

A review of methods to trace material flows into final products in dynamic material flow analysis - from industry shipments in physical units to monetary input-output tables (part I)

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Abstract

Dynamic Material Flow Analysis (dMFA) is widely used to model stock-flow dynamics. To appropriately represent material lifetimes, recycling potentials, and service provision, dMFA requires data about the allocation of economy-wide material consumption to different end-use products or sectors, i.e., the different product stocks, in which material consumption accumulates. Previous estimates of this allocation only cover few years, countries, and product groups. Recently, several new methods for estimating end-use product allocation in dMFA were proposed, which so far lack systematic comparison.

We review and systematize five methods for tracing material consumption into end-use products in inflow-driven dMFA and discuss their strengths and limitations. Widely used data on industry shipments in physical units have low spatio-temporal coverage, which limits their applicability across countries and years. Monetary input-output tables (MIOTs) are widely available and their economy-wide coverage makes them a valuable source to approximate material end-uses. We find four distinct MIOT-based methods: consumption-based, waste-input-output MFA (WIO-MFA), Ghosh absorbing Markov chain, and Partial Ghosh. We show that when applied to a given MIOT, the methods' underlying input-output models yield the same results, with exception of the Partial Ghosh method, which involves simplifications. For practical applications, the MIOT system boundary must be aligned to those of dMFA, which involves the removal of service flows, sector (dis)aggregation, and re-defining specific intermediate outputs as final demand. Theoretically, WIO-MFA, applied to a modified MIOT, produces the most accurate results as it excludes massless and waste transactions. In part II of this work, we compare methods empirically and suggest improvements for aligning MIOT-dMFA system boundaries.

1. Introduction

Dynamic Material Flow Analysis (dMFA) is increasingly used for the mass-balanced modelling of socio-economic material stocks and flows. It allows us to study the biophysical basis of society in great detail, including economy-wide, long-term, high process and product resolution stock-flow dynamics (Haberl et al., 2019; Lanau et al., 2019; E. Müller et al., 2014). Such information offers important insights for sustainability science and high-level political goals like the Sustainable Development Goals or the Paris Climate Agreement (Clark & Harley, 2020; Haberl et al., 2019; Pauliuk & Hertwich, 2015).

Research using dMFA can be divided into stock-driven ('bottom-up') and inflow-driven ('top-down') applications, depending on which exogenous data are used to endogenously derive either stocks or flows (Lanau et al., 2019; E. Müller et al., 2014; Wiedenhofer et al., 2019). We herein focus on inflow-driven 'top-down' dMFA, which draws on widely available data for material or product consumption, production and trade, and models the accumulation of stocks from those physical flows into use (Cao, Shen, Løvik, et al., 2017; Liu & Müller, 2013; Pauliuk et al., 2013; Wiedenhofer et al., 2019). A major drawback of the available material flow data is, that they either refer to specific products or report total economy-wide material consumption without distinguishing any products or end-uses (W.-Q. Chen & Graedel, 2015; Krausmann, Schandl, et al., 2017; Lanau et al., 2019). Improving the resolution and coverage of end-use products in inflow-driven dMFA is therefore an important research frontier.

Material end-use products refer to the type of product stocks as which materials accumulate and which are ultimately used to provide functions and services (e.g. living space provided by buildings, mobility enabled by infrastructure and bicycles, cars, trams, etc.; L. Carmona et al., 2017; Haberl et al., 2017; Kalt et al., 2019; Tanikawa et al., 2021). Improved end-use product resolution would enable progress on, for example: more detailed and robust material stock and end-of-life outflow estimates by product through more accurate lifetime assumptions (W.-Q. Chen & Graedel, 2015; Miatto et al., 2017); better comparison with independently derived 'bottom-up' end-use product estimates; expanded systems modelling, addressing product-level operational energy use, emissions, or circularity; and linkage of stocks and flows with material and energy services, practices and ultimately their contributions to human well-being (Haberl et al., 2021).

To model the end-use products that materials accumulate in, inflow-driven dMFA studies draw on various data sources and methodological options (Figure 1). We focus on the first option in Figure 1, which starts with widely available economy-wide data on production, trade and apparent consumption for multiple materials. Because these data are compiled in an aggregate manner, material end-uses need to be added exogenously, using data on 'end-use shares' as proxy. Ideally, information on 'end-use shares' should be on the product rather than sectoral level, e.g. refer to a

residential building instead of the broader construction sector (Chen and Graedel (2015) and W.-Q. Chen (2017)). When available, sector and product-specific data (Figure 1, options 2/3) directly provide end-use information (reviewed in W.-Q. Chen and Graedel (2015)), but these are often scarce or very labor intensive to compile, rendering economy-wide and long-term coverage across many materials, end-uses and countries hardly achievable.¹

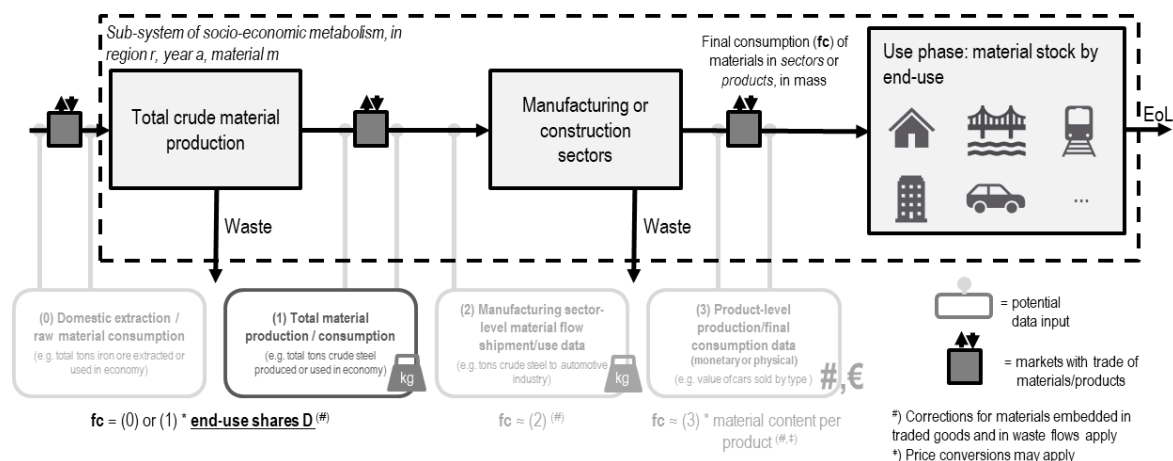


Figure 1: Approaches to utilizing different data sources for inflow-driven dynamic Material Flow Analysis to differentiate material stocks by end-uses at product or sector-level. Material end-uses are defined as the ‘products’ in which materials accumulate, e.g. the steel, aluminum or plastics, accumulated in a bicycle, car, building or infrastructure. Data availability and research scope determine which approach is feasible and useful (W.-Q. Chen & Graedel, 2015; Wiedenhofer et al., 2019). Data sources (0), (1) and (3) are shown with two data entry points (grey lines), as they can be utilized either as material/product production, or at the stage of apparent consumption after trade. This paper focuses on option (1): total material production/consumption multiplied by end-use shares D to distinguish economy-wide material use to end-use products or sectors.

To derive ‘end-use shares’ for economy-wide material flows, several methods and data sources have been used. So far, these methods have not been systematically compared and differing terminology, mathematical notations, and study scopes make it hard to assess their strengths and weaknesses. Additionally, inflow-driven dMFA studies are either increasingly re-using published end-use shares from previous work (e.g. Godoy León et al., 2020; Jarrín Jácome et al., 2021; Klose & Pauliuk, 2021; Wieland et al., 2021), or could gain enhanced insights via the introduction of end-uses to economy-wide dMFA (Streeck et al., 2020; Wiedenhofer et al., 2019). Therefore, it becomes important to comparatively assess end-use estimation methods to inform future work towards building more reliable stock-flow databases across multiple materials, regions and years. Here, we pose the following research questions:

¹ Option 2 are *sector-level* physical flow data (Figure 1, identifier 2), for which end-use is identified by the destination of the destined manufacturing sector or market (e.g. tons crude steel shipped to automotive). Later, we call these ‘industry shipments’ as data source to inform end-use shares. Option 3 are *product-level* flow data (Figure 1, identifier 3) which directly report the sale of specific products in either physical (e.g. number of cars sold) or monetary units (e.g. value of cars sold) for which material use is inferred via material intensities.

- RQ1: Which data sources and methods are used to determine the share of different end-use products in final material consumption ('end-use shares') for inflow-driven dynamic Material Flow Analysis?
- RQ2: What are the rationales and methodological requirements for each method? What are their similarities, differences, strengths and weaknesses regarding consistent system boundaries, end-use resolution, as well as application to many materials, countries and years?

We review and compare five distinct methods for deriving material end-use shares applicable to economy-wide material flows. Data sources include industry shipment data in physical units and monetary input-output tables (MIOTs). We start with an overview of key literature and methods and discuss each method's data requirement, clarity of documentation, system boundaries and potential end-use resolution. We then focus on MIOT-based methods and provide a harmonized description of the procedures, rationales and methodological requirements. In section 3 we conclude on industry shipments vs. MIOTs, and on the different MIOT-based methods, and suggest potential methodological improvements. In part II of this work, we apply the five identified methods, including the suggested improvements, to the data-rich case of the USA, as well as to major regions of a multi-regional input-output model (Streeck et al., in revision_).

2. Reviewing methods to derive end-use shares

To identify all original methods which exogenously derive end-use shares for inflow-driven dMFA, we focused on the English-language peer-reviewed literature as collected by two comprehensive reviews by E. Müller et al. (2014) and Lanau et al. (2019), searched Google Scholar, and applied citation snowballing, with a cut-off in January 2022. We did not aim to systematically cover every single study using these methods, but rather to identify and review pioneering studies and recent prominent applications.

