation Partition Construct

The aggregation partition construct (equation 3.20) may be further simplified in the special cases where the intensive property used for partitioning each activity is equal for all its outputs (Fig. 3.3: ▲). Such a situation would arise, for example, with the volume-based partitioning of an activity whose products all have the same density. A more typical example is the partitioning with respect to economic value of an inventory recorded in monetary terms.[12] In such cases, all the rows of matrix $\boldsymbol{\Psi}_{\bullet *}$ are identical, and $\boldsymbol{\Psi}$ is reduced to a repetition of the row vector $\boldsymbol{\psi}_{*}$ (equation 3.24).

[12] The intensive property that guides partitioning is price — i.e. value per unit amount. If the inventory is recorded in terms of monetary value, however, prices are expressed in terms of dollars (value) per dollar's worth of product (amount). In such a case, prices always equal 1. All entries in a column of $\boldsymbol{\Psi}_{\bullet *}$ are therefore identical to each other.

Special Condition: Identical intensive partition property within each activity

$$\psi_{jJ} = \psi_J \;\; \forall\, j \in \bullet, J \in * \qquad\qquad \boldsymbol{\Psi}_{\bullet *} = \mathbf{e}_{\bullet}\boldsymbol{\psi}_{*} \tag{3.24}$$

Substituting this special condition in equation 3.20 simplifies the aggregation Partition Construct to the industry-technology construct (intermediate steps in the *Derivation of ITC* section):

$$a_{ij} = \sum_{J \in *} \frac{u_{iJ}}{g_J}\frac{v_{jJ}}{q_j} \;\; \forall\, i, j \in \bullet \qquad\qquad \mathbf{A} = \mathbf{U}\hat{\mathbf{g}}^{-1}\mathbf{V}'\hat{\mathbf{q}}^{-1} \equiv \mathbf{A}_{IT} \tag{3.25}$$

The ITC is thus a special case of the more broadly defined aggregation Partition Construct, which is, in turn, based on partition allocation and an aggregation step.

European System Construct as Special Case of the Aggregation Partition Construct

Partitioning may be performed based on the property of being a primary product or not. Such partitioning allocates all requirements to the primary product, rendering the secondary products virtually "free" (Fig. 3.3: ▼). This special case of partitioning has been described as the *surplus method* (Heijungs and Suh, 2002).

Special condition : binary allocation

$$\psi_{jJ} = \begin{cases} 1 & \forall\, (j, J) \in \mathscr{P} \\ 0 & \forall\, (j, J) \in \mathscr{S} \end{cases} \qquad\qquad \boldsymbol{\Psi} = \bar{\mathbf{E}}_{\bullet *} \tag{3.26}$$

Such binary partitioning reduces the aggregation Partitioning Construct to the European-system construct (demonstration in SI, on the web):

$$z_{ij} = a_{ij}q_j = \sum_{J|(j,J) \in \mathscr{P}} u_{iJ} \;\; \forall\, i, j \in \bullet \qquad\qquad \mathbf{Z} = \mathbf{A}\widehat{\mathbf{V}\mathbf{e}} = \mathbf{U}\bar{\mathbf{E}}'_{\bullet *} \tag{3.27}$$

If each commodity is the primary output of exactly one producer (equation 3.28), the European System Construct of equation 3.27 simplifies to the form reviewed by Jansen and Raa (1990b).[13]

The European-system construct is therefore also a special case of the aggregation Partition Construct.

[13]If each commodity is the primary output of exactly one activity, then $\bar{\mathbf{E}}'_{\bullet *}$ simplifies to the identity matrix $\hat{\mathbf{E}}$, which allows for the simplification of equation 3.27 to $\mathbf{A} = \mathbf{U}\widehat{\mathbf{V}\mathbf{e}}^{-1}$. In the case of this construct, however, it makes no difference whether the system is aggregated to a square SUT before the construct is performed or "during" the construct by equation 3.27.

Commodity Technology as Special Case of the Aggregation Alternate-Activity Construct

Through aggregation or disaggregation, a SuUT inventory can usually be rearranged such that each commodity is the primary output of exactly one activity, leading to a square supply table with a fully populated diagonal. In such a case, there exists only one primary production technology for each commodity. This, in turn, reduces the alternate technology matrix to the identity matrix ($\mathbf{\Gamma} = \hat{\mathbf{E}}$). In other words, if there is only one primary producer for a commodity, then the technology of this producer must be the one assumed for all secondary productions of this commodity under alternate-activity construct (AAC) modeling.

Special condition for CTC: Square system of primary production

$$\gamma_{Jj} = \begin{cases} 1 & \forall\ j \in \bullet, J \in *|j = J \\ 0 & \forall\ j \in \bullet, J \in *|j \neq J \end{cases} \qquad \mathbf{\Gamma} = \bar{\mathbf{E}}'_{\bullet *} = \hat{\mathbf{E}} \tag{3.28}$$

In such a case (Fig. 3.3: ■), the aggregation AAC simplifies to the commodity-technology construct (demonstration in section 3.8).

$$\mathbf{A}_{\bullet\bullet} = \mathbf{U}\mathbf{V}^{-1} \tag{3.29}$$

The CTC model is thus a special case of the more broadly defined AAC model, which is in turn based on repeated Alternate-Activity Allocations and an aggregation step.

Byproduct Technology as a Special Case of the Product-Substitution Construct

In the special case where substitution is only possible between identical commodities (e.g. secondary steam production displaces an equal amount of identical steam from primary production), then the substitution matrix is reduced to the identity matrix.

Special condition for byproduct technology construct

$$\xi_{ik} = \begin{cases} 1 & \forall\ i = k \\ 0 & \forall\ i \neq k \end{cases} \quad i, k \in \bullet \qquad \mathbf{\Xi} = \hat{\mathbf{E}}_{\bullet\bullet} \tag{3.30}$$

Which simplifies the product-substitution construct (PSC) aggregation model directly to the BTC:

$$z_{ij} = a_{ij} \sum_{J|(j,J)\in\mathscr{P}} v_{jJ} = \begin{cases} \sum\limits_{J|(j,J)\in\mathscr{P}} (u_{iJ} - v_{iJ}) & \forall\ i \neq j \\ \sum\limits_{J|(j,J)\in\mathscr{P}} u_{iJ} & \forall\ i = j \end{cases} \quad i, j \in \bullet$$

$$\mathbf{Z}_{\bullet\bullet} = \mathbf{A}_{\bullet\bullet}\widehat{\tilde{\mathbf{V}}\mathbf{e}_*} = \left(\mathbf{U} - \hat{\mathbf{E}}\tilde{\mathbf{V}}\right)\bar{\mathbf{E}}'_{\bullet *} = \left(\mathbf{U} - \tilde{\mathbf{V}}\right)\bar{\mathbf{E}}'_{\bullet *} \tag{3.31}$$

A square system of primary production (equation 3.28) reduces this construct to its usual form ($\mathbf{Z}_{\bullet\bullet} = \mathbf{A}_{\bullet\bullet}\hat{\mathbf{V}} = \mathbf{U} - \check{\mathbf{V}}$).[14]

The BTC is thus a special case of a more broadly defined product-substitution construct, which is in turn based on product-substitution allocation and an aggregation step.

3.7 Discussion

Revisiting the Relation Between Models

Starting from a generalized representation, we derived the different practical allocation and construct models applicable SuUT and StUT inventories. This now allows us to clarify the relation between modeling practices in LCA and EEIO.

Each allocation technique underpins two broadly defined constructs: a traceable and an aggregation construct. The traceable construct results directly from the allocation of a traceable inventory —typical of LCA (see "one brand axiom" in Heijungs and Suh (2002))— and requires no further modeling. On the contrary, the allocation of an untraceable inventory —typical of EEIO— requires an an extra modeling step: an aggregation across producing activities to describe average production recipes.

Thus, partition allocation is at the foundation of a traceable and an aggregation partition construct. Both ITC and ESC are special cases of the aggregation partition construct, resulting from different specific partitioning assumptions. ITC is therefore related to partitioning allocation (Suh et al., 2010), but is more narrowly defined and includes an aggregation step.

Similarly, substitution allocation underlies both a traceable and an aggregation product-substitution construct. The traceable PSC describes the displacement of specific primary producers, whereas the aggregation PSC automatically displaces an average primary production mix (Suh et al., 2010). BTC is a special case of the aggregation PSC construct, as it only allows substitution between identical products. BTC is therefore related to substitution allocation, but is more narrowly defined in terms of substitution relations (ideal 1:1 substitution) and displaced producers (average mix).

As for the CTC, it also has an associated allocation technique. This EEIO construct is a special case of a more broadly defined, production-balanced construct, which we named the aggregation Alternate-Activity Construct. This construct is based on Alternate-Activity Allocation, in which the Leontief production functions of secondary products are estimated based on that of alternative primary productions.

CTC and BTC are special cases of different aggregation constructs, which in turn are based on different allocation techniques. In spite of these differences, Suh et al. (2010) elegantly demonstrate that analyses based on CTC and BTC

[14]It makes no difference whether or not the system is aggregated to a square supply before the construct is performed or "during" the construct by equation 3.31.

necessarily calculate identical total lifecycle footprints.[15] This equality between these special cases is not generalizable to other substitution (PSA, PSC) and alternate-activity (AAA, AAC) models.

Alternate-Activity models (AAA, AAC, CTC) all split requirements across coproducts, and are therefore distinct from product-substitution models (PSA, PSC, BTC), in which no such splitting is performed. In fact, as was demonstrated by Cherubini, Strømman, and Ulgiati (2011), it is even possible to calculate "implicit partitioning coefficients" for AAA models.[16]

Alternate-Activity models are also distinct from partition models by virtue of the criteria behind the splitting of the requirements; partition allocation is based on some property of the coproducts, whereas AAA is based on the technical requirements of alternative production routes.

The most popular EEIO constructs —ITC, CTC and BTC— are therefore all derived as special cases of more broadly defined aggregation constructs. These constructs are, in turn, based on three distinct allocation techniques. Two of these allocation models — AAA and PSA— resolve coproduction based on the existence of alternative (competing) activities. In the following section, further analysis of the differences between these two modeling techniques may help clarify the boundary between system expansion and allocation.

Distinction between System Expansion and Modeling

Clear definitions and relations have emerged from our mathematical derivation and taxonomic tree of models. This should prove useful to resolving some of the confusion related to the term "system expansion" (Wardenaar et al., 2012), which has been used in the literature to designate three different things: classical system expansion, alternate-activity allocation, and substitution allocation. We quickly contrast these three concepts.

Classical system expansion avoids any form of modeling by leaving the description of the coproducing activity untouched: the recipe used in the system description is that of the *bundle* of the different coproducts, as observed in the inventory. On the contrary, both AAA and PSA perform some modeling to generate standalone recipes for one or more of the coproducts. Thus, system expansion forces a multifunctional comparison and an explicit modeling of all activities and consumption flows in the expanded system. On the contrary, both AAA and PSA allow for system descriptions with a unique functional output.

PSA also differs from classical system expansion with respect to production balance. Classical system expansion is necessarily production balanced, as all

[15] BTC and CTC necessarily calculate equal *total* impacts but may differ with respect to the breakdown of these impacts across products in the value chain. The two models calculate identical results when lifecycle impacts are split between consumption categories (consumer perspectives), but give different results when splitting lifecycle impacts across production sectors (producer perspective).

[16] The meaningfulness of these "alternate-activity-based" partition coefficients depends on the extent to which the alternate sources of a commodity can be considered as a "property" of this commodity.

the inventoried inputs and outputs are preserved and explicitly described. This is also the case for AAA, but not PSA; substitution necessarily *perturbs* the production balance of the inventory.

AAA differs from system expansion with respect to the strength of the connection between primary and secondary products. As classical system expansion describes the recipe of a bundle of coproducts, it forces a fixed ratio between their production volume (see Heijungs and Frischknecht 1998); for example, it is not possible to demand more electricity from a CHP activity without also demanding more heat. In this respect, PSA is more similar to system expansion, as the ratio between the negative inputs (avoided products) and the main product is fixed. On the contrary, AAA enforces no such ratio; the modeled production function of a commodity is fully independent from the modeled production volume of its coproducts.

Consequently, neither substitution nor alternate-activity models share all the properties of classical system expansion. We recommend use of the term "system expansion" exclusively in cases where allocation is avoided by explicit multi-functional comparisons. Using the same name for three mathematically different approaches is counterproductive.

Gains in Consistency, Flexibility, and Transparency

Our analysis confirms that the modeling phase can be fully dissociated from the inventory phase, and so, just as much in LCA and in EEIO analyses (Suh et al., 2010). Production and consumption systems can be inventoried *as observed* in SUT inventories, sans embedded allocations or assumptions, thus keeping the modeling steps separate, consistent and flexible. The full detail of supply chain descriptions, essential to LCA, can be captured in traceable inventories (StUT).

We found that constructs typically used in EEIO are but special cases of more broadly defined aggregation constructs. This creates an opportunity for more flexible modeling within the IO community; practitioners have more tools at their disposal than simply CTC, BTC and ITC. Furthermore, these broader construct definitions are conceptually closer to modeling practices in LCA, which should improve the consistency of hybrid LCA-EEIO analyses. Our framework should facilitate hybrid analyses in which LCA foregrounds and EEIO backgrounds are constructed with compatible models, based for example on a unique partitioning paradigm or a common substitution matrix.

Contrary to the conventional definitions of CTC and BTC, which require square supply and use tables, the more broadly defined AAC and PSC may be elegantly applied to rectangular SUT. This gain in flexibility may reduce the need for aggregation in the compilation of these inventories.

With the notable exception of BTC (Suh et al., 2010), aggregation constructs typically lead to input structures that are difficult to relate to the original inventory. In this respect, our two-step approach to aggregation constructs offers an opportunity for substantial gains in transparency. Indeed, all aggregation constructs are equally clear and transparent prior to their aggregation step (see demonstration in SI on the web). Regardless of the choice of model, the systematic allocation of the multi-output activities of a system always leads to perfectly clear representations of coproduction structures (e.g. $\mathbf{Z}_{\bullet J \bullet}$), which are then aggregated and obfuscated in the final step of the aggregation construct ($\mathbf{Z}_{\bullet\bullet}$). Different system descriptions may therefore be analyzed pre-aggregation for greater insight.

Conclusion and the Way Forward

The analysis of lifecycle impacts is complicated by the problem of coproduction —where the requirements of a single activity are used to produce more than one product— as well as the problem of traceability —where it is desired to track the use of a commodity to its specific provider rather than use an average mix.

The first objective of this article was to harmonize and improve the description of allocation and construct models used in LCA and EEIO. We have given formal descriptions of the different models and, most importantly, we have bound all these models in a common mathematical derivation. Clear definitions and relations have emerged. The present framework should bring greater transparency and clarity to methodological discussions in LCA and EEIO.

The importance of using this common mathematical framework in LCA and EEIO cannot be overstated. Various forms of hybrid analysis, combining aspects of LCA and EEIO in one assessment, are being increasingly utilized; this can only be done properly if we have consistent inventory structures, and if consistent allocation and construct models are applied to these inventories.

This refined treatment of allocation and construct models should also have important implications both for the interfacing of lifecycle studies with material flow analysis and for the elaboration of consistent attributional and consequential models. We aim to further explore these questions in forthcoming publications.

We found an equivalence between allocation and constructs only when applied to traceable inventories. Such traceable constructs embody maximum information about supply and use of products, and therefore we feel it would be more productive for LCA practitioners, statistical offices, and EEIO analysts to record inventories in a *traceable* Supply and Use framework. Any construct applied to untraceable inventories necessitates a further assumption to that applied in the allocation, that the average (rather than a specific) producer of a product is upstream in the supply chain.

We hope to have clarified some of the confusion surrounding the term *system expansion*, which has been used to designate three different approaches to coproducing activities: "classical" system expansion and two mathematically distinct allocation models. Neither of these two models share all the characteristics of classical system expansion and should be designated under different names.

Finally, we hope to have demonstrated the futility of analyzing the properties of allocations and constructs in dissociation from the properties of the inventories to which they are applied. These properties (traceability, aggregation level, etc.) determine the very relationship between allocations and constructs. We hope that our analysis will guide researchers to first decide on the scope of their analysis; then move on to inventory selection; before finally deciding on what methods of allocation and construct should be applied for their case. The historic method of embedding allocation and construct within an inventory should be forgotten.

3.8 Formal Descriptions and Derivations

Traceable Allocations and Constructs

The section entitled *From Generalized to Practical Allocation Models* describes the allocation of SuUT inventories. Dimensions are simply adjusted as follows for application to traceable inventories (StUT).
PA assumption (equation 3.38) simplifies equation 3.33 to a traceable partition allocation

$$z_{IiJj} = a_{IiJj} v_{jJ} = u_{IiJ} \phi_{Jj} \;\; \forall\, i,j \in \bullet, I, J \in *$$
$$\mathbf{Z}_{I\bullet J\bullet} = \mathbf{A}_{I\bullet J\bullet} \widehat{\mathbf{V}_{\bullet J}} = \mathbf{U}_{I\bullet J} \mathbf{\Phi}_{J\bullet} \;\; \forall\, I, J \in * \quad (3.34)$$

AAA assumption ($\underline{\tilde{\mathbf{A}}} = \mathbf{A}^{\Gamma}$) simplifies equation 3.33 to a traceable alternate-activity allocation

$$z_{IiJj} = \begin{cases} u_{IiJ} - \sum\limits_{k|(k,J)\in\mathscr{S}} a^{\Gamma}_{Iik} v_{kJ} \;\; \forall\, (j,J) \in \mathscr{P}, I \in *, i \in \bullet \\ a^{\Gamma}_{Iik} v_{kJ} \;\; \forall\, (k,J) \in \mathscr{S} | k = j, I \in *, i \in \bullet \end{cases}$$
$$\mathbf{Z}_{I\bullet J\bullet} = \left(\mathbf{U}_{I\bullet J} - \mathbf{A}^{\Gamma}_{I\bullet\bullet} \tilde{\mathbf{V}}_{\bullet J}\right) \bar{\mathbf{E}}'_{\bullet J} + \mathbf{A}^{\Gamma}_{I\bullet\bullet} \widehat{\tilde{\mathbf{V}}_{\bullet J}} \;\; \forall\, I, J \in * \quad (3.35)$$

Traceability has a greater impact on PSA, as it is no longer sufficient to simply displace a commodity; a choice must be made as to the origin of the displaced commodity (first term of equation 3.36). In addition, as PSA does not describe production functions for secondary products, we must redirect to a (competing) primary provider any use of commodity that was traceably sourced from a secondary production in the inventory. As PSA is based on market mechanisms, both choices can be made explicit in a *competing production matrix* $\mathbf{\Theta}$ (second and third terms of equation 3.36). This activity-by-commodity matrix identifies which producer is displaced by a secondary production of a given commodity. Thus, $\theta_{Jj} = 1$ identifies J as the producer of j that is in direct competition with secondary productions of j.

Traceable PSA assumption:

$$\underline{\delta v}_{kJ} = v_{kJ} \;\; \forall\, (k,J) \in \mathscr{S}, J \in * \qquad \underline{\mathbf{\Delta V}}_{\bullet J} = \tilde{\mathbf{V}}_{\bullet J} \;\; \forall\, J \in * \qquad \text{(rep. 3.43)}$$

<u>Generalized allocation of inputs to J traceable to provider I:</u>

$$z_{IiJj} = a_{IiJj}(v_{jJ} - \underline{\delta v}_{jJ}) = \begin{cases} u_{IiJ} - \underline{\delta u}_{IiJ} - \sum_{k|(k,J)\in\mathscr{S}} \underline{a}_{IiJk}(v_{kJ} - \underline{\delta v}_{kJ}) & \forall\,(j,J)\in\mathscr{P} \\ \underline{a}_{IiJk}(v_{kJ} - \underline{\delta v}_{kJ}) & \forall\,(k,J)\in\mathscr{S}|k=j \end{cases} \quad \forall i,j \in \bullet, I,J \in *$$

$$\mathbf{Z}_{I\bullet J\bullet} = \mathbf{A}_{I\bullet J\bullet}(\widehat{\mathbf{V}_{\bullet J} - \underline{\mathbf{\Delta V}}_{\bullet J}}) = \left((\mathbf{U}_{I\bullet J} - \underline{\mathbf{\Delta U}}_{I\bullet J}) - \underline{\tilde{\mathbf{A}}}_{I\bullet J\bullet}(\tilde{\mathbf{V}}_{\bullet J} - \underline{\tilde{\mathbf{\Delta V}}}_{\bullet J})\right)\bar{\mathbf{E}}'_{\bullet J} + \underline{\tilde{\mathbf{A}}}_{I\bullet J\bullet}(\widehat{\tilde{\mathbf{V}}_{\bullet J} - \underline{\tilde{\mathbf{\Delta V}}}_{\bullet J}}) \tag{3.32}$$

<u>Generalized Production-balanced allocation of inputs to J traceable to provider I:</u>

$$z_{IiJj} = a_{IiJj}v_{jJ} = \begin{cases} u_{IiJ} - \sum_{k|(k,J)\in\mathscr{S}} \underline{a}_{IiJk}v_{kJ} & \forall\,(j,J)\in\mathscr{P} \\ \underline{a}_{IiJk}v_{kJ} & \forall\,(k,J)\in\mathscr{S}|k=j \end{cases} \quad \forall I,J \in *, i,j \in \bullet$$

$$\mathbf{Z}_{I\bullet J\bullet} = \mathbf{A}_{I\bullet J\bullet}\widehat{\mathbf{V}_{\bullet J}} = \left(\mathbf{U}_{I\bullet J} - \underline{\tilde{\mathbf{A}}}_{I\bullet J\bullet}\tilde{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J} + \underline{\tilde{\mathbf{A}}}_{I\bullet J\bullet}\widehat{\tilde{\mathbf{V}}_{\bullet J}} \;\; \forall\, I,J \in * \tag{3.33}$$

$$\underline{\delta u}_{IiJ} = \begin{cases} \theta_{Ii} \sum\limits_{k|(k,J)\in\mathscr{S}} \xi_{ik} v_{kJ} - \theta_{Ii} \sum\limits_{K|(i,K)\in\mathscr{S}} u_{KiJ} & \forall\,(i,I)\in\mathscr{P}, J\in * \\ u_{IiJ} & \forall\,(i,I)\in\mathscr{S}, J\in * \end{cases}$$

$$\underline{\mathbf{\Delta U}}_{*\bullet J} = \mathbf{\Theta}\mathbf{\Xi}\widehat{\tilde{\mathbf{V}}_{\bullet J}} + \tilde{\mathbf{U}}_{*\bullet J} - \mathbf{\Theta}\big(\widehat{\mathbf{e}'\tilde{\mathbf{U}}_{*\bullet J}}\big) \quad (3.36)$$

These assumptions reduce equation 3.32 to a traceable PSA.

$$z_{IiJj} = a_{IiJj} v_{jJ} = \begin{cases} u_{IiJ} - \theta_{Ii} \sum\limits_{k|(k,J)\in\mathscr{S}} \xi_{ik} v_{kJ} \\ \qquad + \theta_{Ii} \sum\limits_{K|(i,K)\in\mathscr{S}} u_{KiJ} & \forall\,(i,I),(j,J)\in\mathscr{P}, i\in\bullet \\ 0 \end{cases}$$

$$\mathbf{Z}_{I\bullet J\bullet} = \mathbf{A}_{I\bullet J\bullet}\widehat{\bar{\mathbf{V}}_{\bullet J}} = \Big(\bar{\mathbf{U}}_{I\bullet J} - \mathbf{\Theta}_{I\bullet}\mathbf{\Xi}\widehat{\tilde{\mathbf{V}}_{\bullet J}} + \mathbf{\Theta}_{I\bullet}\big(\widehat{\mathbf{e}'\tilde{\mathbf{U}}_{*\bullet J}}\big)\Big)\,\bar{\mathbf{E}}'_{\bullet J} \quad (3.37)$$

The LSA of a traceable inventory would also require the rerouting of traceable uses of secondary products. Contrary to PSA, however, LSA is not based on any market logic and offers no guidance as to how the rerouting should take place. We therefore did not find Lump-sum modeling to be defined in terms of traceable inventory.

The repeated application of PA, AAA, or PSA to each activity of a StUT inventory yields a symmetric flow matrix and therefore constitutes a valid traceable construct (figure 3.3: dark gray).

Derivations from Generalized Allocation

Derivation of PA

As detailed in the *Generalized Allocation Equations* section, the splitting of requirements across coproducts can be generally represented as exogenously fixing the technological recipe of all coproducts but one ($\underline{\tilde{\mathbf{A}}}$). For partitioning, the requirements artificially assigned to a product are proportional to this product's share of the total output in terms of a chosen partitioning property ($\mathbf{\Psi}_{\bullet J}$). Furthermore, the requirements allocated to each product follow the overall input structure of the joint production, i.e. the ratio between the inputs of i and of j will be the same for all coproducts and for the joint requirements. The technology assumed for "secondary products" can therefore be formalized as the product between [1] a ratio of properties (e.g. $\frac{\psi_{kJ}}{\sum_{j\in\bullet}\psi_{jJ}v_{jJ}}$) and the inputs to the joint production (e.g. u_{iJ}), as in equation 3.38.

<u>Partition Allocation Assumption in terms of decision variable $\underline{\tilde{\mathbf{A}}}$:</u>

$$\underline{a}_{iJk} = u_{iJ}\frac{\psi_{kJ}}{\sum\limits_{j\in\bullet}\psi_{jJ}v_{jJ}} \quad \forall\, k|(k,J)\in\mathscr{S}, i\in\bullet, J\in *$$

$$\underline{\tilde{\mathbf{A}}}_{\bullet J\bullet} = \mathbf{U}_{\bullet J}\big(\widehat{\mathbf{V}'_{\bullet J}\mathbf{\Psi}_{\bullet J}}\big)^{-1}\mathbf{\Psi}'_{\bullet J} \;\; \forall\, J\in * \quad (3.38)$$

Inserting the PA assumption (equation 3.38) in the generalized production-balanced allocation equation (equation 3.7) yields equation 3.39.

$$\begin{aligned}\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet}\widehat{\mathbf{V}_{\bullet J}} &= \left(\mathbf{U}_{\bullet J} - \mathbf{U}_{\bullet J}\left(\widehat{\mathbf{V}'_{\bullet J}\mathbf{\Psi}_{\bullet J}}\right)^{-1}\mathbf{\Psi}'_{\bullet J}\tilde{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J} \\ &+ \mathbf{U}_{\bullet J}\left(\widehat{\mathbf{V}'_{\bullet J}\mathbf{\Psi}_{\bullet J}}\right)^{-1}\mathbf{\Psi}'_{\bullet J}\widehat{\tilde{\mathbf{V}}_{\bullet J}}\end{aligned} \tag{3.39}$$

which may be reorganized

$$\begin{aligned}\mathbf{Z}_{\bullet J \bullet} &= \mathbf{A}_{\bullet J \bullet}\widehat{\mathbf{V}_{\bullet J}} \\ &= \mathbf{U}_{\bullet J}\left(\widehat{\mathbf{V}'_{\bullet J}\mathbf{\Psi}_{\bullet J}}\right)^{-1}\left(\left(\left(\widehat{\mathbf{\Psi}'_{\bullet J}\mathbf{V}_{\bullet J}}\right) - \mathbf{\Psi}'_{\bullet J}\tilde{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J} + \mathbf{\Psi}'_{\bullet J}\widehat{\tilde{\mathbf{V}}_{\bullet J}}\right)\end{aligned} \tag{3.40}$$

The diagonalization is dropped for 1x1 matrix, allowing for further simplification

$$\begin{aligned}\mathbf{Z}_{\bullet J \bullet} &= \mathbf{A}_{\bullet J \bullet}\widehat{\mathbf{V}_{\bullet J}} \\ &= \mathbf{U}_{\bullet J}\left(\widehat{\mathbf{V}'_{\bullet J}\mathbf{\Psi}_{\bullet J}}\right)^{-1}\left(\left(\mathbf{\Psi}'_{\bullet J}\mathbf{V}_{\bullet J} - \mathbf{\Psi}'_{\bullet J}\tilde{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J} + \mathbf{\Psi}'_{\bullet J}\widehat{\tilde{\mathbf{V}}_{\bullet J}}\right)\end{aligned} \tag{3.41}$$

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet}\widehat{\mathbf{V}_{\bullet J}} = \mathbf{U}_{\bullet J}\left(\widehat{\mathbf{V}'_{\bullet J}\mathbf{\Psi}_{\bullet J}}\right)^{-1}\left(\left(\mathbf{\Psi}'_{\bullet J}\bar{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J} + \mathbf{\Psi}'_{\bullet J}\widehat{\tilde{\mathbf{V}}_{\bullet J}}\right) \tag{3.42}$$

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet}\widehat{\mathbf{V}_{\bullet J}} = \mathbf{U}_{\bullet J}\underbrace{\left(\widehat{\mathbf{V}'_{\bullet J}\mathbf{\Psi}_{\bullet J}}\right)^{-1}\mathbf{\Psi}'_{\bullet J}\widehat{\mathbf{V}_{\bullet J}}}_{\mathbf{\Phi}_{J\bullet}} \tag{rep. 3.11}$$

It should be noted that the filter identifying secondary coproducts ($\tilde{\square}$) naturally disappears in the derivation of the partition equation. The choice of the "primary" and "secondary" products for expressing the decision variable $\underline{\tilde{\mathbf{A}}}$ can therefore be completely arbitrary. In other words, and contrary to other models, partition allocation does not require the robust identification of a primary product.

Derivation of PSA

The assumptions of PSA are formalized in terms of decision variables $\underline{\mathbf{\Delta V}}$ and $\underline{\mathbf{\Delta U}}$ in equations 3.43 and 3.44.