We found five original methods to derive material end-use shares, based on two widely used types of data sources (Table 1). Firstly, many studies used industry shipment data in physical units with typically 3-10 end-uses (17 end-uses as exception, see Table 1). Secondly, we found four methods using MIOTs, resulting in 3-33 end-uses. As noted by Nakamura et al. (2014), we found that various terms were used to describe 'end-use shares', which suggests a lack of harmonized definitions. Terms ranged from 'branching ratio' (Spatari et al., 2005), 'sector split' (D. B. Müller et al., 2006), 'distribution of resources among consumption products' (Duchin & Levine, 2010), 'share of each respective end-use' (Hatayama et al., 2010), 'product-to-use matrix' (Cullen et al., 2012; Wang et al., 2007), 'allocation matrix' (Cullen et al., 2012), 'allocation matrix of materials to final products' (Nakamura et al., 2014), to 'split ratio of end-use sectors' (Cao, Shen, Løvik, et al., 2017). The different terms already point towards specific

1 methods and scopes to derive end-use information. Herein, we consistently used the term ‘end-use
2 shares’ and checked if the methods provide information on actual products or product groups, instead
3 of only broad sectors, such as ‘construction’.

4 Industry shipments were reported by statistical bureaus (e.g. International Steel Statistics Bureau),
5 industry associations (e.g. International Wrought Copper Council), or geological surveys (e.g. USGS
6 mineral commodity summaries; Kelly & Matos, 2014). Terminology and definitions varied, from
7 ‘shipments [...] to manufacturing and fabrication’ (Dahlström et al., 2004), ‘shipments by end-use’ (The
8 Aluminum Association, 2009), ‘apparent use [...] by market’ (PCA, 2016), or ‘supply [...] in the end-use
9 markets’ (CDA, 2020). Herein, we used the summary term ‘industry shipments’. Pioneering studies
10 using end-use shares derived from industry shipments started in the 1990s, focusing on single
11 materials and countries with good data availability (Dahlström et al., 2004; Melo, 1999; Zeltner et al.,
12 1999). Several studies followed that approach and extrapolated end-use shares available for only a
13 few years and single countries, to conduct global, country-level, long-term modelling (Cao, Shen, Løvik,
14 et al., 2017; Glöser et al., 2013; Liu & Müller, 2013; D. B. Müller et al., 2006; Pauliuk et al., 2013). See
15 Table 1, and section 2.1. below for details.

16 The second major approach, containing four original methods, utilized monetary input-output tables
17 (MIOTs) to derive end-use shares (Table 1, and section 2.2. below). MIOTs report monetary flows
18 between economic sectors, which can be used as proxy for physical flows, and are available from
19 national statistics offices (e.g. US BEA, 2021). We identified 12 works that used national-level MIOTs
20 to derive end-use shares, thereof 7 for Japan or the USA, which provide the most detailed MIOTs
21 globally. National MIOTs were also integrated into global, multi-regional input-output models (MRIOs),
22 starting in the 1990s (Inomata & Owen, 2014; Tukker et al., 2018), and some already in the 1970s
23 (Lenzen et al., 2013; Lenzen et al., 2021). To our knowledge, Pauliuk et al. (2017) present the only
24 empirical case using an MRIO with coverage of many countries/regions (25) for dMFA purposes.²

² We also identified one study that uses the physical-monetary hybrid unit input-output database EXIOBASE v3.3 instead of its purely monetary version to allocate an extension of material gross additions to stock (GAS) to industry and final demand sectors (Aguilar-Hernandez et al. (2021)). The extension was constructed via mass-balancing resource use and waste accounts (Merciai and Schmidt (2018)). While the extension allows to determine the GAS used in an industry sectors’ products, it cannot directly discern the products that contain GAS in final demand and therefore cannot comprehensively allocate material use to end-use products (final products). Additionally, the construction of the extensions is difficult to repeat, related quality of waste data problematic (Tisserant et al. (2017)), and mixed-unit tables so far only available for a single year. For these reasons we decided to not list this approach as additional data source to derive end-use shares.

Table 1: Overview of selected studies that use industry shipment data in physical units versus input-output tables in monetary units to derive material end-uses or end-use shares for (inflow-driven) dynamic Material Flow Analysis. Only highly cited or recent studies are listed for industry shipment data.

Physical Industry shipments (prominent examples)	Publication	Material flows	Geographical resol.	Time	End-uses	End-use source	Actual data on end-uses for:
	Zeltner et al. (1999)	Copper	USA	1900-2100	10	Black and Lyman (1990)	1975, 1989
	Melo (1999)	Aluminum	Germany	1970-2012	7	Metallgesellschaft and WBMS as cited in Melo 1999	1985-1995
	Dahlström et al. (2004)	Iron & steel, aluminum	UK	1958/68-2001	6/9	Alfed, WBMS, ISSB	1978-2011, 1958-1997, 1970-2000
	Spatari et al. (2005)	Copper	North America	1900-1999	10	various, e.g. U.S. Bureau of Mines (1941), CDA (1980), literature, expert knowledge	unclear
	D. B. Müller et al. (2006)	Iron	USA	1900-2004	4	AISI (domestic shipment), imports as domestic shares	1941-1999
	Daigo et al. (2007)	Steel	Japan	1980-2000	7	JISF, 1971–2003	~1971-2003
	Kapur et al. (2008)	Cement	USA	1900-2005	7	USGS, PCA	unclear
	Hatayama et al. (2010)	Steel	42 countries	1980-2005	8	40 countries with 1-6 datapoints: JISEA, 1980-2005, USA: AISI, 1960-2006, Japan: JISF, 1971-2000	min. 1980, max. 2005, ~1960-2006, ~1971-2000
	Du and Graedel (2011)	15 rare earths	Global, total**	1995-2007	17	USGS, CSRE (2008), JOGMEC (2007), MERI/J (2003), resolution unclear (~China, Japan, USA)	~2007
	Glöser et al. (2013)	Copper	Global, total	1910-2010	17	ICSG, ICA & Ayres et al. (2003), resolution unclear	1912-2008, 2006-2010
	Pauliuk et al. (2013)	Iron & steel	Global, country-level	1700-2008	4	USA: AISI (1941-2005), UK: ISSB (1979) & Dahlström et al. (2004), India: SERC	2004, 1960-65 & 1970-2000, 1995-1999
	Liu and Müller (2013)	Aluminum	Global, country-level	1900-2010	7	19 countries, various sources, e.g. WBMS, GARC, Alfed	min. 1950, max. 2010
	Cao, Shen, Løvik, et al. (2017)	Cement	Global, country-level	1950-2014	3	Statistics by industry experts, e.g. PCA, Cembureau	min. ~1990, max. 2011
	Geyer et al. (2017)	Plastics	Global, total	1950-2015	7	Various, e.g. PlasticsEurope, ACC, CPMAI, for EU, USA, China, India	2002-2014
	L. G. Carmona et al. (2021)	Steel in transport sector	UK	1960-2015	5	WSA and secondary data made available by Dahlström et al. (2004) and Pauliuk et al. (2019)	1978–2011, see Dahlström et al., unclear

** however, some country-level results in text; ~ indicates that the period is not entirely clear from documentation and that primary sources could not be accessed for checking; ACC = American Chemistry Council; Alfed = The Aluminum Federation; AISI = American Iron and Steel Institute; Cembureau = European Cement Association; CDA = Copper Development Association; CPMAI = Chemical and Petrochemicals Manufacturers' Association India; CSRE = Chinese Society of Rare Earths; GARC = Global Aluminum Recycling Committee; ICA = International Copper Association; ICSG = International Copper Study Group; ISSB = Iron and Steel Statistics Bureau; JISEA = Japan Iron and Steel Exporters' Association; JISF = The Japan Iron and Steel Federation; JOGMEC = Japan Oil, Gas and Metals National Corporation; MERI/J = Metal Economics Research Institute, Japan; PCA = U.S. Portland Cement Association; SERC = Spark Steel & Economy Research; USGS = United States Geological Survey; WBMS = World Bureau of Metal Statistics; WSA = World Steel Association

Monetary Input-Output Tables	Methods	Publication	Material flows	Geography/resolution	Time	End-uses	Source for IO table	Validation?*
	Waste Input-Output Approach to Material Flow Analysis (WIO-MFA)*** (Nakamura et al., 2007; Nakamura & Kondo, 2002; Nakamura & Nakajima, 2005)	Nakamura et al. (2014)	Steel in a car	Exemplary/Japanese data	100 years	5	Japanese 2005	Comparison to industry data [†]
		Pauliuk et al. (2017)	Steel	Global, 25 regions	2015-2100	10	EXIOBASE v2 2007	Sensitivity Analysis
		Yokoi et al. (2018)**	Copper	Japan	2011	16	Japanese 2011	No
		Nakatani et al. (2020)	Plastic containers & packaging	Japan	2015	Packaging (1)	Japanese 2000/05/11/15	No
		Helbig et al. (2022)	7 metal elements	Global, global	1000 years	11	Combine EXIOBASE v3 2011 & Japanese 2005	Comparison to USGS 2011 production data
	WIO-MFA + transaction price extension (see S 1.1)	W.-Q. Chen and Graedel (2015)	Aluminum	USA	1963-2007	motor vehicles (1)	U.S. BEA benchmark	Other estimation methods
		W.-Q. Chen (2017)	Aluminum	USA	1963-2007	33 (>100 products)	1963-2007	
	WIO-MFA + investment matrix (see S 1.1)	Kondo et al. (2012)	17 materials	Japan	2000	10 (in 17 sectors)	Japanese 2000	No
		Yokoi et al. (2022)**	Copper	Japan	1960-2015	16 (in 12 sectors)	Japanese (1960-2015, ~5 yearly)	Comparison to literature
	Consumption-based accounting (CBA)	Hashimoto et al. (2007)	Construction minerals	Japan	1995	24	Japanese 1995	2 nd method
	CBA + investment matrix (see S 1.1)	Dombi (2018)	Total domestic extraction	Hungary	1995-2015/ 2001-2015	EXIOBASE v2 sectors (3 further analyzed)	EXIOBASE v2 2007, EU KLEMS, Hungarian statistics	Comparison to literature (Dombi et al., 2018)
	Ghosh-IO Absorbing Markov Chains (AMC)	Duchin and Levine (2010)	Exemplary 'resource'	exemplary	exemplary	3 exemplary	exemplary	-
		Duchin and Levine (2013)	'Ores'	Global, 3 regions	1990	4	WTMBT 3 regions	-
	Partial Ghosh-Input-Output (IO)	Cao, Shen, Liu, et al. (2017)	Cement	China	1970-2013	3	Eora national table 1970-2013	Statistics in mass 1999/2000
		Arypratama and Pauliuk (2019)	Wood	Indonesia	1961-2016	6	Indonesian 2010	No

[†]based on Nakamura and Nakajima (2005), *of end-use shares, **Yokoi et al. (2018,2022) also apply transaction specific prices (in a price extension), ***multiple other studies apply WIO-MFA, mostly in static studies looking at a single year, e.g. in substance case studies Nakamura et al. (2009), as methodological development (Nakamura et al., 2011; Ohno, Matsubae, et al., 2017) or to track material flows through supply networks (W.-Q. Chen et al., 2016; Jiang et al., 2017; Nuss et al., 2019; Ohno et al., 2016). Schiller et al. (2017) also use MIOTs to estimate the direct material input (DMI) of stock-building materials going to 'capital goods'. To the best of our knowledge, the authors understand capital goods as certain types of equipment not falling under buildings, infrastructure or consumer goods. From the documentation in Schiller et al. (2015) it seems that a classical Leontief model (CBA) was used with one particular category of final demand ('Ausrüstung und sonstige Anlagen' = capital goods) to calculate end-uses. However, certain service flows in the inter-industry/technology matrix were not considered, which resembles aspects of WIO-MFA. Furthermore, the authors did not distinguish DMI output by MIOT sector but rather estimated DMI in capital goods by using the final demand category 'capital goods' as final demand vector, which is somewhat similar to disaggregated investment matrices. As the documentation does not give explicit formulas, we cannot surely allocate the cited work to a specific method. Eora = see Lenzen et al., 2013; AMC = Absorbing Markov Chains; KLEMS = see O'Mahony & Timmer, 2009; EXIOBASE = see Stadler et al., 2018; U.S. BEA = United States of America Bureau of Economic Analysis; WTMBT = World Trade Model with Bilateral Trade (Hammer Strømman & Duchin, 2006); USGS = United States Geological Survey

2.1 Assessing industry shipments as approach to derive end-use shares

At first sight, industry shipments are an attractive data source to derive end-use shares, as numerous studies show (Table 1). However, there are a number of critical limitations to be considered. These start with practical data scarcity and inaccessibility, as many times substantial fees or memberships have to be paid for (e.g. The Aluminum Association, 2009), and continue with poor documentation of data generation, system boundaries and end-use definitions, as well as the usually quite low product resolution. Consequently, when such data are applied, various extrapolations and assumptions are required to compensate for these specific limitations:

Scarce coverage of space and time: industry shipment data require use of large-scale extrapolation. Pauliuk et al. (2013) for instance mapped industry shipment data for India (1995-99), the UK (1960-65/1970-2000) and the USA (2004) to three sets of four end-use shares each (transport, construction, machinery, products) and used the derived shares as time-constant for all countries globally. The authors then optimized international end-use shares by selecting those shares resulting in the best scrap market balance.

Incomplete reporting of material flows: data at times reflect only a share of total economy-wide material use or production, which is not always transparently reported, e.g. the inclusion of imports of materials contained in final products (end-uses) can remain unclear (Pauliuk et al., 2013). To nonetheless achieve coverage of economy-wide material flows, end-use shares derived from shipments are often combined with independent estimates of total apparent consumption or gross additions stocks to derive total material end-use.

Ignoring subsequent trade flows: data can either refer to shipments to manufacturing sectors (mostly for highly manufactured materials, e.g. steel to automotive), in which case trade of final products is not included; or to shipments to final markets for which trade is included (mostly for less manufactured materials, e.g. cement to residential buildings). If large quantities of a material are embedded in traded goods, such as electronics, the computation of apparent final consumption as output + imports – exports is essential (Daniel B. Müller et al., 2011).

Ignoring subsequent waste flows: if waste flows are high, such as in aerospace manufacturing or parts of vehicle manufacturing (Milford et al., 2011), they need to be deducted from the materials consumed by end-use sectors, which is seldomly reported in studies.

Ambiguous system boundaries of end-use categories: certain categories such as ‘construction’ are very broad and might contain only the materials used for construction *products* such as buildings, infrastructure, etc., or refer to *sectoral activities* which can for instance also contain construction

machinery and tools. For example, in the USA the latter is the case for copper end-use statistics, while it is not specified for aluminum in the publicly available data sources (CDA, 2020; Kelly & Matos, 2014; The Aluminum Association, 2009).

Incoherent system boundaries across materials: definitions of end-uses differ across materials, e.g. material use for ‘containers and packaging’ is reported as own category in U.S. aluminum, but included in the category ‘others’ for iron and steel statistics (W.-Q. Chen & Graedel, 2015).

Potential for misclassification: reported industry shipments to end-uses might actually be intermediate products, which are supplied to other end-use products. Ohno, Fukushima, et al. (2017) gave the example of ‘electric and electronics equipment’ being delivered to the ‘automobile industry’ in which case part of the material in the first end-use would be misclassified.

Non-descriptive and unclear end-use definitions: where substantial shipments to sectors such as ‘service centers’ or ‘other’ are reported, for which the actual end-use of the respective shipments remains unclear (Pauliuk et al., 2013; USGS, 2018).

Low end-use resolution: the resolution of shipments’ destination (end-use) is often on a more aggregated sectoral rather than product level (W.-Q. Chen & Graedel, 2015; Ohno, Fukushima, et al., 2017).³

2.2 Assessing monetary input-output tables as approach to derive end-use shares (MIOTs)

MIOTs are derived from the System of National Accounts, thereby following a national, economy-wide system boundary, and report on the sectoral interdependencies of an economy (United Nations, 2009, 2014). They are widely available (e.g. US MIOTs since 1947), cover all economic sectors, including material production, and show medium to high sector resolution which enables detailed modelling of end-use sectors or even products (W.-Q. Chen & Graedel, 2015). However, utilizing MIOTs as proxy for physical flows requires several assumptions, the most prominent being the assumption of homogenous prices for each sector and product group output, and assuming proportionality between monetary and physical flows (Bullard & Herendeen, 1975; Weisz & Duchin, 2006).⁴

³ Some studies take additional steps to improve the quality of industry shipment data or fit additional data to their purpose. For instance, as mentioned above, Pauliuk et al. (2013) optimized limited information on end-use shares against scrap market balances. Spatari et al. (2005) consulted with industry and academic experts. Daigo et al. (2007) and Hatayama et al. (2010) refined end-use resolution by splitting Japanese steel industry shipments for ‘automobiles’, into ‘trucks’ and ‘passenger vehicles’, through the assumption of a 2:1 weight ratio derived from the Japan Automobile Manufacturers Association (2000); or by splitting steel industry shipments for 42 countries to the end-use ‘construction’ into ‘civil engineering’ and ‘buildings’, based on the relationship of the two end-uses with population density for Japanese prefectures.

⁴ In reality, prices vary by seller-buyer relationships, commodity type and geography, the aggregation of which can lead to biased estimation of environmental burden (Jakobs et al. 2021). In MRIOs, currency conversion (see, for example, Stadler et al. (2018)) and relative price levels among countries can lead to additional over- or underestimation of environmental burden, if prices deviate from the homogenous sector average. Furthermore, MIOTs represent a model in which primary data collected through national accounting first need to be compiled into supply-use tables and/or balanced MIOTs, with a number of underlying assumptions and resulting caveats, e.g. limited sector resolution due to reasons of confidentiality (Eurostat (2008); R. E. Miller and Blair (2009); United Nations (2009)). Also the import proportionality assumption for trade flows into individual industrial sectors (Schulte et al. (2021)), and, in the case of single-regional MIOTs, the domestic technology assumption apply (Bouwmeester and Oosterhaven (2013); Lenzen et al. (2004)).

To facilitate the description of the four MIOT-based methods to derive end-use shares, Figure 2 illustrates the schematic of a MIOT. In the equations below, non-italic, non-bold lower-case letters (like 'a') denote vectors and italic, non-bold lower-case letters (like 'c') denote scalars or elements of vectors/matrices. Non-italic, bold uppercase letters (like '**B**') stand for matrices. i and j stand for row and column indices respectively. e stands for appropriate column vector for summation that contains only ones. \wedge denotes diagonalization of a vector.

rows <i>i</i> / columns <i>j</i>	materials (producers)	products (manufacturers)	services (providers)	final demand			Σ
				hh	gov	gfcf	
materials (producers)							total output <i>x</i>
products (manufacturers)	interindustry transaction Z (= intermediate demand)			final demand Y (<i>y</i> = Y <i>e</i>)			
services (providers)							
	value added <i>v</i>						
	total input <i>x</i>						
	environmental extension F						

Figure 2: Schematic input-output table (IOT) with exemplary three sectors corresponding to materials, intermediate or consumer products, and services. The labels for the table's compartments are used in subsequent equations. hh = household consumption, gov = government consumption, gfcf = gross fixed capital formation.