Product-Substitution Assumption:

$$\underline{\delta v}_{kJ} = \begin{cases} v_{kJ} & \forall\,(k,J) \in \mathscr{S}, J \in * \\ 0 & \forall\,(k,J) \in \mathscr{P}, J \in * \end{cases} \qquad \underline{\mathbf{\Delta V}}_{\bullet J} = \tilde{\mathbf{V}}_{\bullet J} \;\; \forall\, J \in * \tag{3.43}$$

$$\underline{\delta u}_{iJ} = \sum_{k|(k,J)\in\mathscr{S}} \xi_{ik} v_{kJ} \;\; \forall\, i \in \bullet, J \in * \qquad \underline{\mathbf{\Delta U}}_{\bullet J} = \mathbf{\Xi}\tilde{\mathbf{V}}_{\bullet J} \;\; \forall\, J \in * \tag{3.44}$$

These assumptions first reduce the generalized non-production-balanced allocation equation (3.6) to

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet} \left(\widehat{\mathbf{V}_{\bullet J} - \tilde{\mathbf{V}}_{\bullet J}} \right) = \left(\mathbf{U}_{\bullet J} - \boldsymbol{\Xi} \tilde{\mathbf{V}}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} \quad \forall J \in * \tag{3.45}$$

which simplifies to the PSA equation by virtue of the complementary nature of the set of primary and the set of secondary products

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet} \widehat{\bar{\mathbf{V}}_{\bullet J}} = \left(\mathbf{U}_{\bullet J} - \boldsymbol{\Xi} \tilde{\mathbf{V}}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} \quad \forall J \in * \qquad \text{(rep. 3.18)}$$

Derivation of LSA

The assumptions of lump-sum allocation (LSA) are formalized in terms of decision variables $\underline{\boldsymbol{\Delta}\mathbf{V}}$ and $\underline{\boldsymbol{\Delta}\mathbf{U}}$ in equations 3.46 and 3.47.
Lump-Sum Assumptions:

$$\underline{\delta v}_{jJ} = \begin{cases} - \sum\limits_{k|(k,J) \in \mathscr{S}} v_{kJ} & \forall \, (j, J) \in \mathscr{P} \\ v_{kJ} & \forall (k, J) \in \mathscr{S} | k = j \end{cases}$$

$$\underline{\boldsymbol{\Delta}\mathbf{V}}_{\bullet J} = \tilde{\mathbf{V}}_{\bullet J} - \bar{\mathbf{E}}_{\bullet J} \widehat{\mathbf{e}' \tilde{\mathbf{V}}_{\bullet J}} \;\; \forall \, J \in * \tag{3.46}$$

$$\underline{\delta u}_{iJ} = 0 \;\; \forall \, i \in \bullet, J \in * \qquad\qquad \underline{\boldsymbol{\Delta}\mathbf{U}}_{\bullet J} = \mathbf{0} \;\; \forall \, J \in * \tag{3.47}$$

These assumptions first reduce the generalized non-production-balanced allocation equation (3.6) to

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet} \left(\widehat{\mathbf{V}_{\bullet J} - \tilde{\mathbf{V}}_{\bullet J} + \bar{\mathbf{E}}_{\bullet J} \widehat{\mathbf{e}' \tilde{\mathbf{V}}_{\bullet J}}} \right) = \left(\mathbf{U}_{\bullet J} - \mathbf{0} \right) \bar{\mathbf{E}}'_{\bullet J} \; \forall J \in * \tag{3.48}$$

which simplifies to the LSA equation, by virtue of the complementary nature of the set of primary and the set of secondary products, as follows

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet} \left(\widehat{\bar{\mathbf{V}}_{\bullet J} + \bar{\mathbf{E}}_{\bullet J} \widehat{\mathbf{e}' \tilde{\mathbf{V}}_{\bullet J}}} \right) = \left(\mathbf{U}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} \; \forall J \in * \tag{3.49}$$

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet} \left(\widehat{\bar{\mathbf{E}}_{\bullet J} \widehat{\mathbf{e}' \mathbf{V}_{\bullet J}}} \right) = \left(\mathbf{U}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} \; \forall J \in * \tag{3.49a}$$

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet} \left(\widehat{\bar{\mathbf{E}}_{\bullet J} g_J} \right) = \left(\mathbf{U}_{\bullet J} \right) \bar{\mathbf{E}}'_{\bullet J} \; \forall J \in * \qquad \text{(rep. 3.19)}$$

Compilation of Alternate Technology Matrix

As presented in the *Alternate-Activity Allocation* section, AAA is a production-balanced allocation model that assumes alternate technologies for secondary productions. Given that a matrix of alternate technology coefficients has been compiled ($\mathbf{A}^{\Gamma}$), the assignment of these alternate technologies to secondary products (equation 3.50) directly reduces the generalized production-balanced allocation equation to an AAA model.

$$\underline{\tilde{\mathbf{A}}} = \mathbf{A}^{\Gamma} \tag{3.50}$$

Nothing has been said, however, on he compilation of this $\mathbf{A}^{\Gamma}$ matrix. We now wish to describe this intermediate variable in terms of inventory data ($\mathbf{V}$, $\mathbf{U}$, etc.) and exogenous choices by the practitioners.

With AAA, the practitioner must exogenously select an alternate primary producer that will be used for the description of each secondary product ($\mathbf{\Gamma}$). The compilation of $\mathbf{A}^{\Gamma}$ can therefore be conceptually described as the selection of a given set of technological recipes, amongst all technological recipes of the system ($\mathbf{A}_{\bullet * \bullet}$), to be used as assumptions for secondary products.[17]

$$a^{\Gamma}_{ij} = \sum_{J \in *} a_{iJj}\gamma_{Jj} \ \ \forall \, i, j \in \bullet \qquad \qquad \mathbf{A}^{\Gamma}_{\bullet\bullet} = \sum_{J \in *} \mathbf{A}_{\bullet J \bullet} \widehat{\mathbf{\Gamma}_{J\bullet}} \tag{3.51}$$

Although equation 3.51 is valid, its description is strictly conceptual since, in practice, $\mathbf{A}_{\bullet * \bullet}$ is not known (if it were known we would not need allocation). We therefore need a more practical description.

The calculation of a Alternate Technology matrix is trivial when all the chosen alternate activities are single-output activities ($\mathbf{\Gamma} = \dot{\mathbf{\Gamma}}$). In such a case, the $\mathbf{A}^{\Gamma}$ matrix may be directly calculated by rearranging the normalized use coefficient matrix ($\mathbf{B}$).

$$\mathbf{\Gamma} = \dot{\mathbf{\Gamma}} \quad \rightarrow \quad \mathbf{A}^{\Gamma}_{\bullet\bullet} = \mathbf{B}\mathbf{\Gamma} = \mathbf{U}\hat{\mathbf{g}}^{-1}\mathbf{\Gamma} \tag{3.52}$$

Equation 3.52 takes advantage of the fact that the technology of a single-output activity (e.g. $\mathbf{B}_{\bullet J}$) and the technology for the production of its primary product (e.g. $\mathbf{A}_{\bullet Jj}$) are one and the same.

In the more general case where some alternate activities selected in $\mathbf{\Gamma}$ are multi-output, however, further upstream allocation is necessary. For example, if I produces i and j, and if J is chosen as the alternate technology for the production of j, the technological descriptions $\mathbf{A}_{\bullet Jj}$ will be used to extract $\mathbf{A}_{\bullet Ii}$. If J is in turn a multi-output activity that supplies both j and k, then $\mathbf{A}_{\bullet Jj}$ cannot be known until activity J has been allocated based on activity K... and so on until the allocation process encounters a single-output activity.

In LCA, this procedure has typically been done manually in an *ad hoc* manner. In IO, the various constructs bypassed this step by directly generating aggregated $\mathbf{A}$-matrices, thus making it more difficult to investigate the various

[17] In equation 3.51, the summation term can be applied to normalized coefficients since only one alternate producer is selected per commodity in $\mathbf{\Gamma}$, which entails that no two non-null values are ever summed.

coproduction structures (Suh et al., 2010). Both these approaches are suboptimal. The above calculation procedure may be automated as in equation 3.53.

$$\begin{aligned}\mathbf{A}^{\Gamma}_{\bullet\bullet} &= (\dot{\mathbf{B}} + \ddot{\mathbf{N}}) \sum_{n=0}^{n=\infty} (-1\mathbf{\Gamma M})^n \mathbf{\Gamma} \\ &= (\dot{\mathbf{B}} + \ddot{\mathbf{N}})\mathbf{\Gamma} - (\dot{\mathbf{B}} + \ddot{\mathbf{N}})(\mathbf{\Gamma M})\mathbf{\Gamma} + (\dot{\mathbf{B}} + \ddot{\mathbf{N}})(\mathbf{\Gamma M})^2\mathbf{\Gamma} + \ldots\end{aligned} \tag{3.53}$$

where $\mathbf{N}$ contains the requirements of an activity *per unit of primary product*;

$$\mathbf{N} = \mathbf{U}\widehat{(\mathbf{e}'\bar{\mathbf{V}})}^{-1} \tag{3.54}$$

the matrix $\mathbf{M}$ contains the output of secondary product per unit of primary product;

$$\mathbf{M} = \tilde{\mathbf{V}}\widehat{(\mathbf{e}'\bar{\mathbf{V}})}^{-1} \tag{3.55}$$

and the filter $\ddot{\square}$ indicates that all single-output activities have been filtered out, leaving only multi-output activities.

If all alternate activities selected in the alternate-activity matrix ($\mathbf{\Gamma}$) are single-output, the terms $\ddot{\mathbf{N}}\mathbf{\Gamma}$ and $\mathbf{\Gamma M}$ are null, and equation 3.53 simplifies to equation 3.52.

On the contrary, if an alternate activity selected in $\mathbf{\Gamma}$ is multi-output (e.g. J producing j and k), the technical requirements of its primary output (j) are estimated in the first summation term with $\ddot{\mathbf{N}}\mathbf{\Gamma}$, which ignores the secondary products of this activity and therefore constitutes an overestimation. This overestimation is corrected by the second summation term, where the requirements for producing the secondary products (e.g. k) are subtracted out. However, if some of the industries selected as the alternate producers of those secondary products (e.g. K) are also a multi-output activities, then the initial overestimation is "overcorrected". This "overcorrection" is then corrected in the third summation term, and this goes on until $(\mathbf{\Gamma M})^n$ is null, i.e. until all "allocation paths" reach a single-output activity.

There is no guarantee that $\mathbf{A}^{\Gamma}$ is computable, it is possible that equation 3.53 may not converge. In other words, it may prove impossible to identify a suitable alternate technology for each product of the system. As a reality check, however, it has been successfully applied to the one-region SUT of EXIOPOL (Tukker et al., 2013).

Derivation of ITC

Special Condition: Identical intensive partition property within each activity

$$\psi_{jJ} = \psi_J \ \forall\, j \in \bullet, J \in * \qquad\qquad \mathbf{\Psi}_{\bullet *} = \mathbf{e}_{\bullet}\boldsymbol{\psi}_{*} \tag{rep. 3.24}$$

This assumption modifies the partition aggregation construct (equation 3.20, reproduced below)

$$z_{ij} = \sum_{J\in *} \frac{u_{iJ} v_{jJ} \psi_{jJ}}{\sum\limits_{k\in\bullet} v_{kJ}\psi_{kJ}} \;\forall\, i,j \in \bullet \qquad \mathbf{Z} = \mathbf{U}\left(\widehat{\mathbf{V}'\boldsymbol{\Psi}}\right)^{-1} \boldsymbol{\Psi}' \circ \mathbf{V}' \qquad \text{(rep. 3.20)}$$

by replacing all instances of $\boldsymbol{\Psi}$ by $\mathbf{e}_\bullet \boldsymbol{\psi}_*$, as in equation 3.56,

$$z_{ij} = \sum_{J\in *} \frac{u_{iJ} v_{jJ} \psi_{J}}{\sum\limits_{k\in\bullet} v_{kJ}\psi_{J}} \;\forall\, i,j \in \bullet \qquad \mathbf{Z} = \mathbf{U}\left(\widehat{\mathbf{V}'\mathbf{e}_\bullet\boldsymbol{\psi}_*}\right)^{-1} (\mathbf{e}_\bullet\boldsymbol{\psi}_*)' \circ \mathbf{V}' \qquad (3.56)$$

which is then rearranged

$$z_{ij} = \sum_{J\in *} \frac{u_{iJ} v_{jJ} \psi_{J}}{\psi_J \sum\limits_{k\in\bullet} v_{kJ}} \;\forall\, i,j \in \bullet \qquad \mathbf{Z} = \mathbf{U}\left(\widehat{\mathbf{V}'\mathbf{e}_\bullet}\right)^{-1} \widehat{\boldsymbol{\psi}_*}^{-1} (\boldsymbol{\psi}_*'\mathbf{e}_\bullet') \circ \mathbf{V}' \qquad (3.57)$$

and simplified.

$$z_{ij} = \sum_{J\in *} \frac{u_{iJ} v_{jJ}}{\sum\limits_{k\in\bullet} v_{kJ}} \;\forall\, i,j \in \bullet \qquad \mathbf{Z} = \mathbf{U}\left(\widehat{\mathbf{V}'\mathbf{e}}\right)^{-1} \mathbf{V}' \qquad (3.58)$$

Reformulating in terms of total commodity production ($\mathbf{q} \equiv \mathbf{V}\mathbf{e}_*$) and total activity output ($\mathbf{g} \equiv \mathbf{e}_\bullet'\mathbf{V}$) yields equation 3.59.

$$a_{ij} q_j = \sum_{J\in *} \frac{u_{iJ} v_{jJ}}{g_J} \;\forall\, i,j \in \bullet \qquad \mathbf{A}\hat{\mathbf{q}} = \mathbf{U}\hat{\mathbf{g}}^{-1}\mathbf{V}' \qquad (3.59)$$

Isolating the technical requirement matrix gives the industry-technology construct in its usual form,

$$a_{ij} = \sum_{J\in *} \frac{u_{iJ}}{g_J}\frac{v_{jJ}}{q_j} \;\forall\, i,j \in \bullet \qquad \mathbf{A} = \mathbf{U}\hat{\mathbf{g}}^{-1}\mathbf{V}'\hat{\mathbf{q}}^{-1} \qquad \text{(rep. 3.25)}$$

The industry-technology construct is thus a special case of the more broadly defined aggregation Partition Construct.

Derivation of CTC

In the special case where each commodity is the primary output of exactly one activity, which renders the supply table square with a fully populated diagonal, the AAC equation (equation 3.21, reproduced below)

$$z_{ij} = \sum_{J|(j,J)\in\mathscr{P}} \left(u_{iJ} - \sum_{k|(k,J)\in\mathscr{S}} a_{ik}^{\Gamma} v_{kJ} \right) + \sum_{K|(j,K)\in\mathscr{S}} a_{ij}^{\Gamma} v_{jK} \;\forall\, i,j \in \bullet$$

$$\mathbf{Z}_{\bullet\bullet} = \left(\mathbf{U} - \mathbf{A}_{\bullet\bullet}^{\Gamma}\tilde{\mathbf{V}}\right)\bar{\mathbf{E}}_{\bullet *}' + \mathbf{A}_{\bullet\bullet}^{\Gamma}\widehat{(\tilde{\mathbf{V}}\mathbf{e})} \qquad \text{(3.21, rep)}$$

simplifies to the following form (equation 3.60):

$$z_{ij} = \underbrace{u_{iJ} - \sum_{k|(k,J)\in\mathscr{S}} a^{\Gamma}_{ik} v_{kJ}}_{a_{iJj}v_{jJ}} + \sum_{K|(j,K)\in\mathscr{S}} a^{\Gamma}_{ij} v_{jK} \;\; \forall\, i,j \in \bullet, J|J=j$$

$$\mathbf{Z}_{\bullet\bullet} = \underbrace{\mathbf{U} - \mathbf{A}^{\Gamma}_{\bullet\bullet}\check{\mathbf{V}}}_{\left(\sum_{K\in *} \bar{\mathbf{A}}_{\bullet K \bullet}\right)\hat{\mathbf{V}}} + \mathbf{A}^{\Gamma}_{\bullet\bullet}\widehat{(\check{\mathbf{V}}\mathbf{e})} \quad (3.60)$$

Moreover, as there is only one primary producer for any given commodity, the technology of this sole primary producer will always be the one assumed for the secondary productions. This simplifies the alternate-activity matrix ($\mathbf{\Gamma}$) to an identity matrix. This, in turn, reduces the conceptual description of $\mathbf{A}^{\Gamma}$ (eq 3.51) to the mere collection of all primary productions of the system ($\bar{\mathbf{A}}_{\bullet * \bullet}$).

$$a^{\Gamma}_{ij} = a_{iJj} \;\; \forall\, i,j \in \bullet, J|J=j$$

$$\mathbf{A}^{\Gamma}_{\bullet\bullet} = \sum_{K\in *} \mathbf{A}_{\bullet K \bullet}\widehat{\mathbf{\Gamma}_{K\bullet}} = \sum_{K\in *} \mathbf{A}_{\bullet K \bullet}\widehat{\hat{\mathbf{E}}_{K\bullet}} = \sum_{K\in *} \bar{\mathbf{A}}_{\bullet K \bullet} \quad (3.61)$$

In such a circumstance, the technical requirement ascribed to the production of a commodity will be the same regardless of whether it is produced by its primary producer or by any other activity, which corresponds exactly to the definition of the CTC.

$$a_{ij}q_j = a_{iJj}v_{jJ} + \sum_{K|(j,K)\in\mathscr{S}} a^{\Gamma}_{ij} v_{jK} = a^{\Gamma}_{ij} q_j \;\; \forall\, i,j \in \bullet, J|J=j$$

$$\mathbf{A}_{\bullet\bullet}\widehat{(\mathbf{V}\mathbf{e})} = \left(\sum_{K\in *} \bar{\mathbf{A}}_{\bullet K \bullet}\right)\hat{\mathbf{V}} + \underbrace{\mathbf{A}^{\Gamma}_{\bullet\bullet}}_{\sum_{K\in *} \bar{\mathbf{A}}_{\bullet K \bullet}} \widehat{(\check{\mathbf{V}}\mathbf{e})} = \mathbf{A}^{\Gamma}_{\bullet\bullet}\widehat{(\mathbf{V}\mathbf{e})} \quad (3.62)$$