For transparent comparison of the four methods below, we define the end-use share matrix **D** which satisfies the following conditions: $0 \leq d_{ij} \leq 1$, $\sum_j d_{ij} = 1$. **D** can come in two different forms: for **D**_[Method] an element d_{ij} indicates the share of sector output i (e.g., a material; row) contained in the deliveries of sector j (column) to final demand, j therein identified as end-use sector for i (the index [Method] referring to one of the four identified methods in sections 2.2.1-2.2.4: WIO-MFA, CBA, Ghosh-IO AMC, and Partial Ghosh-IO). For **D**_{[Method].res} an element d_{ij} states the share of a natural resource or material (e.g., an ore) listed in the extension table **F** that is allocated to the deliveries of sector j to final demand. In here, we primarily show the calculation of **D**_[Method]. The two forms of **D** can be transformed into each other, using a matrix of allocation factors of environmental indicators in satellite **F** to sectors j (\tilde{S} , for details see supplementary information two (SI 1b)).

2.2.1 The Waste Input-Output Approach to Material Flow Analysis (WIO-MFA)

WIO-MFA was first presented in Nakamura and Nakajima (2005), introducing a mass-balanced material flow analysis perspective to MIOTs. WIO-MFA uses monetary transaction data to approximate the flow of materials into downstream supply chain products at their actual mass. For this purpose, WIO-MFA introduces filter matrices which exclude all monetary inputs that do not

become part of the physical product output of an industrial sector (e.g., automobile production produces automobiles). The mass filter matrix ϕ_{Mass} excludes all monetary inputs that represent non-physical transactions (i.e. service transactions in unmodified MIOTs in Figure 2), and the yield factor matrix Γ deducts part of the monetary transactions as processing waste, the remainder of which $(1-\Gamma)$ defines a waste fraction. Both matrices are multiplied element-wise (Hadamard product \odot) with the technology matrix \mathbf{A} to exclude non-physical transactions and separate waste flows (Equation 1):

$$\tilde{\mathbf{A}} = \mathbf{A} \odot \phi_{\text{Mass}} \odot \Gamma \quad \text{Equation 1}$$

$\tilde{\mathbf{A}}$ is furthermore partitioned according to the degree of the sector output's fabrication. $\tilde{\mathbf{A}}_{m,p}$ is a matrix with only non-zero elements for those transactions where 'materials' i become part of 'products' j (see Figure 2). $\tilde{\mathbf{A}}_{p,p}$ is a matrix with only non-zero elements for 'products' i becoming part of other 'products' j .⁵ This partition is crucial to enforce mass-balance across the WIO-MFA model (Nakamura et al., 2007).

From these two matrices, a material composition matrix \mathbf{C} is calculated (Equation 2). Each coefficient of \mathbf{C} states the concentration of materials in product output to final demand, i.e. the material input i per (monetary) output of product j leaving the inter-industry system towards final demand.

$$\mathbf{C} = \tilde{\mathbf{A}}_{m,p} (\mathbf{I} - \tilde{\mathbf{A}}_{p,p})^{-1} \quad \text{Equation 2}$$

To obtain \mathbf{C} , a calculation similar to obtaining the Leontief inverse is conducted, with the difference that the inter-industry system is cut off towards upstream material sectors. Thus \mathbf{C} does not represent supply chain wide requirements, but a material concentration matrix, in which the exogenous direct material input i to product j ($\tilde{\mathbf{A}}_{m,p}$) is delivered to an industry subsystem ($\tilde{\mathbf{A}}_{p,p}$), which traces product-to-product flows only. \mathbf{C} coefficients can be in either monetary, hybrid or physical units depending on the original units of the partitioned $\tilde{\mathbf{A}}$ matrix. WIO-MFA equation 2 is the analogue of a Leontief price model, just that the material concentration table \mathbf{C} is substituted for the commodity price and exogenous material input for value added (for detailed explanation, see SI 1b).

To calculate the end-use share matrix \mathbf{D}_{WIO} , i.e., the output share of material i (e.g. cement) as product j (e.g. a house) to final demand \mathbf{y} , material composition \mathbf{C} is post-multiplied with final demand $\hat{\mathbf{y}}$ and divided by total output of material i contained in all products j (Equation 3, Nakamura et al., 2014).

$$\mathbf{D}_{\text{WIO}} = (\widehat{\mathbf{C} \mathbf{y}})^{-1} \mathbf{C} \hat{\mathbf{y}} \quad \text{Equation 3}$$

⁵ In how far 'service' sectors can also be classified as 'products' and thus have non-zero sector in/outputs is discussed in section 3.2

Below, we briefly discuss studies that used WIO-MFA to split aggregate material flows to end-uses (see Table 1).

Nakamura et al. (2014) developed the MaTrace model, a combination of dMFA and a linear IO-model, to trace material flows through their lifecycle, amongst others, to end-use products. The authors applied the model to trace ferrous materials in Japanese passenger cars and used the WIO-MFA method together with the Japanese MIOT for the year 2005 to generate an end-use share matrix for refined materials. Pauliuk et al. (2017) extended the model by Nakamura et al. (2014) to MaTrace Global which covers steel flows in the global economy in 25 regions. They used the MRIO database EXIOBASE v2 for the year 2007 in combination with WIO-MFA to calculate the end-use share matrix for all regions. Several other studies used and extended upon the original MaTrace model, including MaTrace-alloy (Nakamura et al., 2017), MaTrace-multi (Helbig et al., 2022), and various case studies (e.g. Godoy León et al., 2020; Jarrín Jácome et al., 2021; Klose & Pauliuk, 2021; Takeyama et al., 2016; not all of them used WIO-MFA to derive end-use shares). Nakamura and Kondo (2018) presented a dynamic model for the Waste-Input-Output method by integrating it with MaTrace-alloy, which also comprised an end-use share matrix.

Yokoi et al. (2018) proposed an approach to distinguish pathways of material flows which accumulate as end-use products in final demand versus in endogenous (inter-industry) sectors, those that are accompanying product flows (e.g. packaging), and those which dissipate within industries. They applied it for WIO-MFA and copper flows in Japan (2011). Additionally, the authors proposed a new approach to distinguish materials in different processing forms for WIO-MFA (2.1.4. in Yokoi et al.), which is similar to the Hypothetical Extraction Method that has been proposed for the Leontief model (Dietzenbacher et al., 2019; Hertwich, 2021) and with similar outcome to a method already introduced in the original WIO-MFA publication by Nakamura et al. (2007). The approaches to distinguish materials in different processing forms are also important for differentiating end-uses and are further elaborated on in section 3.2. The approach of Yokoi et al. (2018) was furthermore applied by Nakatani et al. (2020) who traced the flows of plastic containers and packaging in Japan.⁶

2.2.2 Consumption-based accounting (CBA)

CBA is widely used to estimate so-called environmental footprints (Galli et al., 2012; Wiedmann et al., 2006; Wiedmann & Lenzen, 2018). Here, environmental burdens from socio-economic activity are allocated to categories of final demand, depicting the ‘embodied’ environmental burdens

⁶ Building upon WIO-MFA, also problems other than end-use shares can be tackled, e.g. by relating the flows of materials in MIOTs to a product unit, similar to the functional unit in Life Cycle Assessment (‘UPIOM = unit physical input-output by materials; Nakamura et al. (2011)), using WIO-MFA for linear optimization of vehicle recycling (Ohno, Matsubae, et al. (2017)), and for tracing material flows through supply chain networks (e.g. W.-Q. Chen et al. (2016); Nuss et al. (2019); Ohno et al. (2016)).

accumulating along (global) supply chains. To estimate the flow of embodied environmental burdens per sector, i.e. sector *footprint* \mathbf{F}_s , an environmental extension \mathbf{F} (expressing the absolute environmental burden by sector) is divided by total output \mathbf{x} , and multiplied with the total requirement matrix \mathbf{L} and the vector of final demand \mathbf{y} (Equation 4):

$$\mathbf{F}_s = \mathbf{F} \hat{\mathbf{x}}^{-1} \mathbf{L} \hat{\mathbf{y}} \quad \text{Equation 4}$$

The environmental extension \mathbf{F} can be constructed either as supply or as use-extension (Owen et al., 2017; Wieland et al., 2020). For materials, a supply-extension translates to the supply or extraction of raw materials (e.g. limestone) by different sectors which is distributed to the economy. A use-extension refers to semi-manufactured goods that are used further downstream the supply chain (e.g., cement made from limestone and used in construction), and whose corresponding row in the \mathbf{Z} matrix is replicated as row in the \mathbf{F} matrix. Depending on extension choice, the footprint \mathbf{F}_s has different interpretations: for the supply-extension, element $f_{i,j}$ of matrix \mathbf{F}_s represents the accumulated amount of natural resource i (e.g. limestone or iron ore), while for the use-extension the accumulated amount of material i (e.g. cement or steel), that is required for producing the final demand for sector j .

From equation 4, the end-use share matrix $\mathbf{D}_{\text{CBA_res}}$, can be calculated via Equation 5, with coefficients $d_{i,j}$ representing the share of environmental burden \mathbf{F} that is embodied in final demand of sector j . \mathbf{D}_{CBA} , i.e. the share of sector output i that is embodied in final demand of sector output j , can be calculated via Equation 6. Compared to WIO-MFA, \mathbf{D}_{CBA} does not solely contain end-use shares for ‘materials’ but also for all other MIOT sectors (potentially including both ‘products’ and ‘services’ in the sense of Figure 2).

$$\mathbf{D}_{\text{CBA_res}} = (\mathbf{F}_s \mathbf{e})^{-1} \mathbf{F}_s \quad \text{Equation 5}$$

$$\mathbf{D}_{\text{CBA}} = (\mathbf{L} \mathbf{y})^{-1} \mathbf{L} \hat{\mathbf{y}} \quad \text{Equation 6}$$

For CBA, the end-use shares \mathbf{d}_{CBA} calculated for sector output j include all upstream direct and indirect (raw) material, product and service inputs, also those that might not become physical part of the output to final demand j . These include both, monetary transactions that have been assigned physical material via the proportionality assumption of monetary and physical flows, but are most likely not of physical nature (i.e. services), and monetary transactions (or fractions of those) that are physical, but refer to waste flows which do not become part of end-use products (e.g. new scrap during manufacturing). Thus, the end-use share for a physical product j represents embodied material

use, different from the actual material mass of the physical product like for WIO-MFA. In effect, these properties lead to misclassifications of material end-uses.^{7,8}

Hashimoto et al. (2007) used CBA with a type of use-extension for a Japanese MIOT for 1995 to allocate the Japanese domestic production of construction minerals (cement, sand and gravel, crushed stone) to 24 material end-uses. The authors compared end-use results with a second estimation method, which they deemed more reliable than CBA. Also Dombi (2018) used CBA with supply-extension to distribute total domestic extraction to end-uses (for details see S 1.2).

2.2.3 Ghosh Input-Output Absorbing Markov Chains (Ghosh-IO AMC)

Duchin and Levine (2010) proposed an input-output notation to Absorbing Markov Chains (AMC) and introduced a framework to trace the number of times a resource flows through the industrial network ('resource-specific networks'). Duchin and Levine (2013) extended this approach to only track those flows going to a single final product ('resource end-use networks'), which can be used to calculate end-use shares.

The AMCs' central element is the so called *transition matrix*, i.e. documenting the probability of transitioning between two previously defined states, e.g. the transformation of a resource into an intermediate product. Duchin and Levine (2010) proposed that for IOA, the transition coefficients represent the proportion of a resource transitioning to a product. This definition in IOA terms can be understood as the *direct output coefficients matrix* $\mathbf{B} = \hat{\mathbf{x}}^{-1}\mathbf{Z}$.

Similar to WIO-MFA, Duchin and Levine (2010) introduced supply-chain directionality according to the degree of a product's fabrication into their model. They achieved this by partitioning the matrix \mathbf{Z} 's sectors into resources (which we here call materials m to align with WIO-MFA notation) and products p where only the two right-sided quadrants are non-zero (Equation 7). The *direct output coefficients matrix* \mathbf{Q} denotes that materials can become part of intermediate products ($\mathbf{Z}_{m,p}$) and the latter can become part of the same or other intermediate products ($\mathbf{Z}_{p,p}$), while excluding other directionalities:

⁷ An example would be monetary transactions recorded between 'physical materials' (e.g. cement) to a non-physical service (e.g. government services), which in turn delivers a service transaction to another physical end-use product (e.g. a house). Through the physical extension in CBA, the service-input 'government services' to the 'house' would then be associated with a physical 'cement' flow and thus add to the footprint of the 'house', although the service-transaction does not contain a physical flow in reality.

⁸ As extension to CBA, the endogenization of capital flows into footprints of final consumption, i.e. the treatment of capital goods not as final demand but as intermediate inputs to production, has been discussed in the literature and applied for materials (T. R. Miller et al. (2019); C.-J. H. Södersten et al. (2018)). This method was termed 'capital-augmented material footprints' (C.-J. Södersten et al. (2020)) and allocates resource use embodied in capital goods used by industry (e.g. machinery and buildings), to the respective industry output to final consumption. The system boundaries of this method are not suited to determine material end-uses in actual mass, because in addition to the embodied perspective of CBA, it allocates materials embodied in the endogenized capital goods downstream to goods and services for final consumption (i.e. gross fixed capital formation 'gfcf' allocated to consumption of households 'hh' and government 'gov' in Figure 2).

$$\mathbf{Q} = \hat{\mathbf{x}}^{-1} \begin{pmatrix} 0 & \mathbf{Z}_{m,p} \\ 0 & \mathbf{Z}_{p,p} \end{pmatrix} \quad \text{Equation 7}$$

Additionally to directionality, the IO-AMC defines absorbing states which once entered, ‘capture’ associated flows (‘consumption goods’). Duchin and Levine (2010) defined these states as matrix \mathbf{R} (Equation 8) which gives the share of final demand y in total gross production of products (p). Materials (m) are assumed to not directly transition to final demand, but first become part of intermediate products (thus zero). If transactions in original \mathbf{Z} and y are deleted, \mathbf{x} requires recalculation before calculating \mathbf{Q} and \mathbf{R} .

$$\mathbf{R} = \hat{\mathbf{x}}_p^{-1} \hat{\mathbf{y}}_p \quad \text{Equation 8}$$

To trace flows over the whole supply chain, the inverse of \mathbf{Q} is calculated (which is similar to the Ghosh inverse \mathbf{G}). Multiplying this inverse with \mathbf{R} yields the distribution of sector outputs i to final demand as product j (Equation 9). Like for CBA, \mathbf{D}_{AMC} includes shares for all sectors defined in the MIOT used.

$$\mathbf{D}_{\text{AMC}} = (\mathbf{I} - \mathbf{Q})^{-1} \mathbf{R} \quad \text{Equation 9}$$

Duchin and Levine (2013) applied the framework to the world trade model with bilateral trade (Hammer Strømman & Duchin, 2006), tracing the use of ores to four end-uses. Besides this study, we are not aware of any other application of this framework.

In the distinction of materials, intermediate and consumption products, the proposed Ghosh-IO AMC corresponds closely to WIO-MFA. In contrast, like for CBA, Ghosh-IO AMC does not remove waste flows and, depending on the definition of sectors, might also include services (which would translate to a consumption-based footprint perspective).

2.2.4 Partial Ghosh Input-Output (IO)

In their work on stocks and flows of cement and wood, Cao, Shen, Liu, et al. (2017) and Aryapratama and Pauliuk (2019) used procedures that are similar to the first steps of the Ghosh-IO AMC in order to derive end-use shares \mathbf{D} . However, the authors used a modified version of the *direct output coefficients matrix* \mathbf{B} , which is why we termed their approach *Partial Ghosh-IO*. While in the Ghosh model, \mathbf{B} is calculated with gross output \mathbf{x} , the two studies only used the intermediate output, i.e. summing over the row elements in the inter-industry transaction matrix \mathbf{Z} ($\mathbf{x}_{\text{INTER}}$). Hereafter, this matrix is termed $\mathbf{B}_{\text{INTER}}$ in which the resulting coefficients give the direct allocation of a sectors output to all inter-industry sectors (Equation 10). Thus, the summation of elements in rows adds up to one.

$$\mathbf{B}_{\text{INTER}} = \hat{\mathbf{x}}_{\text{INTER}}^{-1} \mathbf{Z} \quad \text{Equation 10}$$

To calculate the distribution over supply chain steps, Cao, Shen, Liu, et al. (2017) and Aryapratama and Pauliuk (2019) defined sectors as either intermediate or end-use: intermediate sectors deliver 100% of their output further downstream the supply chain to other intermediate or end-use sectors; end-use sectors only receive inputs from intermediate sectors, which are assumed to be delivered in full to final demand (the absorbing state in AMC terms). Materials (m), like defined in the Ghosh-IO AMC, are part of intermediate products (p) in this method. Material flows are traced manually to several downstream steps in the supply chain until they reach end-use. Here, we formalized the procedure using matrix notation: analogous to Equation 7, we first partitioned $\mathbf{B}_{\text{INTER}}$ into $\mathbf{Q}_{\text{INTER}}$ with the individual rows/columns reflecting intermediate (p) and end-use products (c), respectively. Only flows of intermediates (to intermediate use and end-use) were non-zero (Equation 11):

$$\mathbf{Q}_{\text{INTER}} = \begin{matrix} \mathbf{B}_{\text{INTER}_{p,p}} & \mathbf{B}_{\text{INTER}_{p,c}} \\ 0 & 0 \end{matrix} \quad \text{Equation 11}$$

Second, we computed the Ghosh-inverse of $\mathbf{Q}_{\text{INTER}}$ i.e. $\mathbf{D}_{\text{P-GHOSH}}$ where the top right quadrant $\mathbf{D}_{\text{P-GHOSH}_{p,c}}$ contained the end-use share matrix, reflecting the flow of intermediates (p , for this method including materials m) to end-uses (c , Equation 12):

$$\begin{matrix} \mathbf{D}_{\text{P-GHOSH}_{p,p}} & \mathbf{D}_{\text{P-GHOSH}_{p,c}} \\ 0 & 0 \end{matrix} = (\mathbf{I} - \mathbf{Q}_{\text{INTER}})^{-1} \quad \text{Equation 12}$$

Cao, Shen, Liu, et al. (2017) applied this method to the Chinese inter-industry transaction matrices for 1970-2013 from the global MRIO Eora (Lenzen et al., 2013). The authors distributed the apparent consumption of cement according to the derived end-use shares along up to two intermediate supply-chain steps, before arriving at end-use, and deducted 1.5% material losses during transportation. Out of a total of 122 sectors in the Eora MIOTs, the authors aggregated 113 sectors to three end-use sectors (agriculture, buildings, infrastructure). For the years 1999 & 2000, the authors found a close fit between the derived cement use in buildings and statistics from the China Building Industry Yearbook (NBSC, 2002).

Aryapratama and Pauliuk (2019) used the inter-industry matrix of the Indonesian national MIOT for 2010 and distributed the apparent consumption of wood/roundwood, pulp, sawnwood and wood-based panels to six end-use categories (paper & packaging, furniture, buildings, infrastructure, agriculture, others). Export of end-use products was only considered for furniture, as for other end-uses, monetary export flows reported in the MIOT were small compared to final demand.

In addition to the four methods described here, we found dMFA studies that applied extra modifications to MIOTs (i.e. use of investment matrices & transaction specific prices). These are described in SI 1a.