Which in turn demonstrates that this special case renders the alternate technical coefficient matrix ($\mathbf{A}^{\Gamma}_{\bullet\bullet}$) equal to the symmetric technical coefficient matrix of the whole system ($\mathbf{A}_{\bullet\bullet}$):

$$a_{ij} = a^{\Gamma}_{ij} = a_{iJj} \;\; \forall\, i,j \in \bullet, J \in *|J=j \qquad \mathbf{A}_{\bullet\bullet} = \mathbf{A}^{\Gamma}_{\bullet\bullet} = \sum_{K\in *} \bar{\mathbf{A}}_{\bullet K \bullet} \quad (3.63)$$

This allows us to drop the activity dimension of the A-matrix in equation 3.60, yielding the CTC:

$$z_{ij} = u_{iJ} - \sum_{k|(k,J)\in\mathscr{S}} a_{ik} v_{kJ} + \sum_{K|(j,K)\in\mathscr{S}} a_{ij} v_{jK} \;\; \forall\, i,j \in \bullet, J|J=j$$

$$\mathbf{Z}_{\bullet\bullet} = \mathbf{U} - \mathbf{A}_{\bullet\bullet}\check{\mathbf{V}} + \mathbf{A}_{\bullet\bullet}\widehat{(\check{\mathbf{V}}\mathbf{e})} \quad (3.64)$$

$$a_{ij} = \frac{u_{iJ} - \sum\limits_{k|(k,J)\in\mathscr{S}} a_{ik}v_{kJ} + a_{ij}\sum\limits_{K|(j,K)\in\mathscr{S}} v_{jK}}{\sum\limits_{K\in *} v_{jK}} \quad \forall\, i,j \in \bullet, J|J=j$$

$$\mathbf{A} = \left(\mathbf{U} - \mathbf{A}\check{\mathbf{V}} + \mathbf{A}\widehat{\check{\mathbf{V}}\mathbf{e}}\right)\widehat{(\mathbf{V}\mathbf{e})}^{-1} \tag{3.65}$$

Which simplifies to equation 3.66, (see Raa and Rueda-Cantuche (2007) for details):

$$a_{ij} = \frac{u_{iJ} - \sum\limits_{k|(k,J)\in\mathscr{S}} a_{ik}v_{kJ}}{v_{jJ}} \quad \forall\, i,j \in \bullet, J|J=j \quad \mathbf{A} = \left(\mathbf{U} - \mathbf{A}\check{\mathbf{V}}\right)\left(\widehat{\hat{\mathbf{V}}\mathbf{e}}\right)^{-1} \tag{3.66}$$

$$a_{ij}v_{jJ} + \sum_{k|(k,J)\in\mathscr{S}} a_{ik}v_{kJ} = u_{iJ} \;\; \forall\, i,j \in \bullet, J|J=j \quad \mathbf{A}\hat{\mathbf{V}} + \mathbf{A}\check{\mathbf{V}} = \mathbf{U} \tag{3.67}$$

commodity-technology construct:

$$\mathbf{A} = \mathbf{U}\mathbf{V}^{-1} \qquad \text{(rep. 3.29)}$$

The CTC model is thus equivalent to an Alternate-Activity aggregation Construct applied to the special case of an inventory with exactly one primary producer per commodity.

Chapter 4

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

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4.1 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 analysis (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 analysis (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, Suh, and Huppes, 2005; Majeau-Bettez, Strømman, and Hertwich, 2011), multiple hybrid analyses take advantage of the completeness of EEIO and the specificity of LCA (Suh et al., 2004; Suh and Huppes, 2005; Strømman, Peters, and Hertwich, 2009; Lenzen and Crawford, 2009; Peters and Hertwich, 2006; Suh, 2004b; Suh, 2006; Nakamura and Kondo, 2002; Nakamura et al., 2008; Nakamura et al., 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, Hammervold, and Brattebø, 2009; Graedel et al., 2012; Pauliuk, Sjöstrand, and Müller, 2013). Similarly, Waste-IO extends traditional EEIO models with MFA capabilities (Nakamura and Nakajima, 2005; Nakamura et al., 2011; Nakamura et al., 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; United Nations, 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, Weidema, and Suh, 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, and 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), and the byproduct-technology construct (BTC) (Stone, 1961; Jansen and Raa, 1990b; 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, Wood, and Strømman (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, 1990b; Rueda-Cantuche and Raa, 2009), their generation of negative coefficients (Raa and Van der Ploeg, 1989; Almon, 2000; Suh et al., 2010), and their representation of different types of coproduction (Raa and Chakraborty, 1984; Londero, 1999a; Bohlin and Widell, 2006; Smith and McDonald, 2011). Similarly, the LCA allocation problem has been discussed in terms of the level of subjectivity, transparency, data requirements, compliance with ISO standards, and physical realism of the different models (Frischknecht 1994; Weidema 2000; ISO 2006; Heijungs and Guinée 2007; Cherubini, Strømman, and Ulgiati 2011; Ardente and Cellura 2012; Jung, Assen, and Bardow 2012, among others). Allocation choices pertaining to waste treatment and recycling have been evaluated somewhat separately, both in the ISO standard (ISO 2006; Weidema 2014) and in the literature (Ekvall and Tillman, 1997; Ekvall, 2000; Huppes, 2000; Werner and Richter, 2000; Finnveden, 1999; Johnson, McMillan, and Keoleian, 2013).

Some of these evaluations of allocations and constructs focused specifically on the respect of balances. Jansen and Raa (1990b) and Rueda-Cantuche and 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, Weidema, and Suh, 2010; Merciai et al., 2013; Ecoinvent Centre, 2014), and despite ongoing efforts to track material stocks and flows through lifecycle economic models (cf. Kytzia, Faist, and Baccini, 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, 1990b)? 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 (IE) 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, Wood, and Strømman, 2014). Conversely, because industry-by-industry constructs do not explicitly represent product groups (European Commission, 2008; Rueda-Cantuche and 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 IE systems. The vast literature on balancing algorithms (e.g., Lenzen, Wood, and Gallego, 2007; Lenzen, Gallego, and Wood, 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, 2000b), 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 section 4.6 and appendix B.6).

There exist two popular notation conventions for calculating lifecycle requirements and impacts: the Leontief (1936) and Leontief (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, Assen, and Bardow, 2013; Majeau-Bettez, Wood, and Strømman, 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 supporting information (SI) (appendix A). To not overburden the main text, the mathematical proofs are also presented in SI.

Section 4.2 presents the defining characteristics and balances of a multilayered SUT. We then derive in sections 4.4 and 4.5 the necessary and sufficient conditions for the respect of these balances by the different LCA and EEIO models. This allows for a complete overview of modeling options, notably for representing waste treatment and exclusive secondary products, in section 4.6. We then explore practical implications for various research questions in section 4.7.

4.2 SUT inventory

Mixed-unit SUT

Both LCA and EEIO inventories describe the technosphere in terms of a set of activities ($*$) and a set of products ($\bullet$). The supply of these products by these activities may be conveniently regrouped in a product-by-activity supply table ($\mathbf{V}_{\bullet *}$). The requirements of these activities are then recorded in two separate tables: a use table ($\mathbf{U}_{\bullet *}$)[1] for product requirements and an extension

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

table ($\mathbf{G}_{\star *}$) 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, Wood, and Hertwich, 2014), mineral ores, skilled labor, oxygen (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, Wood, and Hertwich, 2014).

The main benefit of such an 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, 2012b). For example, the supply of electricity and heat by a CHP plant would be recorded as separate flows in the supply table, and the total use of fuel by this plant would simply be noted as one entry in the use table, without having to decide what share of the fuel should be ascribed to what coproduct. This modeling decision can thus remain fully dissociated from the observation phase for greater transparency and flexibility (Suh et al., 2010).

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

The obvious disadvantage with mixed-unit SUT inventories is that the system is never completely described in terms of any of its dimensions. Flows described uniquely in terms of mass cannot be included in cost calculations; flows accounted only in terms of their energy content cannot be used to check the carbon balance, 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, Weidema, and Suh, 2010; Ecoinvent Centre, 2014). The carbon content of the fuel used in a CHP plant, for example, is recorded in the carbon layer of the use table $\left(u_{fuel,CHP}^{carbon}\right)$, whilst the economic value of this same fuel input would be found in the monetary layer $\left(u_{fuel,CHP}^{monetary}\right)$.[2]

Upgrading a mixed-unit inventory to a multi-unit inventory is performed by acquiring additional data on the composition of each product and factors of production. These may be described in terms of their mass, elementary content,

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

energy content, or economic value. We refer to such dimensions of products and factors of production as *properties*. If it is expected that these properties are conserved —i.e., that they survive the transformation of the products or factors without alteration to their quantity— these properties are characterized as *conservative*. For the sake of this article, mass, energy, elementary content and value are all *conservative properties*.

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

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

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

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 4.1 with a mass and a monetary layer (pale and dark gray) derived from a mixed-unit layer (hatched).

[3] In addition to simplifying notation, the assumption of homogeneous product groups ensures that allocations and constructs are the only sources of imbalances in this study, which allows us to focus on the specific contribution of these modeling choices to balance issues. The sensitivity of our results to this fundamental assumption of LCA and EEIO (Viet, 1994; Konijn and Steenge, 1995; Weisz and Duchin, 2006) is discussed in appendix B.6.

[4] The conversion between a mixed-unit layer and property layers of different signs is

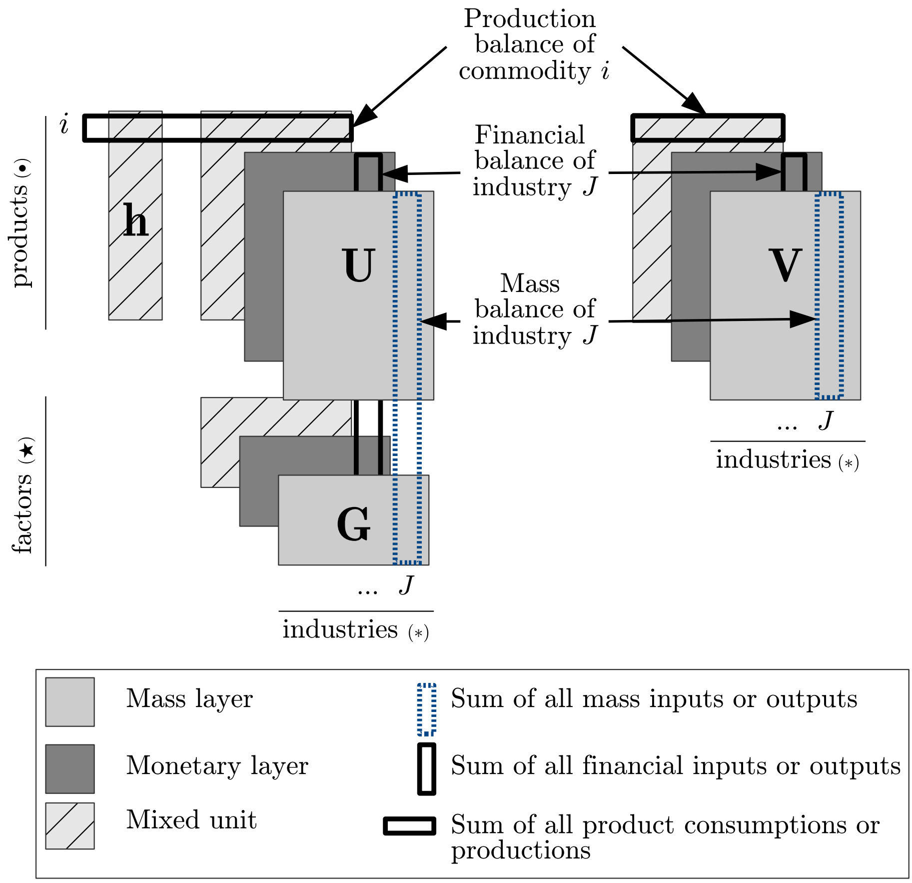

Figure 4.1: Multilayered supply (**V**) and use (**U**) inventory tables (SUTs), with environmental extensions (**G**) and final consumption (**h**), derived from a mixed-unit layer (hatched). Column sums in the different layers assess the financial and mass balances in the different industries, and row sums in the mixed-unit layer assess production balance (a.k.a. market balance) for the different commodities.

The column sums within a given layer should balance if the different industries conserve this layer's defining property (Schmidt, Weidema, and Suh, 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:

$$\underbrace{\sum_{i \in \bullet} u_{iJ}^m + \sum_{c \in \star} g_{cJ}^m}_{\text{total amount in requirement flows}} = \underbrace{\sum_{i \in \bullet} v_{iJ}^m}_{\text{total amount in supply flows}} \qquad m \in \triangle, J \in * \quad (4.1)$$

For greater convenience, each industry's balance may be reformulated in terms of the original mixed-unit SUT ($\mathbf{U}$, $\mathbf{V}$, $\mathbf{G}$) and the unit conversion tables ($\mathbf{\Lambda}_{\triangle\bullet}$, $\mathbf{\Lambda}_{\triangle\star}$), as shown in equation (4.2).

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

$$\underbrace{\sum_{i \in \bullet} \lambda_{mi} u_{iJ} + \sum_{c \in \star} \lambda_{mc} g_{cJ}}_{\text{total amount in requirement flows}} = \underbrace{\sum_{i \in \bullet} \lambda_{mi} v_{iJ}}_{\text{total amount in supply flows}} \qquad m \in \triangle, J \in * \quad (4.2)$$

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 $\left(\sum_{J \in *} v_{iJ}\right)$ must be met by an equal total consumption, either intermediate $\left(\sum_{J \in *} u_{iJ}\right)$ or final (h_i) (equation (4.3)).

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

$$\underbrace{\sum_{J \in *} u_{iJ} + h_i}_{\text{total consumption}} = \underbrace{\sum_{J \in *} v_{iJ}}_{\text{total supply}} \qquad i \in \bullet \qquad (4.3)$$

simply performed by allowing for negative values in property tables $\mathbf{\Lambda}_{\triangle\bullet}$.

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.

4.3 From SUT to technical recipes

Both LCA and EEIO rely on system descriptions that are articulated in terms of "recipes," also known as Leontief production functions (Miller and Blair, 2009). Defining such recipes from the inventory of a multifunctional activity constitutes a challenge, however, because such an inventory describes not the production of a single, homogeneous product but rather the coproduction of multiple products, potentially used in different ratios by different industries (Guinée, 2002).

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

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

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

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

flows $\mathbf{Z}_{\bullet Ji}$, $\mathbf{Z}_{\bullet Jj}$, and $\mathbf{Z}_{\bullet Jk}$ (equation (4.4)).[6]

$$allocation : \mathbf{U}_{\bullet J} \, , \mathbf{V}_{\bullet J} \rightarrow \mathbf{Z}_{\bullet J \bullet} \tag{4.4}$$

Whereas allocations are models applicable to individual activities, constructs are rather applicable to complete system inventories. In this article, the term *construct* designates the modeling of a symmetric, self-contained[7] and complete system of monofunctional recipes from an 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 (**Z**) and normalized to a square technical coefficient matrix (**A**). Various aggregation constructs — notably the CTC, ITC, ESC, and BTC — thus produce product-by-product representations (equation (4.5)) based on different assumptions (United Nations, 1999; European Commission, 2008).[8]

$$aggregation\ construct : \mathbf{U}_{\bullet *} \, , \mathbf{V}_{\bullet *} \rightarrow \mathbf{Z}_{\bullet \bullet} \tag{4.5}$$

From functions 4.4 and 4.5, it is clear that the concept of allocations and constructs are intimately related. Both convert descriptions of industries (**U**, **V**) into recipes for the production of commodities (**Z**, **A**). In doing so, how are the balances of the SUT preserved or discarded?

4.4 Recipe balances

In this section, we ask when the different models generate recipes that are simultaneously balanced with respect to multiple conservative properties. We first investigate allocation models in sections 4.4 to 4.4. We then extend our analysis to IO constructs in section 4.4, making use of the fact that all constructs can be expressed either as multiple repeated or aggregated allocations (Majeau-Bettez, Wood, and Strømman, 2014) (see appendix B.1).

Equation (4.6) defines the balance of a given property in an allocated recipe. The recipe for the production of commodity j by industry$J$ is balanced in terms of property m when the total amount of m in the supply of j ($\lambda_{mj} v_{jJ}$) equals the net total amount of m in allocated requirement flows, taking into account both flows of commodities (e.g., z_{iJj}) and of factors of production (e.g., g_{cJj}).