3. Discussion

3.1 Using industry shipment and monetary input-output data for global end-use shares

If available at sufficient detail and suitable sectoral resolution, end-use shares derived from industry shipments in physical units are superior to monetary data as they resemble more closely the biophysical flows modeled in dMFA. In practice, however, industry shipment data are scarce in terms of tempo-spatial coverage, usually yield low end-use resolution, and are prone to misclassification of end-use categories and partial system coverage (see section 2.1). For individual countries with good data availability, industry shipments are well suited to differentiate end-uses. For the systematic compilation of end-use shares for economy-wide material use across multiple materials, years, and countries, available data are limited and their potential largely exploited (Table 1).

Therefore, monetary input-output tables (MIOTs) represent a complementary data source due to their global availability, often relatively high resolution of countries and sectors, and their economy-wide coverage. The few studies that compared end-uses derived from MIOTs with other methods for a handful of years and three countries, mostly found good agreement (Cao, Shen, Liu, et al., 2017; W.-Q. Chen, 2017; W.-Q. Chen & Graedel, 2015; Hashimoto et al., 2007). However, the assumptions that apply to the environmental extension of MIOTs, as described in section 2.2, need to be considered when evaluating results. Additionally, the following specifics of MIOTs call for further investigation:

Firstly, the quality and differentiation of end-use data relies on the quality of specific MIOTs, for both the number of sectors and the way these are defined. While previous work mostly utilized high-resolution country-level MIOTs (i.e. USA and Japan, see Table 1), such detailed MIOTs are hardly available for other countries. For MRIOs, substantial efforts have been made to improve sectoral resolution, especially in the primary extractive industries. This influences two properties which can strongly impact results: first, how environmental extensions can be matched to MIOT sectors and which assumptions are required to allocate materials or energy, which are usually reported with system boundaries different from those of MIOT sectors (Inomata & Owen, 2014; Owen et al., 2017; Tukker et al., 2018; Wieland et al., 2020); and second, the accuracy of downstream tracing (i.e. the more disaggregated the supply-chain of materials, the better suited are assumed average material intensities and output structure, leading to more accurate tracing (Lenzen, 2011)).⁹ For end-use

⁹ Consider, for example, the flows of indium and iron through the MIOT. Indium quickly changes form and becomes part of electronics and other manufactured goods, so that the MIOT has no accurate data on the whereabouts of indium, but uses proxy data on the whereabouts of electronics to trace the estimate use

sectors, however, the resolution is often quite low. For instance, ‘construction’ is responsible for the lions share of global material use, but represents only one sector in many MRIOs, which is problematic if one wants to distinguish between residential buildings, infrastructure, etc. (Krausmann, Wiedenhofer, et al., 2017; Lenzen et al., 2013; Stadler et al., 2018). Only the recently published GLORIA MRIO at least distinguishes ‘all buildings’ and civil engineering (Lenzen et al., 2021). Also at high MIOT product resolution, some end-use product stocks can show large differences to physical accounts (W.-Q. Chen, 2017), which merits the question how reliable the interpretation of results for individual MIOT sectors is.¹⁰ In part II of this review, we empirically investigate these issues (Streeck et al., in revision_).

Secondly, the system boundaries of MIOTs differ from those of dMFA. On an aggregate level, MIOT transactions are similar to dMFA flows, except for that they also contain waste (Figure 3: 1) and service flows (Figure 3: 2). For instance, final demand \mathbf{Y} is similar to the gross additions to stock (GAS) in dMFA, while including demand for services and waste treatment.

On a fine-grained level, dMFA is interested in tracing material flows into use either as a *product* (e.g. steel use in a building), an *activity* (e.g. steel use in health care), or a *product* within an *activity* (e.g. steel in buildings used in health care). In their default configuration, MIOTs take a *product* perspective by tracking materials into products for final use when these enter final demand (United Nations, 2009). The physical use of MIOT *products* in different *activities* cannot be identified with standard input-output analysis but would require augmentation with further data.¹¹ Rather, the in-use stock requirements for *activities* are assumed to be provided by industrial assets and other durable products in the form of services.

shares of indium. For iron, which mostly ends up in steel, the situation is different, since steel is a separate product category in most MIOTs (sometimes even several downstream processing forms of iron distinguished), and the table data thus more accurately reflects whereabouts and average material intensities.

¹⁰ Additionally, while national MIOTs follow internationally harmonized principles (United Nations (2009)), national specificities apply, regarding national statistical efforts and procedures in data gathering and aggregation as well as estimation procedures, nationally specific decisions for sectoral (dis)aggregation (e.g. confidentiality and/or national interests), or issues of ownership (e.g. state-owned housing vs privately-owned buildings means that substantial final demand is either part of households, or government expenditures). Available MRIOs try to reconcile national definitions, data gaps, as well as often mismatching and conflicting data using various techniques (Tukker et al. (2018)).

¹¹ To identify the physical material flows into *activities*, the material deliveries to these accounts would require re-routing to using industries via the use of capital flow/investment matrices (Lenzen and Treloar (2005); Pauliuk et al. (2015)), which could happen in a particular configuration of capital-augmented material flow tracing (in contrast to capital-augmented footprints; C.-J. Södersten et al. (2020)).

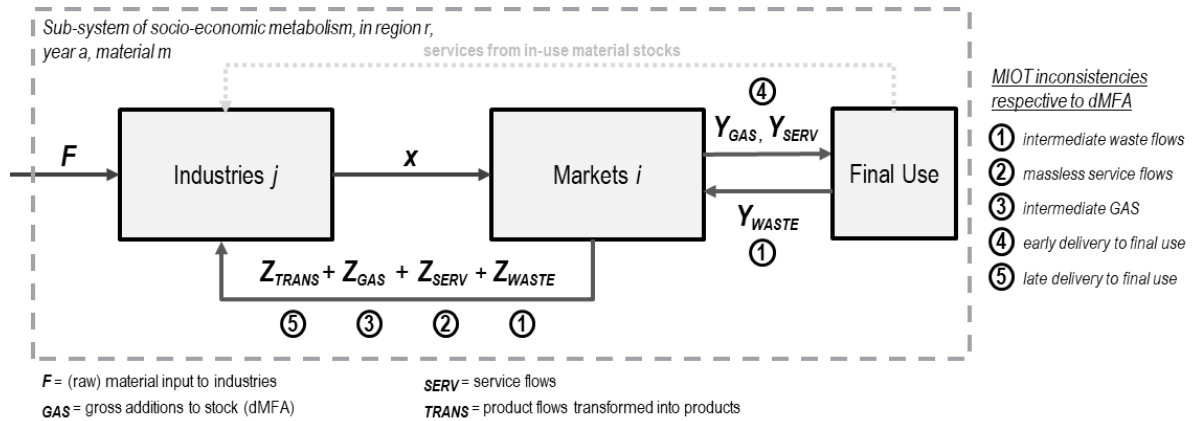


Figure 3: Schematic representation of monetary input-output table (MIOT) structure and identified points for potential inconsistencies with system boundaries of dynamic Material Flow Analysis when determining end-use as sector output deliveries from the inter-industry system to final demand/use. GAS = gross additions to stock, SERV = service flows, TRANS = product flows transformed into products.

Small discrepancies exist that complicate matching MIOTs to dMFA system boundaries: intermediate demand refers to the transactions that are input to an industry and are either ‘entirely used up’ or ‘transformed’ and become part of the industry’s output (United Nations, 2009: 6.224, 10.35). However, it also includes smaller maintenance, repairs and tools (United Nations, 2009: 6.225, 6.226). Therefore, when using MIOTs, we cannot be sure exactly which part of the flow remains as gross additions to stock (GAS) within the receiving industry activity as e.g. small repairs or hand tools, and which part is contained in the industries product output (Figure 3: 3).¹²

Other than that exception, both MIOTs and dMFA can have an aligned system definition regarding products when the definitions of product groups match, or if the dMFA products are simply a (partial) aggregation of the MIOT products. If a MIOT-product is delivered to final demand and matches the dMFA-product definition, the dMFA-coherent tracing of material flows into products with MIOTs is feasible. However, two cases of mismatch can occur:

- (1) The material flow in MIOTs is routed into the ‘wrong’ product group as it is delivered to final demand early and does not reach the matching dMFA product/sector (Figure 3: 4): for example, a boiler is delivered to final demand as investment (GFCF) and is thus identified as end-use category ‘machinery’. In contrast, in dMFA, we might want to account the boiler as part of the end-use ‘buildings’. However, the flows to trace the boiler from GFCF into ‘buildings’ are not present in standard MIOTs.
- (2) The material flow in MIOTs is propagated too far downstream and skips the matching dMFA product/sector classification (Figure 3: 5): for example when ‘construction machinery’ is an

¹² Following SNA definitions, one would however expect that the majority of flows in intermediate demand are either used up or transformed and contained in a sectors output. Yokoi et al. (2018) documented an attempt to tackle this problem (see section 2.2): by referring to the Japanese MIOT definition of fixed capital assets in final demand (unit price >100,000 Yen and durability of over one year), the authors used the purchaser unit prices for products to identify the transactions not meeting these criteria and labeled them as accumulating within sectors of intermediate demand. For accumulations in intermediate demand, one cannot always be sure in which product the flow ends up, thus corresponding to an activity perspective (e.g. cement as GAS to agricultural industry).

intermediate input to ‘building construction’, the MIOT approach would identify the latter sector as end-use category. This categorization of ‘construction machinery’ corresponds rather to an *activity* (construction) than a *product* (machinery). For the intended accounting as product, the items would need to be delivered to final instead of intermediate demand.

Some products, for example packaging, are always identified as MIOT intermediate use and thus systematically propagated too far downstream compared to dmFA categories. These products will never show up as distinct end-use in any MIOT-based method that defines end-use according to the product transactions to final demand (also see section 3.2, point (3)).