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

$$\underbrace{\sum_{i \in \bullet} \lambda_{mi} z_{iJj} + \sum_{c \in \star} \lambda_{mc} g_{cJj}}_{m \text{ in requirements allocated to } j} = \underbrace{\lambda_{mj} v_{jJ}}_{m \text{ in supply of } j} \qquad \forall j \in \bullet \tag{4.6}$$

---

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

[7] In a product-by-product **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.

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

Because equation (4.6) — which mirrors equation (4.2) for unallocated flows — explicitly includes the unit conversion coefficients (λ_{mi}, λ_{mc}, and λ_{mj}), variables z, g, and v can be conveniently defined in mixed units.

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 4.1 and 4.2. The former presents a CHP plant that requires coal to coproduce heat and electricity. The latter reports the flows associated with raising a dairy cow and raising a steer for slaughter;[9] cow farming coproduces milk and cow meat, whereas steer farming solely produces steer meat.

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

Table 4.1: 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_2	kg					−4420	−754
O_2	kg					1690	385
labor	$					1820	320

Table 4.2: 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.

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

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 4.3.

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

Table 4.3: 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 $\mathbf{\Lambda}$ matrices (Tables B.1, B.2, B.6 and B.7), and all properties are normalized relative to the units of inventory for each product/factor in the mixed-unit SUTs (tables 4.1 and 4.2).

The different layers of the multi-unit SUTs of these two examples are presented in appendix B.5. 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, and 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, as shows in equation (4.7).

$$\text{requirements of } j = \text{requirements of } J \times j\text{'s share of partitioning property} \tag{4.7}$$

We substitute the equations representing partition-allocated flows (equations (B.7) and (B.8)) in the equation defining the balance of property m in allocated flows (equation (4.6)). The resulting equation (B.24) thus defines the criterion for the balance of property m in partition-allocated flows, and its solution set then necessarily corresponds to all situations where PA leads to balanced recipes. This solution set is expressed in words by proposition 1, with the associated proof in appendix B.2.

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

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

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

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

Let us examine the *value-based partition allocation* of the example CHP plant. According to proposition 1, any property that is found in a fixed proportion to the financial value (partitioning property) in all coproducts will be balanced in the allocated flows. Trivially, the financial value is proportionate to itself and should be conserved in this allocation. In addition, table 4.3 shows that the carbon content of electricity and heat is "proportionate" to financial

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

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 4.3), 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 4.4. 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.

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

Table 4.4: 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, as shown by equation (4.8).

$$\text{requirements of } j = \text{requirements of } J - \text{products avoided} \qquad (4.8)$$

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

Although this modeling technique is not identical to the classical definition of system expansion, it is often referred to as such (Wardenaar et al., 2012; Heijungs, 2013), along with another modeling technique (see section 4.4) (Majeau-Bettez, Wood, and Strømman, 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 (B.9) and (B.10)) with the equation defining the balance of property m in allocated flows (equation (4.6)), and the resulting equation then necessarily represents the criterion for the balance of property m in substitution-allocated flows (equation (B.30)), as expressed in proposition 2.

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

Because the sufficient and necessary condition for PSA balance is expressed in terms of a sum total amount of m over all substitutions, there is a possibility for multiple imbalanced substitutions to cancel one another out 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 appendix B.2).

In the dairy farm example, milk is the primary product, as it provides the majority of the revenues (Londero, 1999a). 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 4.3. Let us assume that $1 of cow meat can substitute $1 of steer meat in this fictional market.[11] Given these parameters, we investigate which balances will be respected by PSA in table 4.5.

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 4.3 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 4.5.

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

Table 4.5: 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, Wood, and Strømman, 2014). The technology assumptions for secondary products are based on the technological description of alternate, primary productions, hence the name

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

(equation (4.9)).

$$\text{requirements of } j = \text{requirement of } J - \text{assumed requirements for coproducts} \quad (4.9)$$

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 (4.8) and (4.9)).

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 (B.11) and (B.12)) with the equation defining the balance of property m in allocated flows (equation (4.6)) yields an equation representing the balance of m in alternate-activity-allocated flows (equation (B.33)). The solution set of this equation, which necessarily corresponds to the set of all situations where AAA leads to balanced recipes (appendix B.2), is expressed in proposition 3.

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

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

For the AAA of dairy cow raising, let us use steer meat production as the best technological proxy for cow meat growth. Furthermore, we assume that these animals' requirements for muscle growth are most similar per kg of muscle (rather than per energy content or protein content, for example). We therefore assume the same requirements to produce a certain mass of meat, regardless of whether it is steer or cow meat. We analyze which balances are upheld by such a coproduction model in table 4.6.

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. 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), whereas 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.

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

Table 4.6: 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.

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 (appendix B.1).

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, Wood, and Strømman, 2014). As the sum of any two balanced recipes will itself be balanced (lemma 3, appendix B.2), 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-partition 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, Wood, and Strømman, 2014). Regardless, any property layer that does respect the ITC definition is also necessarily balanced, following proposition 1.

Beyond traditional SUT, some inventories contain additional data and record use flows that are traceable to a specific supplier, thus adding an extra dimension to the use table ($\mathbf{U}_{*\bullet*}$) (Majeau-Bettez, Wood, and Strømman, 2014). In this case, the coefficient u_{IiJ} denotes the use by activity J of product i sourced specifically from industry I, rather than from the average production mix.[12] From such a StUT, a symmetric system description is simply obtained

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

by applying allocation to each industry in turn, without need for aggregation or any further modeling (see appendix B.1). As traceable constructs are simply repeated allocations, the insights from sections 4.4 to 4.4 directly apply to traceable-partition construct (tPC), traceable-product-substitution construct (tPSC), and traceable-alternate-activity construct (tAAC).

4.5 Production balances

In the previous section, we examined how different models generate balanced recipes across multiple property layers from initially balanced industry descriptions (figure 4.1, 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 4.1, 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 (i.e., $\mathbf{Ve}$) when it is applied to a final demand ($\mathbf{y}$) equal to the original inventoried final demand ($\mathbf{h}$)? Thus, the criterion can be expressed as follows:

$$\mathbf{Ve} = \left(\hat{\mathbf{E}} - \mathbf{A}\right)^{-1} \mathbf{h} \tag{4.10}$$

This test, which can be simplified to equation (4.11) as shown in appendix B.3,

$$\mathbf{AVe} = \mathbf{Ue} \tag{4.11}$$

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

The simplification to equation (4.11) 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 (4.12))? If yes, the allocation in question does not perturb the system's production balance, and vice versa otherwise (proposition 5).

$$\mathbf{A}_{\bullet J \bullet} \mathbf{V}_{\bullet J} = \mathbf{U}_{\bullet J} \tag{4.12}$$

As demonstrated in appendices B.3 and B.3, PA and AAA are always production-balanced. On the contrary, PSA necessarily perturbs the production balance (appendix B.3).

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

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 (appendix B.3). This broad assessment of production balance in the different allocation and construct families extends, and is in accord with, the analysis of ITC, CTC and BTC by Jansen and Raa (1990b).

4.6 Result synthesis

Overview of Balances in Allocations and Constructs

Table 4.7 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. None of the model

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

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

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

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

Table 4.7: 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), partition 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).

families investigated can be said to always yield balanced recipes (table 4.7, column 1). They all have the capacity to do so, however, depending on special characteristics of the SUT inventories (table 4.7, 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 4.7, third column). Alternate-activity and product-substitution models cannot be fully balanced if a secondary product is unique in terms of any of the conservative properties of interest.

The balance across multiple layers in modeled recipes is thus function of the similarity between products: similarity between coproducts in PA, between substituting products in PSA, and between technological proxies in AAA. In practice, however, the similarity between product groups is largely a question of classification and aggregation, as explored in section 4.6.

The question of market balances is more clear cut (table 4.7, second column): partition and alternate-activity models are production-balanced, whereas substitution models are not. Contrary to mass or energy balance, however, the disruption of market balances can be intentional, depending on the question at hand, as explored in section 4.7.

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 or not each waste flow should be considered a functional flow.

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

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

The original Leontief (1970) Pollution Abatement Model, the waste-IO models (Nakamura and Kondo, 2002), ecoinvent 2 (2010), ecoinvent 3.1 consequential or cut-off (2014), and FORWAST (Schmidt, Weidema, and Suh, 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 (4.2) remains valid as long as signs are chosen correspondingly in the property table $\mathbf{\Lambda}$ (see appendix B.4). Our analysis of the different allocations and constructs in table 4.7 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, Wang, and Müller, 2012). The so-called "value-corrected substitution" (Werner and Scholz, 2002; Huppes, 2000), "market-based" (Ekvall, 2000), and "end-of-life recycling" (Atherton, 2006) methods —reviewed by (Johnson, McMillan, and Keoleian, 2013)— also all apply substitution models to multifunctional waste treatment; they only differ in terms of how the substitution coefficients are determined. From table 4.7, 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, McMillan, and Keoleian, 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 4.7 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 4.7, 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 (1990b)), the trade-offs 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." Because 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, Schildhauer, and Biollaz, 2009)— this aggregation will lead to a mismatch between the recorded fuel inputs to district heating and its observed outputs (e.g., SO_2 emissions). A similar mismatch would exist between the recorded inputs to construction and the actual composition of the building.

There is thus potential for problem shifting: in order for allocation and construct models to respect all balances of the inventory, practitioners must somehow work at a coarser resolution level, which in turn causes imbalances of its own in the inventory. Forcing the data collection in the straightjacket that is a "square SUT," where each commodity is the primary product of exactly one activity, seems counterproductive: 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?

4.7 Discussion: What balance for what question?

In response to the title question of this article, we found that none of the allocation or construct model families are unconditionally balanced; only special cases can guarantee the simultaneous respect of all balances (table 4.7). 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; Nakamura et al., 2011) constitutes a good example of such an analysis. More generally, any study at the frontier between MFA and LCA/EEIO must be particularly mindful of these balances. A computer manufacturer claiming that its products do not *contain* more than x% conflict metals, for example, is making a statement about the *accumulation* of materials through the lifecycle value chain of their product, and this certainly requires mass balances.

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

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

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

4.8 Conclusion

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

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

Chapter 5

On the financial balance of input–output constructs: revisiting an axiomatic evaluation

Guillaume Majeau-Bettez, Richard Wood, and Anders Hammer Strømman

Submitted for publication at *Economic Systems Research*

Is not included due to copyright

Chapter 6

Balance issues in monetary input-output tables: a comment on physical inhomogeneity, aggregation bias, and coproduction

Guillaume Majeau-Bettez, Stefan Pauliuk, Richard Wood, Evert A. Bouman, Anders Hammer Strømman

Submitted for publication at *Ecological Economics*

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Chapter 7

Choice of allocations and constructs for attributional and consequential life cycle assessment and input–output analysis

Guillaume Majeau-Bettez, Thomas Dandres, Stefan Pauliuk, Richard Wood, Edgar G Hertwich, Anders Hammer Strømman

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Chapter 8

Lifting industrial ecology modeling to a new level of quality and transparency: a call for more transparent publications and a collaborative open source software framework

Stefan Pauliuk, Guillaume Majeau-Bettez, Christopher Mutel, Bernhard Steubing, Konstantin Stadler

In press at *Journal of Industrial Ecology*

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Chapter 9

Conclusion

9.1 Gains in efficiency and consistency through integration of methods? Return on research objectives

This thesis offers but a small contribution to the long-term development of research on sustainability. It nonetheless addressed key issues pertaining to the integration of core industrial ecology (IE) research methods, principally life-cycle assessment (LCA) and environmentally extended input–output analysis (EEIO), but also material flow analysis (MFA). Through such an integration, important gains in clarity, efficiency, and consistency seem possible for the analysis of our socio-economic metabolism.

Despite sharing most of their calculation routines, the LCA and EEIO communities rely on distinct coproduction modeling traditions that are formulated and justified quite differently. By formally bridging allocation and construct models (chapter 3) and jointly analyzing their properties (chapters 4, 5 and 7), this thesis takes a significant step not only toward more consistent hybrid LCAs, but potentially toward the complete integration of LCA and EEIO research.

Such an integration would likely bring about important efficiency and consistency gains in terms of data collection and consolidation (sub-question Q1). The analysis in chapter 2 brings further confirmation that LCA and EEIO databases are complementary in terms of their coverage of the economy, their scale and resolution, and their level of physical and financial detail. In an integrated LCA-EEIO database development, all process data collections would progressively introduce disaggregations in the economic supply and use table (SUT) representation of the socioeconomic metabolism. This would potentially avoid work done in double by each sub-community, would subject LCA and EEIO inventories to the same checks and balances, would force the consideration of scale and production volumes in LCA, and would bring more physical detail to EEIO system descriptions. This integrated development would also likely alleviate many of the methodological complications of "ad hoc" hybrid LCAs (chapter 2), such as issues of double-counting (Strømman, Peters, and

Hertwich, 2009). However, chapters 3 and 7 point to the need to reconcile different levels of traceability of transactions, as the assumption of an untraceable homogeneous market is not as prevalent in the LCA practice as in EEIO.

The integration of coproduction models already allows for important clarifications for near-future LCA and EEIO development (sub-question Q2). By taking a perhaps more "EEIO perspective" on LCA practice, this thesis identified two different models that had previously been collectively described under the umbrella term of "system expansion" (chapter 3). These models differ from each other and from the original definition of system expansion in terms of their underlying logic, their respect of balances, and the level of technological link that they assume between coproducts (chapters 4 and 7).

The integration of coproduction models also clarifies the link between different allocations and constructs (sub-question Q2), notably demonstrating that typical EEIO constructs can be expressed as the combination of repeated allocations and an aggregation model. It then becomes clear that the dominant EEIO constructs are based on special cases of allocation and can be generalized, giving rise to a broader choice of modeling options (chapter 3).

The combined perspectives of LCA and EEIO on the issue of coproduction thus gives rise to a wider range of modeling options than had been previously recognized by either community, which forces a renewed reflection as to the appropriate choice of coproduction models for different research objectives (sub-question Q3). Most coproduction models are inconsistent with the tracking of flows and stock accumulations because of their incapacity to simultaneously conserve multiple physical and economic dimensions; yet, some special cases do allow for fully balanced production functions and a further integration with multi-layered MFA (chapters 4 and 5). For attributional and marginal-consequential questions, clear compatibility rules were identified based on the respect or perturbation of production balance, the generation of negative flows, the assumed technological link between coproducts, and the capacity to generate technologically credible production functions (chapter 7). This thesis should therefore enable more coherent matches between research objectives and methodological choices.

This impact of coproduction models on the internal consistency of research endeavors should encourage practitioners to be both coherent and flexible in their application of allocations and constructs. The practice of compiling pre-allocated inventories should be abandoned (chapter 3). Rather, a consistent set of rules and assumptions should guide a systematic mix of allocations throughout each system representation (chapter 7). With appropriate software, this can be done efficiently and without obscuring traceability of flows or technological linkage in coproductions. Working in such a modular manner, separating data collection from coproduction modeling, should also allow for gains in flexibility, greater transparency, and more thorough sensitivity analyses (chapter 8).

In summary, chapters 2 to 8 build upon each other to point out avenues for further convergence of core IE methods, providing partial answers to sub-questions Q1 to Q3. This thesis thus offers methodological clarifications, practical prescriptions, and long-term recommendations for more consistent and efficient analyses of our socio-economic metabolism.

9.2 Glimpses of the road ahead

In addition to the potential gains in efficiency and rigor stemming from the integration of IE methods, the present thesis also identified challenges and obstacles. For example, product group inhomogeneities introduce aggregation biases and imbalances across property layers, the latter which hinders the capacity of in LCA, EEIO or MFA to simultaneously conserve more than one physical dimension (chapter 6). Similarly, industry sector aggregations can artificially introduce coproductions through coarse-grain aggregation. Because of such problems, the challenges associated with the integration of very detailed and very aggregated data in a single framework should not be underestimated.

This forces a long-term reflection as to the design of a common database structure for core IE research. Ongoing research efforts in this direction extend the present thesis and that of Pauliuk (2013). An IE database would require a general system structure and a common accounting framework capable of comprehensively and coherently representing unallocated product and waste flows, use phase, factor flows, additions to different types of stocks, factor flows and other exchanges with nature, etc (Pauliuk, Majeau-Bettez, and Müller, 2015).

A common accounting framework would also require the flexible treatment of defining artifacts of IE research, such as boundaries between the socioeconomic metabolism and nature, or the boundary between final and intermediate consumptions. Furthermore, a certain degree of consensus would also be required concerning which types of objects, events, and properties are of interest to the analysis of the socioeconomic metabolism. Such integration efforts could be based on a hierarchical system of definitions, a practical ontology of the socioeconomic metabolism (appendix C).

More work is required in this direction. The quest for a more coherent and integrated study of our metabolism is, if successful, a necessarily dynamic and open-ended process, much like our pursuit of sustainability and balance.

Appendix A

Terminology and notation

A.1 Term definitions

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[1].

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 typically its *primary product* (Londero, 1999a), 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).

A.2 Notation

Table A.1 summarizes the notation and variables used in this article. Some equations are best expressed in coefficient notation, others follow a matrix

[1] 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.

notation, and others are presented with both notations in parallel for greater convenience to the reader.

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	$\in *$
$\mathscr{P}$		Set of all combinations of commodities and activities that are primary production	
$\mathscr{S}$		Set of all combinations of commodities and activities that are *not* primary production	
$\star$		Set of all factors of production (also whole matrix factor-dimension)	
c		indice representing specific factor of production	$\in \star$
$\triangle$		Set of all conservative properties (also whole matrix property-dimension)	
m		indice representing a specific property	$\in \triangle$
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)	
$\circ$		Hadamard multiplication	
Modifiers and Filters:			
$\square'$		transpose	
$\tilde{\square}$		secondary products only	
$\bar{\square}$		primary products only	
$\hat{\square}$		diagonalization of vector OR filter-out off-diagonal elements of matrix	
$\check{\square}$		off-diagonal elements only	
$\dot{\square}$		single-output activities only	
$\ddot{\square}$		multi-output activities only	
Inventory Data			
$\mathbf{U}_{\bullet *}$	u_{iJ}	untraceable Use matrix	
$\mathbf{U}_{* \bullet *}$	u_{IiJ}	traceable Use matrix	
$\mathbf{V}$	v_{iJ}	supply matrix	
$\mathbf{h}$	h_i	inventoried final consumption	
$\mathbf{G}_{\star *}$	g_{cJ}	net use of factors of production	
$\mathbf{\Lambda}_{\triangle \bullet}$	λ_{mj}	conservative properties of products	
$\mathbf{\Lambda}_{\triangle \star}$	λ_{mc}	conservative properties of factors	
Intermediate, Calculated Variables			
$\mathbf{g}$	$g_{1,J}$	Total activity output	$= \mathbf{e}_\bullet' \mathbf{V}$
$\mathbf{q}$	$q_{i,1}$	Total product output	$= \mathbf{U}\mathbf{e}_* + \mathbf{h}$
$\mathbf{B}$	$b_{i,J}$	normalized product use by industries	$= \mathbf{U}\widehat{(\mathbf{e}_\bullet' \mathbf{V})}^{-1}$
$\mathbf{M}$	m_{iJ}	Secondary product per unit of primary production	$= \tilde{\mathbf{V}}\widehat{(\mathbf{e}' \bar{\mathbf{V}})}^{-1}$
$\mathbf{N}$	n_{iJ}	Requirements per unit of primary production	$= \mathbf{U}\widehat{(\mathbf{e}' \bar{\mathbf{V}})}^{-1}$
$\mathbf{S}$	s_{cJ}	normalized factor use by industries	$= \mathbf{G}\widehat{(\mathbf{e}_\bullet' \mathbf{V})}^{-1}$
Decision variables of generalized models			
$\underline{\mathbf{\Delta V}}$	$\underline{\delta v}_{iJ}$	Alteration to the inventoried Supply	
$\underline{\mathbf{\Delta U}}$	d.s.	Alteration to the inventoried Use	
$\underline{\tilde{\mathbf{A}}}$	d.s.	Assumed technical requirements for secondary products	
Intermediate Variables for Specific Models			
$\mathbf{\Psi}$	$\psi_{i,J}$	partitioning (intensive) property	
$\boldsymbol{\psi}$	ψ_J	activity-wide unique intensive property	
$\mathbf{\Phi}$	$\phi_{J,i}$	partitioning coefficient	
$\mathbf{\Gamma}_{* \bullet}$	γ_{Ji}	alternate activity matrix	mapping, 1 or 0
$\mathbf{\Gamma}_{* \triangle \bullet}$	γ_{Jmi}	alternate activity matrix (with explicit production equivalence property)	mapping, 1 or 0
$\mathbf{A}^{\Gamma}$	d.s.	alternate technology coefficient matrix	
$\mathbf{\Xi}$	ξ_{ji}	substitution table	
$\mathbf{\Theta}$	θ_{Ji}	Competing/substituted producer for traceable products	mapping, 1 or 0
Final Variables			
$\mathbf{y}$	y_i	exogenously defined final demand	
$\mathbf{Z}$	d.s.	modeled intermediate flows	
$\mathbf{A}$	d.s.	modeled technical coefficient	
$\mathbf{L}$	l_{ij}	Leontief Inverse	$= (\hat{\mathbf{E}} - \mathbf{A})^{-1}$
$\mathbf{x}$	x_i	total calculated production	$= \mathbf{Ly}$
$\mathbf{G}_{\star * \bullet}$ or $\mathbf{G}_{\star \bullet}$	d.s.	Modeled (allocated or constructed) factors of production	
$\mathbf{F}_{\star * \bullet}$ or $\mathbf{F}_{\star \bullet}$	d.s.	Modeled and normalized factors of production	
d.s. = dimensions specified with subscripts ($\bullet$, $*$, 1) depending on situation			

Table A.1: Notation and variables

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 $*$). Indice c designates an individual factor, element of $\star$.

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 $\mathbf{U}_{\bullet *}$. Furthermore, these indices can also be used to "slice" specific sections of matrices. For example, $\mathbf{U}_{\bullet J}$ designates the $\mathrm{J^{th}}$ column of matrix $\mathbf{U}$, thus selecting the use of all products by industry J.

The set $\mathscr{P}$ is the set of all primary production flows in the system, whereas the set $\mathscr{S}$ 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 $\mathscr{P}$, otherwise it belongs to $\mathscr{S}$. The two sets are thus complementary.[2]

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 ($\hat{\square}$), off-diagonal elements ($\check{\square}$), secondary product entries ($\tilde{\square}$), primary product entries ($\bar{\square}$), single-output industries ($\dot{\square}$), or multi-output industries ($\ddot{\square}$). 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, $\bar{\mathbf{E}}_{\bullet *}$ is the 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] In this way, $\mathscr{S}$ is defined as also including productions of magnitude zero. If k is not produced by J, the pair (k, J) is an element of $\mathscr{S}$.

Appendix B

Supporting information to Article 3

B.1 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* SUT to a *multilayered* SUT, and then proceeds to define the different allocation models and construct models.

Multilayered SUT

Given property matrices ($\mathbf{\Lambda}_{\triangle\bullet}$ and $\mathbf{\Lambda}_{\triangle\star}$) 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 (B.1) to (B.3).

<u>The layer of property m in a multi-unit SUT, defined from the mixed-unit inventory:</u>

$$u_{iJ}^{m} = \lambda_{mi} u_{iJ} \quad m \in \triangle, \forall (i, J) \in (\bullet, *) \tag{B.1}$$

$$v_{iJ}^{m} = \lambda_{mi} v_{iJ} \quad m \in \triangle, \forall (i, J) \in (\bullet, *) \tag{B.2}$$

$$g_{cJ}^{m} = \lambda_{mc} g_{cJ} \quad m \in \triangle, \forall (c, J) \in (\star, *) \tag{B.3}$$

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 (λ_{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 EEIO and LCA (Duchin, 2009; European Commission, 2008; Merciai and Heijungs, 2014) ensures that coproduction modeling choices are the only source of imbalances (see appendix B.6 for sensitivity analysis).

The above equations allow for the conversion between equation (4.1) and equation (4.2) in the main article.

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 ($\mathbf{U}_{*\bullet*}$), 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 ($\mathbf{U}_{\bullet*}$) that industry J uses a certain amount of commodity i (u_{iJ}) 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 (4.4) and (B.4), reproduced below).

$$allocation : \mathbf{U}_{\bullet J}\ , \mathbf{V}_{\bullet J}\ \ \rightarrow \mathbf{Z}_{\bullet J \bullet} \qquad \text{(rep. 4.4)}$$

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

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 (4.5) and (B.5), reproduced below).

$$aggregation\ construct : \mathbf{U}_{\bullet*}\ , \mathbf{V}_{\bullet*}\ \ \rightarrow \mathbf{Z}_{\bullet\bullet} \qquad \text{(rep. 4.5)}$$

$$traceable\ construct : \mathbf{U}_{*\bullet*}\ , \mathbf{V}_{\bullet*}\ \rightarrow \mathbf{Z}_{*\bullet*\bullet} \qquad \text{(B.5)}$$

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 (B.4) and (B.5)). 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, Wood, and Strømman, 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-partition construct (tPC), a traceable-product-substitution construct (tPSC), or a traceable-alternate-activity construct (tAAC), respectively.

Alternatively, an aggregation-partition 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, Wood, and Strømman, 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 homogogeneous, as explored in appendix B.6.

Partition allocation equations

Partition allocation splits requirements across coproducts based on a common property that they share (equation (4.7)) (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* $\mathbf{\Psi}$. In other words, the descriptions of the coproducts are recorded in the column-vector $\mathbf{\Psi}_{\bullet J}$.

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* ($\mathbf{\Phi}$), as expressed in equation (B.6) (Majeau-Bettez, Wood, and Strømman, 2014).

$$\phi_{Jj} = \frac{v_{jJ}\psi_{jJ}}{\sum\limits_{k\in\bullet} v_{kJ}\psi_{kJ}} \quad \forall j \in \bullet \qquad \mathbf{\Phi}_{J\bullet} = \left(\widehat{\mathbf{V}'_{\bullet J}\mathbf{\Psi}_{\bullet J}}\right)^{-1} \mathbf{\Psi}'_{\bullet J}\widehat{\mathbf{V}_{\bullet J}} \tag{B.6}$$

Partitioning coefficients for industry J are then used to partition its use of products (equation (B.7)) and of factors of production (equation (B.8)). The outer vector-product of use flows ($\mathbf{U}_{\bullet J}$) and partitioning coefficients ($\mathbf{\Phi}_{J\bullet}$) leads to a product-by-product representation of the allocated flows at industry J ($\mathbf{Z}_{\bullet J\bullet}$).

$$\mathbf{Z}_{\bullet J\bullet} = \mathbf{A}_{\bullet J\bullet}\widehat{\mathbf{V}_{\bullet J}} = \mathbf{U}_{\bullet J}\mathbf{\Phi}_{J\bullet} \tag{B.7}$$

$$\mathbf{G}_{\star J\bullet} = \mathbf{F}_{\star J\bullet}\widehat{\mathbf{V}_{\bullet J}} = \mathbf{G}_{\star J}\mathbf{\Phi}_{J\bullet} \tag{B.8}$$

Definition 1. Let equations (B.6) to (B.8) collectively define partition allocation.

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 (4.8)) (Guinée, 2002).

Let the substitutability between products be recorded in a product-by-product *substitution matrix* ($\boldsymbol{\Xi}$). 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 4.1). This substitution matrix then allows for the general representation of PSA by equations (B.9) and (B.10) (Majeau-Bettez, Wood, and Strømman, 2014).

$$\mathbf{A}_{\bullet J \bullet}\widehat{\mathbf{V}_{\bullet J}} = \mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet}\widehat{\bar{\mathbf{V}}_{\bullet J}} = \left(\mathbf{U}_{\bullet J} - \boldsymbol{\Xi}\tilde{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J} \tag{B.9}$$

$$\mathbf{F}_{\star J \bullet}\widehat{\mathbf{V}_{\bullet J}} = \mathbf{G}_{\star J \bullet} = \mathbf{F}_{\star J \bullet}\widehat{\bar{\mathbf{V}}_{\bullet J}} = \mathbf{G}_{\star J}\bar{\mathbf{E}}'_{\bullet J} \tag{B.10}$$

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

Definition 2. Let equations (B.9) and (B.10) collectively define product-substitution allocation. Consequently, let $\boldsymbol{\Xi}\tilde{\mathbf{V}}_{\bullet J}$ represent the product flows substituted by the secondary products of an activity J.

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 (4.9)). Each technology assumption is based on the technology of an alternative production route for a similar or identical product (Majeau-Bettez, Wood, and Strømman, 2014).

Thus, in equation (B.11), product requirements are assumed for all secondary productions of J $\left(\mathbf{A}^{\Gamma}_{\bullet\bullet}\widehat{\tilde{\mathbf{V}}_{\bullet J}}\right)$ based on an alternate technology description ($\mathbf{A}^{\Gamma}_{\bullet\bullet}$), and the primary product is allocated the remainder of the joint requirements ($\mathbf{U}_{\bullet J} - \mathbf{A}^{\Gamma}_{\bullet\bullet}\tilde{\mathbf{V}}_{\bullet J}$).

$$\mathbf{Z}_{\bullet J \bullet} = \left(\mathbf{U}_{\bullet J} - \mathbf{A}^{\Gamma}_{\bullet\bullet}\tilde{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J} + \mathbf{A}^{\Gamma}_{\bullet\bullet}\widehat{\tilde{\mathbf{V}}_{\bullet J}} \tag{B.11}$$

Equation (B.12) applies the same allocation modeling to the use of factors of production.

$$\mathbf{F}_{\star J \bullet} = \left(\mathbf{G}_{\star J} - \mathbf{F}^{\Gamma}_{\star\bullet}\tilde{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J} + \mathbf{F}^{\Gamma}_{\star\bullet}\widehat{\tilde{\mathbf{V}}_{\bullet J}} \tag{B.12}$$

Definition 3. Let equations (B.11) and (B.12) 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 $\mathbf{\Gamma}_{*\triangle\bullet}$. 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.

$$\gamma_{Jk} = \sum_{m\in\triangle} \frac{\gamma_{Jmk}\lambda_{mk}}{\lambda_{mj}} \quad \forall (j,J) \in \mathscr{P}, k \in \bullet \quad \mathbf{\Gamma}_{*\bullet} = \sum_{m\in\triangle} \widehat{\mathbf{\Lambda}_{m\bullet}\bar{\mathbf{E}}}^{-1} \mathbf{\Gamma}_{*m\bullet} \widehat{\mathbf{\Lambda}_{m\bullet}} \tag{B.13}$$

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 ($\mathbf{B}_{\bullet *} = \mathbf{U}\widehat{(\mathbf{e}'\mathbf{V})}^{-1}$) of these industries,

$$\mathbf{A}^{\Gamma} = \mathbf{B}\dot{\mathbf{\Gamma}}_{*\bullet} \tag{B.14}$$

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

$$\mathbf{F}^{\Gamma} = \mathbf{S}\dot{\mathbf{\Gamma}}_{*\bullet} \tag{B.15}$$

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, Wood, and Strømman, 2014, for automation of this process).

B.2 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.

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 (4.2). Furthermore, let equation (4.6) 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 (4.6)) is reproduced below.

$$\underbrace{\sum_{i\in\bullet}\lambda_{mi}z_{iJj}+\sum_{c\in\star}\lambda_{mc}g_{cJj}}_{m\text{ in requirements allocated to }j} = \underbrace{\lambda_{mj}v_{jJ}}_{m\text{ in supply of }j} \qquad \forall j\in\bullet \qquad \text{(rep. 4.6)}$$

It may be reformulated in matrix notation as in equation (B.16).