For detailed MIOTs with suitable product labels (e.g. ‘boiler’), these issues can in theory be identified by tracing individual supply-chain steps. However, this gets more difficult, the more aggregated the product groups (e.g. ‘heating equipment’ can be both an input to a building or purchase by consumer).

Additional problems emerge as MIOTs follow an economic and not a biophysical logic. For instance, product transactions are accounted for in either intermediate or final demand, depending on the type of use: if a product is purchased for final consumption or investment, the product transaction is reported in final demand and thus classified as end-use product (e.g. a boiler purchased by a private household); if a product is purchased by a third party to install the product in mandate of a final consumer/investor, the transaction might be accounted for in intermediate demand (e.g. a boiler purchased by a plumber (part of a service sector) for installation in the private household (E. Kolleritsch & Statistik Austria, personal communication, June 30, 2022)). In the second case, the end-use of materials in the boiler would be classified according to the label of the respective plumbing service sector. Additionally, ownership changes of already existing fixed assets might be accounted for in GFCF, which were produced from material consumption in an earlier and not the present year (United Nations, 2009: 10.38/39).

In summary, while the System of National Accounts provides an overarching systematic, in practice, the concrete implementation of the mentioned points in national accounting might vary substantially (e.g. United Nations, 2009: 1.51/53). This might introduce unsystematic differences into MIOTs, which complicates the formulation of a generalized matching to dmFA system boundaries, leaving some remaining mismatches untackled by the MIOT-based methods reviewed herein.

3.2 Comparison of MIOT-based methods and their strengths and weaknesses

The four methods to distinguish material end-use shares from MIOTs presented in section 2.2 are different in two ways: they make use of different input-output (IO) models, and they apply different kinds of data manipulation to original MIOTs. These differences raise the question of how strongly these two elements influence end-use results. Table 2 summarizes differences between methods and

the following text elaborates on these (roman letters in the text below refer to row identifiers in Table 2).

Table 2: MIOT-based methods for deriving the end-use share matrix D and their characteristics. For literature studies that apply the four methods please see Table 1 and section 2.2. Dark orange x = criterion applies, light orange p = criterion can potentially be applied, but few studies do (see Table 1).

Attributes/method	WIO-MFA	CBA	Ghosh-IO AMC	Partial Ghosh-IO
(I) Use intermediate demand only (Z)				yes
(II) Use intermediate & final demand (Z,Y)	yes	yes	yes	
(III) Materials external to industry supply chain wide tracing* (no p->m flows)⊗	yes		yes	
(IV) Yield filter**	yes			
(V) Mass filter (≠ non-physical)***	yes			
(VI) Exclude ‘materials’ from final demand*** (sector demand set to zero)			yes	yes
(VII) Use vs. supply-extension*	potentially			
(VIII) Transaction specific prices**	potentially			
(IX) Investment matrix***	potentially			
Underlying input-output model†	Leontief price	Leontief quantity	Ghosh quantity + market balance	Ghosh quantity (partially)
Advantages	<ul style="list-style-type: none">• Mass-balanced MFA logic excluding waste and service flows	<ul style="list-style-type: none">• Time-efficient application (no filter matrices required)	<ul style="list-style-type: none">• Introduction of processing degrees	<ul style="list-style-type: none">• Applicable with little IOA knowledge• Products that are intermediate demand in MIOTs can easily be defined as end-use (e.g. packaging)
	<ul style="list-style-type: none">• Simultaneous sector output to both intermediate and final demand• Convenient handling of imports/export in final demand			
Challenges/disadvantages	<ul style="list-style-type: none">• Assumptions for processing degrees and filters (deleting data)• Complexity as entry threshold for MFA practitioners	<ul style="list-style-type: none">• Footprints (‘embodied perspective’) = misallocations	<ul style="list-style-type: none">• Dependent on definition of ‘products’: footprints (‘embodied perspective’) = misallocations	<ul style="list-style-type: none">• Only uses information in inter-industry transaction matrix• Assumptions on cutting the supply-chain by defining intermediate and end-use products• Imports/export not automatically considered
	<ul style="list-style-type: none">• ‘Functionality’ of product outputs that in MFA logic are end-uses (=final demand), but are intermediate demand in MIOTs is lost (e.g. packaging)			
	<ul style="list-style-type: none">• MIOT system boundaries of intermediate demand challenge application to material flows (section 3.1)• Assumptions on price homogeneity & physical-monetary proportionality (if no transaction specific prices)• Domestic technology assumption for single-region MIOTs			

Comments: can also be considered as change of *the input-side system boundaries of the industry system (partitioning the A matrix for WIO-MFA and Ghosh-IO AMC, or using different kind of satellites assigned to different MIOT sectors), **the inter-industry system boundaries, *** the output-side system boundaries (either cut off where physical flows end and service flows start, or applying different vectors of final demand); †see supplementary information 1b for further explanation; ⊗ no reverse flows of products (p) to materials (m) – see section 2.2.1 for details

The most prominent distinction of the four methods can be drawn between CBA, WIO-MFA and Ghosh-IO AMC, which use full input-output models corresponding to either the input-output market or industry balance; and the Partial Ghosh-IO which only uses the MIOT inter-industry matrix Z and represents a partial IO-model not fulfilling any IO-balance (see I-II Table 2; SI 1b). Within the first group, the individual methods of CBA, WIO-MFA and Ghosh-IO AMC in turn, correspond to fundamentally different underlying IO-models: the Leontief quantity (CBA), Leontief price (WIO-MFA) and Ghosh quantity (Ghosh-IO AMC) model (for detailed explanation see SI 1b). Despite these different models, the three methods yield the exact same end-use share matrix D , if applied at scale, i.e. to fully

quantified MIOT systems, and with no or equivalent manipulation of MIOT data as specified in Table 2 III-IX (for proof see sections 6 and 7 of SI 1b). Discrepancies between the end-use shares **D** of CBA, WIO-MFA and Ghosh-IO AMC can thus be attributed solely to the differences in manipulation of MIOT data, like the mass-filtering of flows.

Below, we discuss the differences and similarities that arise from (non)-manipulation of monetary data for all four MIOT-based methods identified from literature:

(1) First, the reviewed methods apply different definitions of material end-uses (or in AMC language: the absorbing state). While for Partial Ghosh-IO the practitioner defines the absorbing state by selecting products in the inter-industry matrix (Aryapratama & Pauliuk, 2019; Cao, Shen, Liu, et al., 2017), all other methods refer to the final demand matrix/vector from MIOTs.

For Partial Ghosh-IO, the transition of intermediate products to an absorbing, end-use state is not dependent on values in the matrix of final demand, but selected products in intermediate demand are assumed to directly reflect end-use and 100% of related materials being delivered to this category (see section 2.2). For MIOTs with high product resolution, products might be identifiable as either intermediate or end-use. However, most often MIOT products represent a product mix, which is supplied to both intermediate and final demand (e.g. electric machinery as input to the automotive industry and investment in a fixed asset). Thus, if misclassification occurs, the supply-chain is either artificially elongated (misclassified as intermediate use) and all material distributed downstream, or cut off (misclassified as end-use) and all material considered as end-use. Thereby, this method is particularly sensitive to a practitioner's decision.¹³

All remaining methods make use of final demand data to define the share of the absorbing states in total industry output. In MIOTs, final demand consists of different categories, including 'consumption' and 'gross fixed capital formation' (GFCF, see Figure 2). For GFCF, the "*asset boundary for fixed assets consists of goods and services that are used in production for more than one year*" (United Nations, 2009: 10.33) and thus matches with the definition of material stocks in dMFA research (Fischer-Kowalski et al., 2011). Expenditures on consumer durables (e.g. washing machines and small tools) are accounted for under consumption expenditures. Some expenditure on goods (e.g., a car) might be defined as either GFCF or another category of final demand, depending on whether they are for private or commercial use (United Nations, 2009: 10.34, 10.35, 10.41).

¹³ In support of their categorization of intermediate and end-use products, Aryapratama and Pauliuk ((2019)) take the ratio of intermediate versus final demand, thus somewhat reducing this bias. The exclusion of final demand in Partial Ghosh-IO also impedes the method-immanent inclusion of imports and exports of final end-use products (which are reported in the final demand matrix).

Different studies use varying categories of final demand as absorbing state, the use of a particular sort of these data not tied to one particular of the methods reviewed herein. Most of the reviewed studies use the sum of all final demand accounts from MIOTs as absorbing state, while some only use data on GFCF, sometimes from sources other than MIOTs (W.-Q. Chen, 2017; W.-Q. Chen & Graedel, 2015). Kondo et al. (2012) and Yokoi et al. (2022) use a breakdown of GFCF into the ‘investment matrix’ (Pauliuk et al., 2015), which not only distinguishes investments into products but also the industry sector where the investment occurs, thus allowing conclusion about which industry uses the end-use products (Table 2 IX, see SI 1a).¹⁴ Additionally, GFCF endogenization was discussed in literature, however, it is unsuited for calculation of end-use shares (see footnote 8 and section 2.2.2).

From above definitions, we see that only using GFCF neglects material stocks accumulating in ‘consumption’ of households and governments (might depend on national GFCF definitions). In summary, we propose that, when determining the end-uses within a region, all final demand accounts referring to use within the respective region and time should be used, i.e. including accounts for both ‘consumption’ and GFCF, while excluding accounts for exports and inventory changes.¹⁵

(2) Second, some methods calculate embodied materials (‘raw material equivalents’ or ‘material footprints’), while others aim to track material flows at their actual mass by following dMFA principles. Consumption-based accounting (CBA) calculates material footprints by assigning material use to MIOT-sectors and linking them to final demand through monetary inter-sectoral transactions that are partially also non-physical and waste (e.g. service-flows and processing waste, see section 2.2). When accounting for material end-use shares, however, one is interested in a final product’s actual mass. Thus, following a mass-balanced MFA perspective like WIO-MFA, through locating resources/materials outside of the industry system (III), as well as the introduction of mass and yield filters (IV-V), is superior to CBA.¹⁶ This applies in particular, if supply-extensions of raw materials are used instead of use-extensions of engineering materials (VII; Owen et al., 2017; Wieland et al., 2020). The two Ghosh model methods can calculate either footprints or actual mass, depending on the definition of materials and products (e.g. service

¹⁴ However, despite few data sources like EU KLEMS (O’Mahony and Timmer (2009)), data on investment matrices is scarce, low in resolution, and lacking details on investments for buildup & maintenance vs. demolition (Pauliuk et al. (2015); C.-J. Södersten et al. (2020)).

¹⁵ Also the use of all compartments of MIOT final demand might cause problems: Nakamura et al. (2014) describe that through the vector of exports and inventory changes, also intermediate products are reported in final demand. The authors use a type of output coefficient matrix of the Ghosh model (similar to equation 10) to allocate deliveries of intermediate to final products in a secondary calculation. To avoid the same problem for ‘materials’, the Ghosh-IO AMC method prohibits flows of materials to final demand by partitioning the latter (VI, Equation 7).

¹⁶ Nakamura et al. (2009) compared the material mass of iron, aluminum and polyvinyl chloride in a Japanese passenger car for the year 2000 via CBA and WIO-MFA with data from JAMA (2003) for 1997/2001. They found that CBA overestimated material content by 18-47% while WIO-MFA was fairly close to JAMA data (2-6% deviation).

transactions included as ‘products’ or not) and application of filter matrices (not mentioned in the original studies).

However, also the methods that aim to track actual mass come with their own challenges in manipulating MIOT data (see Equations 2, 7 and 11). When defining different degrees of fabrication, e.g. materials, intermediate and consumption products, as well as filter matrices that exclude non-physical and waste flows (WIO-MFA), monetary transactions need to be deleted from the MIOT, which influences the resulting end-use shares. The definition of filter matrices requires expert knowledge and is to some degree up to assumptions (e.g. when is a transaction non-physical). Specifically, the decision on excluding transactions with service sectors (see compartment in Figure 2), i.e., whether to only filter service sector outputs (non-physical assumption likely) or also service-sector inputs (non-physical assumption precarious), can give wrong results, for example, when large material flows to service sectors like repair are ignored (Streeck et al., in revision_). Additionally, filter matrix compilation can be tedious and filters are hardly available in published works, which complicates comparing different studies. Making these filters available through more transparent publication would benefit re-use, open and cumulative science.

(3) Third, the MIOT system boundaries present a challenge for tracking material use to particular end-use products. The functionality of products that are end-use products in the sense of dMFA, but are intermediate products in the definition of MIOTs (e.g. packaging), is lost during the calculation of the Ghosh/Leontief inverse (e.g. plastic in computer packaging identified as plastic in a computer; see section 2.1.1 in Streeck et al. (in revision_)). This problem applies to all reviewed methods except for the Partial Ghosh-IO, where end-uses are defined by the practitioner (see point (1) above).

In theory, the correct end-use can be re-identified via secondary calculations. Nakamura et al. (2007), Yokoi et al. (2018: section 2.1.4), Dietzenbacher et al. (2019) and Hertwich (2021) propose distinct methods to calculate materials in a final product’s sub-components (e.g. to determine product packaging). However, to our knowledge none of these methods is capable of doing that without facing issues of double counting. Nakamura et al. (2007) propose an approach similar to production layer decomposition (Wieland et al., 2018) for WIO-MFA, in which supply chain layers are decomposed one supply chain step at a time. Dietzenbacher et al. (2019) and Hertwich (2021) propose different variations of the Hypothetical Extraction Method (HEM) to the Leontief quantity model, in which the effect of one product/sector is evaluated by comparing a counterfactual in which this sector is removed from the unperturbed system. Yokoi et al. (2018) propose an

approach similar to HEM for WIO-MFA. However, unless the inter-industry matrix is perfectly directional (triangular, which requires assumptions, Nakamura et al., 2007), all of these approaches lead to double counting if one subsequently wants to decompose into individual sectors/products. Hertwich (2021) corrected for double counting in a downstream step through identifying the amount of environmental burden that is allocated more than once, using a decomposition approach inspired by footprint studies that aim to resolve, i.e. avoid, double counting in footprints (Cabernard et al., 2019; Dente et al., 2018). In theory, above methods could be applied to re-identify end-use functionality for selected products, do however exclude certain sector interactions to avoid double-counting. Further developing these methods towards tracing material flows into sub-components of end-use products without exclusion of sector interactions, thus yielding a three dimensional array version of the end-use share matrix **D**, would be an interesting next step. In the empirical part II of this review (Streeck et al., in revision_), we take a pragmatic stance and propose a simple method to re-define selected intermediate products such as packaging as end-use. We achieve this by altering the system boundaries of the MIOT industry system towards the output-side and call the approach 'End-Use Transfer'.

- (4)** Fourth, most of the studies that used above methods suffer from the price homogeneity assumption inherent to MIOTs, which assumes that the individual products contained in the aggregate product mix delivered by a sector have the same unit price (Weisz & Duchin, 2006). This introduces bias, when prices of individual products in the mix differ substantially (see footnote four for potential reasons). In the studies of W.-Q. Chen and Graedel (2015) and W.-Q. Chen (2017) on aluminum products in the USA, that does not seem to be a large issue, as supposed by the good fit of WIO-MFA results with results of other estimation methods. However for materials like steel, which strongly differ in quality and price (e.g. for automotive versus construction steel), this might be more important.¹⁷ Principally there are two ways to tackle above assumption: first by disaggregating sectors in the MIOT (e.g. Nakajima et al., 2013; Ohno et al., 2015); and second by using transaction-specific prices (Table 2: VIII) for the output of sector *i* to different sectors *j*. The latter was done in Yokoi et al. (2018, 2022), which are the only studies we found that applied this approach. However, the scarcity of price data for different material applications, which additionally matches the product average assumed for MIOT's sector output product mixes, are major limitations for wider application.

¹⁷ For example, high value steel alloys have a high value but relatively low mass flow and hence, the estimation of end-use shares with a monetary table will overestimate the physical end-use share of sectors that consume a lot of high value steel alloys. This problem becomes smaller if sectors are more disaggregated and less price inhomogeneity occurs.

(5) Fifth, the reviewed methods differ regarding ease of use and required Input-Output Analysis (IOA) proficiency. Partial Ghosh-IO can be implemented without detailed knowledge of IOA (like done in Aryapratama & Pauliuk, 2019; Cao, Shen, Liu, et al., 2017), however this method is very sensitive to practitioner decisions (see point (1) above). All other methods require at least basic IOA operations. From these, CBA is the easiest and most efficient method to apply, but is problematic for calculating end-uses due to its consumption-based footprint perspective. WIO-MFA closely follows a physical dMFA logic, but is comparatively complex and data-intensive, which can represent an entry barrier. However, this point might partially be resolved by making available WIO-MFA filter matrices and underlying code scripts via platforms like Zenodo and Github.

There are several additional points to consider when applying the different methods, like choosing the MIOT sectors corresponding to 'materials', the exact design of filter matrices and so on, which will be discussed in the comparative application of methods in part II of this review (Streeck et al. (in revision_)).

4. Conclusions and next steps

The use of monetary input-output tables (MIOTs) to derive end-use shares can help overcome limited data availability in physical units. The reviewed methods can be applied to any MIOT, for which the widely used Waste Input-Output approach to (d)MFA theoretically leads to the most accurate end-use shares by applying corrections to align MIOTs with dMFA system boundaries. We showed that improvements in accuracy of end-use shares arise from the alignment of system boundaries between MIOTs and dMFA, and not from different underlying input-output models (section 3.2).

Beyond theoretical considerations, we see the need to empirically compare end-use shares derived from MRIOs, national MIOTs and physical unit industry shipments, to assess the accuracy and robustness of results from these data sources. To that end, in part II of this review, we apply the methods presented here to investigate and improve upon the theoretical drawbacks (Streeck et al., in revision_). In addition, the wide use of end-use shares in dMFA warrants further comparison and validation efforts with independently obtained estimates, e.g. from bottom-up dMFA.

This review described some of the potentials and drawbacks that come with using monetary proxy data to model physical flows. To enable more accurate assessment of production and consumption, resource efficiency, the circular economy, or integrated modeling of monetary and physical capital, we require a political process that pushes stakeholders and statistical agencies to compile more information on material end-uses in physical units, and to make these data publicly available. Ideally, such a process would enable the compilation of purely physical IOTs, independent accounts of

materials in product stocks, and their integration with dMFA to comprehensively represent the stocks and flows of the biophysical basis of society, including information on end-use products.

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Conflict of Interest Statement

The authors declare no conflict of interest.

Data Availability Statement

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

CRediT author statement

JS: Conceptualization, Investigation, Formal analysis, Visualization, Writing – Original Draft, Review & Editing, **SP:** Formal analysis, Supervision, Writing – Original Draft, Review & Editing, **HW:** Supervision, Writing - Review & Editing, **DW:** Conceptualization, Supervision, Writing - Review & Editing, Project administration

Supporting information

Supporting information is linked to this article on the *JIE* website:

Supporting information SI 1: This supporting information provides potential additional configurations of methods to trace material flows into products, using monetary input-output tables (MIOTs) in SI 1a;

as well as seminal documentation of methods, including formal proof of equivalence of underlying input-output models in SI 1b.

Supporting information SI 2: This supporting information provides examples corresponding to the documentation of methods' underlying input-output models in SI 1b.

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