Conservation of property m in the allocated flows of industry J

$$\underbrace{\mathbf{\Lambda}_{m\bullet}\mathbf{Z}_{\bullet Jj}+\mathbf{\Lambda}_{m\star}\mathbf{G}_{\star Jj}}_{m\text{ in requirements allocated to }j} = \underbrace{\lambda_{mj}v_{jJ}}_{m\text{ in supply of }j} \qquad \forall j\in\bullet \qquad \text{(B.16)}$$

This balance can also be expressed in a normalized form, as in equation (B.17). 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

$$\mathbf{\Lambda}_{m\bullet}\mathbf{A}_{\bullet Jj}+\mathbf{\Lambda}_{m\star}\mathbf{F}_{\star Jj}=\lambda_{mj} \qquad \forall j\in\bullet|v_{jJ}\neq 0 \qquad \text{(B.17)}$$

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 (B.16) is further simplified to equation (B.18).

Conservation of property m in constructed flows

$$\underbrace{\mathbf{\Lambda}_{m\bullet}\mathbf{A}_{\bullet j}+\mathbf{\Lambda}_{m\star}\mathbf{F}_{\star j}}_{m\text{ in requirements to production of }j} = \underbrace{\lambda_{mj}}_{m\text{ in }j} \qquad \forall j\in\bullet \qquad \text{(B.18)}$$

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 (B.7) and (B.8)) with the definition of balanced allocated flows (equation (B.17)) necessarily leads to an equation defining balanced partition-allocated flows (equation (B.19)).

$$\mathbf{\Lambda}_{m\bullet}\mathbf{U}_{\bullet J}\frac{\phi_{Jj}}{v_{jJ}} + \mathbf{\Lambda}_{m\star}\mathbf{G}_{\star J}\frac{\phi_{Jj}}{v_{jJ}} = \lambda_{mj} \qquad \forall j \in \bullet | v_{jJ} \neq 0 \tag{B.19}$$

This equation may be rearranged as in equation (B.20).

$$\left(\mathbf{\Lambda}_{m\bullet}\mathbf{U}_{\bullet J} + \mathbf{\Lambda}_{m\star}\mathbf{G}_{\star J}\right)\frac{\phi_{Jj}}{v_{jJ}} = \lambda_{mj} \qquad \forall j \in \bullet | v_{jJ} \neq 0 \tag{B.20}$$

Since it is given that the inventory of activity J is initially balanced with respect to m, from equation (4.2) the term in parenthesis is equal to the total amount of property m in the supply flows of industry J ($\mathbf{\Lambda}_{m\bullet}\mathbf{V}_{\bullet J}$).

$$\mathbf{\Lambda}_{m\bullet}\mathbf{V}_{\bullet J}\frac{\phi_{Jj}}{v_{jJ}} = \lambda_{mj} \qquad \forall j \in \bullet | v_{jJ} \neq 0 \tag{B.21}$$

From equation (B.6), we reformulate the partition coefficient (ϕ_{Jj}) in terms of intensive properties ($\mathbf{\Psi}$), and we simplify. The braces {} indicate that the inner vector-product results in a scalar.

$$\left\{\mathbf{\Lambda}_{m\bullet}\mathbf{V}_{\bullet J}\right\}\frac{\psi_{jJ}}{\left\{\mathbf{\Psi}'_{\bullet J}\mathbf{V}_{\bullet J}\right\}} = \lambda_{mj} \qquad \forall j \in \bullet | v_{jJ} \neq 0 \tag{B.22}$$

This equation may then be rearranged as in equation (B.23).

$$\frac{\left\{\mathbf{\Lambda}_{m\bullet}\mathbf{V}_{\bullet J}\right\}}{\left\{\mathbf{\Psi}'_{\bullet J}\mathbf{V}_{\bullet J}\right\}} = \alpha = \frac{\lambda_{mj}}{\psi_{jJ}} \qquad \forall j \in \bullet | v_{jJ} \neq 0 \tag{B.23}$$

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 (α). This condition is equivalently expressed in coefficient notation.

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

$$\frac{\lambda_{mj}}{\psi_{jJ}} = \alpha = \frac{\sum\limits_{k\in\bullet}\lambda_{mk}v_{kJ}}{\sum\limits_{k\in\bullet}\psi_{kJ}v_{kJ}} \qquad \forall j \in \bullet | v_{jJ} \neq 0 \tag{B.24}$$

Equation (B.24) thus expresses the necessary and sufficient condition for balanced PA. Equation (B.24) 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., $\forall j \in \bullet | v_{jJ} \neq 0$). □

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.

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., $(j, J) \in \mathscr{P}$). Combining the equations that generally represent substitution-allocated flows (equations (B.9) and (B.10)) with the definition of balanced allocated flows (equation (B.16)) necessarily leads to the definition of balanced substitution-allocated flows (equation (B.25)).

$$\mathbf{\Lambda}_{m\bullet}\left(\mathbf{U}_{\bullet J} - \mathbf{\Xi}\tilde{\mathbf{V}}_{\bullet J}\right) + \mathbf{\Lambda}_{m\star}\mathbf{G}_{\star J} = \lambda_{mj} v_{jJ} \tag{B.25}$$

This equation may be rearranged as follows.

$$\left(\mathbf{\Lambda}_{m\bullet}\mathbf{U}_{\bullet J} + \mathbf{\Lambda}_{m\star}\mathbf{G}_{\star J}\right) - \mathbf{\Lambda}_{m\bullet}\mathbf{\Xi}\tilde{\mathbf{V}}_{\bullet J} - \lambda_{mj} v_{jJ} = 0 \tag{B.26}$$

Since it is given that the inventory of activity J is initially balanced, from equation (4.2) the term in parenthesis equals the total amount of property m in the supply flows of industry J.

$$\mathbf{\Lambda}_{m\bullet}\mathbf{V}_{\bullet J} - \mathbf{\Lambda}_{m\bullet}\mathbf{\Xi}\tilde{\mathbf{V}}_{\bullet J} - \lambda_{mj} v_{jJ} = 0 \tag{B.27}$$

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.

$$\mathbf{\Lambda}_{m\bullet}\tilde{\mathbf{V}}_{\bullet J} - \mathbf{\Lambda}_{m\bullet}\mathbf{\Xi}\tilde{\mathbf{V}}_{\bullet J} = 0 \tag{B.28}$$

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

$$\mathbf{\Lambda}_{m\bullet}\tilde{\mathbf{V}}_{\bullet J} = \mathbf{\Lambda}_{m\bullet}\mathbf{\Xi}\tilde{\mathbf{V}}_{\bullet J} \tag{B.29}$$

Equation (B.29) 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 ($\mathbf{\Lambda}_{m\bullet}\tilde{\mathbf{V}}_{\bullet J}$) equal the sum total amount of m in the substituted products ($\mathbf{\Lambda}_{m\bullet}\mathbf{\Xi}\tilde{\mathbf{V}}_{\bullet J}$). □

Equation (B.29) may be reformulated in coefficient notation for greater convenience.

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

$$\sum_{k|(k,J)\in\mathscr{S}} \lambda_{mk} v_{kJ} = \sum_{k|(k,J)\in\mathscr{S}} \sum_{i\in\bullet} \lambda_{mi} \xi_{ik} v_{kJ} \tag{B.30}$$

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.

Balanced recipes from alternate-activity allocation

Since AAA treats primary and secondary products differently but presents recipes for both, the proof of its balance in 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 (B.11), the requirements that will be allocated to its production will equal those of the assumed equivalent technology.

$$\mathbf{A}_{\bullet Jk} = \mathbf{A}^{\Gamma}_{\bullet k} \tag{B.31}$$

$$\mathbf{F}_{\star Jk} = \mathbf{F}^{\Gamma}_{\star k} \tag{B.32}$$

This allows for the reformulation of the balanced allocation equation (equation (B.17)) as equation (B.33). 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.

$$\mathbf{\Lambda}_{m\bullet}\mathbf{A}^{\Gamma}_{\bullet k} + \mathbf{\Lambda}_{m\star}\mathbf{F}^{\Gamma}_{\star k} = \lambda_{mk} \tag{B.33}$$

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 (B.33) to equation (B.34).

$$\mathbf{\Lambda}_{m\bullet}\bar{\mathbf{E}}\mathbf{\Gamma}_{*k} = \lambda_{mk} \tag{B.34}$$

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

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 (B.11) and (B.12), this product flow is allocated the remainder of the requirements of J after technologies have been assumed for each secondary product.

$$\mathbf{Z}_{\bullet Jj} = \mathbf{U}_{\bullet J} - \mathbf{A}^{\Gamma}\tilde{\mathbf{V}}_{\bullet J} \tag{B.35}$$

$$\mathbf{G}_{\star Jj} = \mathbf{G}_{\star J} - \mathbf{F}^{\Gamma}\tilde{\mathbf{V}}_{\bullet J} \tag{B.36}$$

Combining equations (B.35) and (B.36) with the equation for balanced allocation (equation (B.16)) then defines the criterion for the balance of the AAA-based recipe of a primary product (equation (B.37)).

$$\mathbf{\Lambda}_{m\bullet}\left(\mathbf{U}_{\bullet J} - \mathbf{A}^{\Gamma}\tilde{\mathbf{V}}_{\bullet J}\right) + \mathbf{\Lambda}_{m\star}\left(\mathbf{G}_{\star J} - \mathbf{F}^{\Gamma}\tilde{\mathbf{V}}_{\bullet J}\right) = \lambda_{mj}v_{jJ} \tag{B.37}$$

It is simply rearranged as follows.

$$(\mathbf{\Lambda}_{m\bullet}\mathbf{U}_{\bullet J} + \mathbf{\Lambda}_{m\star}\mathbf{G}_{\star J}) - \left(\mathbf{\Lambda}_{m\bullet}\mathbf{A}^{\Gamma} + \mathbf{\Lambda}_{m\star}\mathbf{F}^{\Gamma}\right)\tilde{\mathbf{V}}_{\bullet J} = \lambda_{mj}v_{jJ} \tag{B.38}$$

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., $\mathbf{\Lambda}_{m\bullet}\mathbf{V}_{\bullet J}$).

$$\mathbf{\Lambda}_{m\bullet}\mathbf{V}_{\bullet J} - \left(\mathbf{\Lambda}_{m\bullet}\mathbf{A}^{\Gamma} + \mathbf{\Lambda}_{m\star}\mathbf{F}^{\Gamma}\right)\tilde{\mathbf{V}}_{\bullet J} = \lambda_{mj}v_{jJ} \tag{B.39}$$

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.

$$\mathbf{\Lambda}_{m\bullet}\mathbf{V}_{\bullet J} - \left(\mathbf{\Lambda}_{m\bullet}\bar{\mathbf{E}}\mathbf{\Gamma}\right)\tilde{\mathbf{V}}_{\bullet J} = \lambda_{mj}v_{jJ} \tag{B.40}$$

As it is given that all secondary product allocations are balanced, equation (B.40) is further simplified based on equation (B.34),

$$\mathbf{\Lambda}_{m\bullet}\mathbf{V}_{\bullet J} - \mathbf{\Lambda}_{m\bullet}\tilde{\mathbf{V}} = \lambda_{mj}v_{jJ} \tag{B.41}$$

which simplifies in turn to

$$\lambda_{mj}v_{jJ} = \lambda_{mj}v_{jJ} \tag{B.42}$$

□

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 technolgy.

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.

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 $\mathbf{Z}_{\bullet Ki}$.

$$\mathbf{a} = \mathbf{Z}_{\bullet Jj} + \mathbf{Z}_{\bullet Ki} \tag{B.43}$$

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 ($\mathbf{G}_{\star Ki}$).

$$\mathbf{b} = \mathbf{G}_{\star Jj} + \mathbf{G}_{\star Ki} \tag{B.44}$$

From equation (B.16), the criterion for the conservation of property m in this aggregation may be represented as follows.

$$\lambda_{mj} v_{jJ} + \lambda_{mi} v_{iK} = \mathbf{\Lambda}_{m\bullet}\mathbf{a} + \mathbf{\Lambda}_{m\star}\mathbf{b} \tag{B.45}$$

It may be reformulated based on equations (B.43) and (B.44),

$$\lambda_{mj} v_{jJ} + \lambda_{mi} v_{iK} = \mathbf{\Lambda}_{m\bullet}\left(\mathbf{Z}_{\bullet Jj} + \mathbf{Z}_{\bullet Ki}\right) + \mathbf{\Lambda}_{m\star}\left(\mathbf{G}_{\star Jj} + \mathbf{G}_{\star Ki}\right) \tag{B.46}$$

and further rearranged.

$$\lambda_{mj} v_{jJ} + \lambda_{mi} v_{iK} = \left(\mathbf{\Lambda}_{m\bullet}\mathbf{Z}_{\bullet Jj} + \mathbf{\Lambda}_{m\star}\mathbf{G}_{\star Jj}\right) + \left(\mathbf{\Lambda}_{m\bullet}\mathbf{Z}_{\bullet Ki} + \mathbf{\Lambda}_{m\star}\mathbf{G}_{\star Ki}\right) \tag{B.47}$$

As it is given that each allocated recipe individually conserves m, equation (B.16) allows for further simplification.

$$\lambda_{mj} v_{jJ} + \lambda_{mi} v_{iK} = \lambda_{mj} v_{jJ} + \lambda_{mi} v_{iK} \tag{B.48}$$

As equation (B.48) necessarily always holds, m is always conserved in the sum of two balance recipes. □

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 (B.5)), 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. □

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.

B.3 Proofs of production balances

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

General

Definition 6. Let equation (4.10), 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 (4.10) and will thereby be production balanced if and only if equation (4.11) holds true when applied to the same data.

Proof. Equation (4.11) is a direct simplification of equation (4.10). Indeed, the criterion for production balance,

$$\mathbf{Ve} = \left(\hat{\mathbf{E}} - \mathbf{A}\right)^{-1} \mathbf{h} \qquad \text{(rep. 4.10)}$$

may be rearranged as follows.

$$\left(\hat{\mathbf{E}} - \mathbf{A}\right)\mathbf{Ve} = \mathbf{h} \tag{B.49}$$

$$-\mathbf{AVe} = -\mathbf{Ve} + \mathbf{h} \tag{B.50}$$

$$\mathbf{AVe} = \mathbf{Ve} - \mathbf{h} \tag{B.51}$$

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 (B.51) to equation equation (4.11), reproduced below.

$$\mathbf{AVe} = \mathbf{Ue} \tag{rep. 4.11}$$

□

Equation (4.11) is identical to the test presented by Jansen and Raa (1990b) 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 (4.12) ($\mathbf{A}_{\bullet J \bullet}\mathbf{V}_{\bullet J} = \mathbf{U}_{\bullet J}$), then the resulting aggregation construct will respect equation (4.11) and will be production balanced.

Proof. We reformulate equation (4.11), based on the fact that a column vector ($\mathbf{Ve}$) is necessarily equal to the row-sum of its diagonalization ($\widehat{\mathbf{Ve}}\mathbf{e}$).

$$\mathbf{AVe} = \mathbf{Ue} \tag{rep. 4.11}$$

$$\mathbf{A}_{\bullet\bullet}\widehat{\mathbf{Ve}}\mathbf{e} = \mathbf{Ue} \tag{B.52}$$

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

$$\mathbf{Z}_{\bullet\bullet}\mathbf{e} = \mathbf{Ue} \tag{B.53}$$

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

$$\sum_{J\in *}\mathbf{Z}_{\bullet J \bullet}\mathbf{e} = \mathbf{Ue} \tag{B.54}$$

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

$$\sum_{J\in *}\mathbf{Z}_{\bullet J \bullet}\mathbf{e} = \sum_{J\in *}\mathbf{U}_{\bullet J} \tag{B.55}$$

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

$$\sum_{J\in *} \mathbf{A}_{\bullet J \bullet} \widehat{\mathbf{V}_{\bullet J}} \mathbf{e} = \sum_{J\in *} \mathbf{U}_{\bullet J} \tag{B.56}$$

and simplifying,

$$\sum_{J\in *} \mathbf{A}_{\bullet J \bullet} \mathbf{V}_{\bullet J} = \sum_{J\in *} \mathbf{U}_{\bullet J} \tag{B.57}$$

leads to an equation that must be true if equation (4.12) ($\mathbf{A}_{\bullet J \bullet} \mathbf{V}_{\bullet J} = \mathbf{U}_{\bullet J}$) is true.

$$\sum_{J\in *} \mathbf{U}_{\bullet J} = \sum_{J\in *} \mathbf{U}_{\bullet J} \tag{B.58}$$

□

Thus, if each allocation respects equation (4.12), 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 (4.12) 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 (4.12).

Production balance of partition allocation

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

Proof. Combining equations (B.6) and (B.7), which collectively define PA of product flows (definition 1), yields a representation of partition-allocated flows ($\mathbf{A}_{\bullet J \bullet} \widehat{\mathbf{V}_{\bullet J}}$) in terms of SUT and intensive partitioning properties ($\mathbf{\Psi}$).

$$\mathbf{A}_{\bullet J \bullet} \widehat{\mathbf{V}_{\bullet J}} = \mathbf{U}_{\bullet J} \left(\widehat{\mathbf{V}'_{\bullet J} \mathbf{\Psi}_{\bullet J}} \right)^{-1} \mathbf{\Psi}'_{\bullet J} \widehat{\mathbf{V}_{\bullet J}} \tag{B.59}$$

The left-hand side of this equation may be rendered identical to that of equation (4.12) by multiplying both sides of the equation by the summation vector $\mathbf{e}$,

$$\mathbf{A}_{\bullet J \bullet} \widehat{\mathbf{V}_{\bullet J}} \mathbf{e} = \mathbf{U}_{\bullet J} \left(\widehat{\mathbf{V}'_{\bullet J} \mathbf{\Psi}_{\bullet J}} \right)^{-1} \mathbf{\Psi}'_{\bullet J} \widehat{\mathbf{V}_{\bullet J}} \mathbf{e} \tag{B.60}$$

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

$$\mathbf{A}_{\bullet J \bullet} \mathbf{V}_{\bullet J} = \mathbf{U}_{\bullet J} \left(\widehat{\mathbf{V}'_{\bullet J} \mathbf{\Psi}_{\bullet J}} \right)^{-1} \mathbf{\Psi}'_{\bullet J} \mathbf{V}_{\bullet J} \tag{B.61}$$

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

$$= \mathbf{U}_{\bullet J} \left(\mathbf{\Psi}'_{\bullet J}\mathbf{V}_{\bullet J}\right)^{-1} \left(\mathbf{\Psi}'_{\bullet J}\mathbf{V}_{\bullet J}\right) \tag{B.62}$$

This simplifies the right-hand side of the equation to that of equation (4.12)

$$= \mathbf{U}_{\bullet J} \tag{B.63}$$

Equation (B.63) is equal to equation (4.12) □

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.

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 (B.11), which defines the AAA of product flows (definition 3), by a vertical summation vector **e**,

$$\mathbf{A}_{\bullet J \bullet}\widehat{\mathbf{V}_{\bullet J}}\mathbf{e} = \left(\mathbf{U}_{\bullet J} - \mathbf{A}^{\Gamma}\tilde{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J}\mathbf{e} + \mathbf{A}^{\Gamma}\widehat{\tilde{\mathbf{V}}_{\bullet J}}\mathbf{e} \tag{B.64}$$

(B.65)

renders the left-hand side of this equation equal to that of the equation defining production-balanced allocation (equation (4.12)).

$$\mathbf{A}_{\bullet J \bullet}\mathbf{V}_{\bullet J} = \left(\mathbf{U}_{\bullet J} - \mathbf{A}^{\Gamma}\tilde{\mathbf{V}}_{\bullet J}\right)\bar{\mathbf{E}}'_{\bullet J}\mathbf{e} + \mathbf{A}^{\Gamma}\tilde{\mathbf{V}}_{\bullet J} \tag{B.66}$$

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

$$= \left(\mathbf{U}_{\bullet J} - \mathbf{A}^{\Gamma}\tilde{\mathbf{V}}_{\bullet J}\right)\{1\} + \mathbf{A}^{\Gamma}\tilde{\mathbf{V}}_{\bullet J} \tag{B.67}$$

the right-hand side of the equation then also simplifies to that of equation (4.12).

$$= \mathbf{U}_{\bullet J} - \mathbf{A}^{\Gamma}\tilde{\mathbf{V}}_{\bullet J} + \mathbf{A}^{\Gamma}\tilde{\mathbf{V}}_{\bullet J} \tag{B.68}$$

$$= \mathbf{U}_{\bullet J} \tag{B.69}$$

Equation (B.69) is equal to equation (4.12) □

AAA therefore always respects equation (4.12), and it is always necessarily production balanced. It should be noted that the proof holds regardless of the value of $\mathbf{A}^{\Gamma}$.

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 (B.9), which defines PSA of product flows (definition 2), is first multiplied on both sides by the summation vector **e** to transforms the left-hand side of this equation to that of equation (4.12).

$$\mathbf{Z}_{\bullet J \bullet} = \mathbf{A}_{\bullet J \bullet} \widehat{\mathbf{V}_{\bullet J}} = \left(\mathbf{U}_{\bullet J} - \boldsymbol{\Xi}\tilde{\mathbf{V}}_{\bullet J}\right) \bar{\mathbf{E}}'_{\bullet J} \tag{B.70}$$

$$\mathbf{A}_{\bullet J \bullet} \widehat{\mathbf{V}_{\bullet J}} \mathbf{e} = \left(\mathbf{U}_{\bullet J} - \boldsymbol{\Xi}\tilde{\mathbf{V}}_{\bullet J}\right) \bar{\mathbf{E}}'_{\bullet J} \mathbf{e} \tag{B.71}$$

$$\mathbf{A}_{\bullet J \bullet} \mathbf{V}_{\bullet J} = \left(\mathbf{U}_{\bullet J} - \boldsymbol{\Xi}\tilde{\mathbf{V}}_{\bullet J}\right) \bar{\mathbf{E}}'_{\bullet J} \mathbf{e} \tag{B.72}$$

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

$$= \left(\mathbf{U}_{\bullet J} - \boldsymbol{\Xi}\tilde{\mathbf{V}}_{\bullet J}\right) \{1\} \tag{B.73}$$

$$= \mathbf{U}_{\bullet J} - \boldsymbol{\Xi}\tilde{\mathbf{V}}_{\bullet J} \tag{B.74}$$

Except in the trivial case where secondary products displace nothing ($\boldsymbol{\Xi}\tilde{\mathbf{V}}_{\bullet J} = \mathbf{0}$), equation (B.74) will always differ from equation (4.12), and PSA is therefore never production balanced. □

B.4 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 B.1-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 B.1-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 B.1-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.

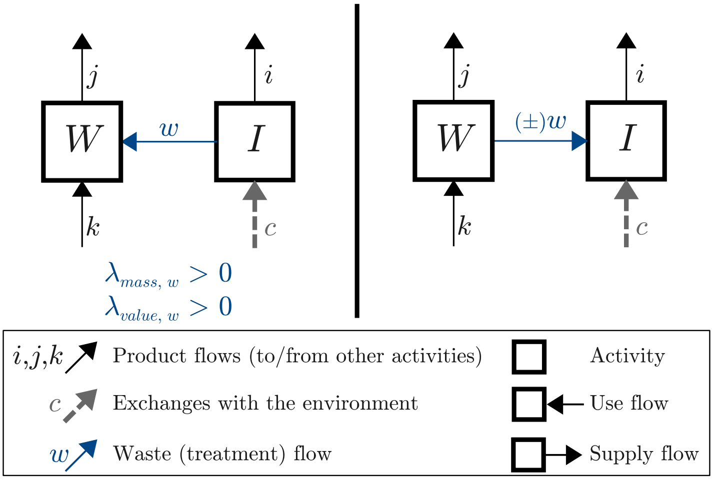

Figure B.1: Two different system representations of waste treatment. Left: waste as byproduct supplied by activity I and used as input by the waste-treating activity W. Right: waste treatment as a useful service supplied by the waste-treating activity W and used by activity I.

Many models follow the logic of figure B.1-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 B.2-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 B.2-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 ($\lambda_{value,w} < 0$).

The opposing signs in the property tables ($\mathbf{\Lambda}$) under the two conventions

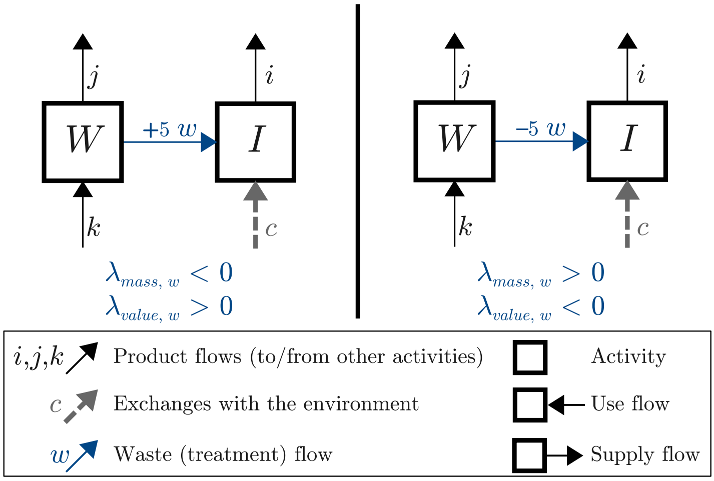

Figure B.2: Two different sign conventions for representing waste treatment as a supply flow from the waste-treating industry, with the corresponding sign change in the property table ($\mathbf{\Lambda}$). Left: a positive supply of waste treatment service. Right: a negative supply of waste material.

of figure B.2 ensures that equation (4.2) (reproduced below) is always directly applicable, regardless of sign conventions, to assess activity balances across all layers.

$$\underbrace{\sum_{i\in\bullet}\lambda_{mi}u_{iJ}+\sum_{c\in\star}\lambda_{mc}g_{cJ}}_{\text{total amount in requirement flows}} = \underbrace{\sum_{i\in\bullet}\lambda_{mi}v_{iJ}}_{\text{total amount in supply flows}} \qquad m\in\triangle, J\in * \tag{rep. 4.2}$$

B.5 Numerical examples: Balanced layers of SUT inventories

Combined heat and power example

Tables B.1 and B.2 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 4.1).

Based on these properties, and following equations (B.1) to (B.3), we separate the mixed-unit flows of the CHP plant (table 4.1) in monetary, energy, and mass layers in tables B.3 to B.5.

$\mathbf{\Lambda}_{\triangle\bullet}$ =

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

Table B.1: Value, energy and carbon contents per unit of the different products of the CHP system.

$\mathbf{\Lambda}_{\triangle\star}$ =

		CO_2 kg^{-1}	O_2 kg^{-1}	waste heat kJ^{-1}	labor $\$^{-1}$
value	\$	0	0	0	1.00
energy	kJ	0	0	1.00	0
carbon	kg	0.273	0	0	0

Table B.2: Value, energy and carbon contents per unit of the different factors of production of the CHP system.

value (\$)	Use flows CHP	Supply flows CHP	Factor requirements CHP	Residual
electricity	0	24		
heat	0	2.1		
coal	10	0		
CO_2			0	
O_2			0	
waste heat			0	
labor			16	
total	10	26	16	0

Table B.3: 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_2			0	
O_2			0	
waste heat			−1042	
labor			0	
total	3474	2432	−1042	0

Table B.4: 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_2			−89	
O_2			0	
waste heat			0	
labor			0	
total	89	0	−89	0

Table B.5: 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 it financial, energy and carbon dimensions.

Cattle example

Tables B.6 and B.7 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 4.2).

Based on these properties, and following equations (B.1) to (B.3), we separate the mixed-unit flows of the cattle farming activities (table 4.2) in monetary, mass and carbon layers (tables B.8 to B.10).

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.

$\Lambda_{\triangle\bullet}$ =

		milk kg^{-1}	cow meat kg^{-1}	steer meat kg^{-1}	feed kg^{-1}
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 B.6: Value, dry mass, and carbon contents per unit of the different products of the cattle example.

$\Lambda_{\triangle\star}$ =

		manure kg^{-1}	respiratory water kg^{-1}	CO_2 kg^{-1}	O_2 kg^{-1}	labor $\$^{-1}$
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 B.7: Value, dry mass and carbon contents per unit of the different factors of production of the cattle example.

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_2					0	0	
O_2					0	0	
labor					1820	320	
total	7350		9170		1820		0
total		1520		1840		320	0

Table B.8: 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_2					-4420	-754	
O_2					1690	385	
labor					0	0	
total	29389		4410		-24978		0
total		6090		304		-5790	0

Table B.9: 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_2					-1210	-206	
O_2					0	0	
labor					0	0	
total	11807		2390		-9420		0
total		2450		189		-2260	0

Table B.10: 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)

B.6 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 ($\mathbf{\Lambda}_{\triangle\bullet}$) 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 (B.1) and (B.2)) 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 ($\mathbf{\Lambda}_{\triangle *\bullet}$), and transforms equations equations (B.1) and (B.2) to equations (B.75) and (B.76).

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

$$u_{iJ}^{m} = \lambda_{mJi} u_{iJ} \quad m \in \triangle, \forall (i, J) \in (\bullet, *) \tag{B.75}$$

$$v_{iJ}^{m} = \lambda_{mJi} v_{iJ} \quad m \in \triangle, \forall (i, J) \in (\bullet, *) \tag{B.76}$$

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 equation (B.77) (instead of equation (4.2)).

$$\sum_{i \in \bullet} \lambda_{mJi} u_{iJ} + \sum_{c \in \star} \lambda_{mc} g_{cJ} = \sum_{j \in \bullet} \lambda_{mJj} v_{jJ} \qquad m \in \triangle, J \in * \tag{B.77}$$

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 (B.78) (instead of equation (4.6)).

$$\sum_{i \in \bullet} \lambda_{mJi} z_{iJj} + \sum_{c \in \star} \lambda_{mc} g_{cJj} = \lambda_{mJj} v_{jJ} \qquad m \in \triangle, J \in *, \forall j \in \bullet \tag{B.78}$$

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 (B.78) and $\mathbf{\Lambda}_{\triangle * \bullet}$. 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, Wood, and Strømman, 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.

Appendix C

Abstract of ongoing work extending the thesis

Stefan Pauliuk, Guillaume Majeau-Bettez, Daniel B. Müller, Edgar G. Hertwich

Abstract

The complexity of data and methods in industrial ecology keeps growing and the demand for comprehensive and interdisciplinary assessments increases. To keep up with this development, the field needs a data infrastructure that allows researchers to annotate, store, retrieve, combine, and exchange data at low cost, without loss of information, and across disciplines and model frameworks.

Prior to the development of data structures and databases, there needs to be consensus about how to describe the common object of study, society's metabolism (SEM). We review the definitions of basic concepts to describe SEM in industrial ecology and related fields like integrated assessment modeling. We find that many definitions are not compatible, implicit, and sometimes lacking.

To resolve the conflicts and inconsistencies with current definitions we propose a hierarchical system of terms and definitions, a practical ontology, for describing objects, their properties, and events in SEM. We propose a typology of object properties and use sets to group objects into a hierarchical, mutually exclusive and collectively exhaustive (H-MECE) classification. This grouping leads to a general definition of stocks. We show that an MECE representation of events necessarily requires two complementary concepts: processes and flows, for which we also propose general definitions based on sets. Using these definitions, we show that the system structure of any interdisciplinary model of SEM can be formulated as directed graph. We propose guidelines for semantic data annotation and database design, which can help to turn the vision of a powerful data infrastructure for SEM research into reality.

List of Acronyms

AAA alternate-activity allocation.

aAAC aggregation-alternate-activity construct.

AAC alternate-activity construct.

ALCA attributional lifecycle assessment.

aPC aggregation-partition construct.

aPSC aggregation-product-substitution construct.

BTC byproduct-technology construct.

CHP combined heat and power.

CLCA consequential lifecycle assessment.

CTC commodity-technology construct.

EEIO environmentally extended input–output analysis.

ESC European-system construct.

IE industrial ecology.

IO input–output analysis.

ITC industry-technology construct.

kg kilogram.

kJ kilojoule.

LCA lifecycle assessment.

LSA lump-sum allocation.

LSC lump-sum construct.

MFA material flow analysis.

MJ megajoule.

mlCLCA *marginal, long-term* consequential lifecycle assessment.

PA partition allocation.

PC partition construct.

PSA product-substitution allocation.

PSC product-substitution construct.

SI supporting information.

StUT supply and *traceable* use table.

SUT supply and use table.

SuUT supply and *untraceable* use table.

tAAC traceable-alternate-activity construct.

tPC traceable-partition construct.

tPSC traceable-product-substitution construct.

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