Deriving life cycle assessment coefficients for application in integrated assessment modelling

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Abstract

The fields of life cycle assessment (LCA) and integrated assessment (IA) modelling today have similar interests in assessing macro-level transformation pathways with a broad view of environmental concerns. Prevailing IA models lack a life cycle perspective, while LCA has traditionally been static- and micro-oriented. We develop a general method for deriving coefficients from detailed, bottom-up LCA suitable for application in IA models, thus allowing IA analysts to explore the life cycle impacts of technology and scenario alternatives. The method decomposes LCA coefficients into life cycle phases and energy carrier use by industries, thus facilitating attribution of life cycle effects to appropriate years, and consistent and comprehensive use of IA model-specific scenario data when the LCA coefficients are applied in IA scenario modelling. We demonstrate the application of the method for global electricity supply to 2050 and provide numerical results (as supplementary material) for future use by IA analysts.

1 Introduction

1.1 Motivation and aims

Curbing greenhouse gas (GHG) emissions is a necessary requirement for achieving the international policy objectives of avoiding dangerous interferences with the climate system (UNFCCC, 1992). Life cycle assessment (LCA) and integrated assessment models (IAMs) are two complementary tools for assessing the GHG emission reduction potential of technologies (Edenhofer et al., 2014; Hertwich et al., 2016a). LCA offers a systematic, bottom-up framework and process for attributing environmental impacts that occur in complex international supply chains to one product. LCA strives to achieve extensive coverage of supply chain activities associated with production, use and waste handling of products. It also strives to achieve extensive coverage of types of environmental impacts, including toxic effects on humans and ecosystems, and natural resource use or depletion (Hauschild et al., 2013; Hauschild and Huijbregts, 2015; Hellweg and Milà i Canals, 2014). IAMs are widely used to explore potential strategies to mitigate future climate change (Krey, 2014; O'Neill et al., 2014; Schwanitz, 2013)[1]. Under the principal assumption that different combinations of primary energy resources and energy transfers and transformations can provide substitutable energy services, the models select (and substitute) resource and technology alternatives so that costs are minimized or welfare is maximized, subject to constraints (e.g., on emissions allowances, resource availability or technology availability). Important reports targeted to policy makers and the public devote significant attention to scenarios produced by IAMs (Edenhofer et al., 2014; IEA, 2014; Johansson et al., 2012).

Existing LCA literature is for the most part concerned with assessing environmental impacts associated with one (small) reference unit (e.g., 1 kWh of electricity) in a static framework. While such assessments can offer useful insights, they carry no notion of absolute magnitude or timing of effects at regional or global levels. Hence, they provide limited basis for assessing long-term technology transformation pathways, especially under scenarios of rapid and large-scale deployment of new technologies (Arvesen and Hertwich, 2011; Dale and Benson, 2013). Also, while any LCA attributes effects occurring in various supply chains to a specific product, most LCAs do not capture other types of consequences of products that one may infer considering broader economic or policy contexts, such as indirect land use change emissions induced by bioenergy products[2]. IAMs, on the other hand, put their focus on representing the dynamics that shape natural and human systems over long time-scales and under large-scale changes in the economic setting. However, IAMs have more narrow boundaries in terms of environmental impacts and do not represent life cycle effects of products, or represent such effects only partially and/or only implicitly via interactions between energy system and macro-economy modules (Pauliuk et al., 2017).

We see two principal ways in which LCA can be useful for IA modelling. One is to integrate LCA results in IA modelling so that indirect emissions of technology and scenario alternatives can be explored, and potentially taken into account in the decision-making routines of the IAMs. Technology selection in state-of-the-art IAMs typically considers some types of indirect emissions, such as methane leakages from fossil fuel production and land use change-related emissions from biomass production, while not considering many other indirect emissions (e.g., emissions from producing metals for power plants). More fully considering indirect emissions

[1] In this work, by IAMs we refer broadly to models that are used to explore transformation pathways and to evaluate climate mitigation policies (Clarke et al., 2014; Riahi et al., 2012), as distinct from aggregated models that monetize climate change impacts in order to perform cost-benefit analysis of climate policy. AIM, GCAM, IMAGE, MESSAGE and REMIND are examples of models that fall into the former category (Edmonds et al., 2012). In addition, we are concerned with models that carry explicit representations of individual energy technologies, as distinct from models lacking technology-level detail.

[2] So-called consequential LCA (CLCA) is an exception (Zamagni et al., 2012). CLCA is much less frequently applied than conventional (sometimes termed attributional) LCA, but a significant number of CLCA studies do exist. Perhaps in particular, CLCA is used in literature to study bioenergy (Creutzig et al., 2015).

of technology alternatives can yield more consistent evaluations, and thus potentially affect optimal technology selection or overall effectiveness of mitigation strategies in IAMs. The relative importance of indirect emissions may increase over time and increasingly stringent emission reduction targets, as technologies with zero or low direct emissions (e.g., electric vehicles, fossil fuel combustion with carbon capture) gradually replace those using fossil fuels. The second way LCA can be useful is to improve environmental impact assessment or broaden the range of environmental concerns addressed in IAMs. Most state-of-the art IAMs have an explicit description of non-CO_2 greenhouse gas emissions and air pollution (e.g, Strefler et al. (2014), Gernaat et al. (2015), Rao et al. (2017)), and recently have also considered water demands (e.g., Mouratiadou et al. (2016)), but lack many other crucial environmental impact dimensions. LCA routinely supports assessment of the effects of hundreds of pollutants, resource flows and land, incorporating environmental mechanisms (e.g., toxic effects on ecosystems or humans) not currently addressed by IAMs (Masanet et al., 2013). When we refer to impact indicator results in this article, we refer broadly to any indices of environmental impacts or natural resource requirements computed using impact assessment methods from LCA (Frischknecht et al., 2016).

The aims of this article are the following:

i) To develop a general method for deriving energy and impact indicator results from detailed, bottom-up LCA such that the results are suitable for application by IA modellers.
ii) To apply the method to calculate energy and impact indicator results for the global electricity system to 2050, for future use by IA practitioners.

The method allows for capturing technology variations and changes between geographical regions and over time. It enables consistent use of IAM-specific scenario data (e.g., emission factors, lifetime, load factors) in combination with LCA coefficients. This is achieved mainly by a separate treatment of main life cycle stages with a unit conversion adapted to the stage and technology in question, and by a decomposition of coefficients into individual energy carriers, industries and energy service types. IA modellers may combine the energy results derived from LCA with IAM-specific emission factors so as to determine emissions related to combustion of energy fuels on a life cycle basis. They may use the impact indicator results derived from LCA to address types of impact other than those commonly associated with combustion, such as toxic effects of pollution loads.

1.2 Existing literature

A few attempts have been made in literature to combine LCA and IAM perspectives for the purpose of long-term and large-scale assessment. A notable study by Daly et al. (2015) couples a national United Kingdom energy system optimization model with a multiregional economic input-output model in order to investigate the significance of indirect emissions for national energy system transformations, explicitly accounting for domestic and nondomestic indirect emissions associated with energy supply. Their results indicate that domestic indirect emissions have little significance, while nondomestic indirect emissions appear significant and would, if included in an ambitious domestic emission reduction target and in absence of commensurate non-domestic mitigation, double the marginal abatement cost of meeting the target. The study assumes non-domestic emission intensities follow baseline trends, i.e. that no climate policies are implemented outside the United Kingdom. An accompanying study by the same authors identifies that the optimization model selects increased electrification and use of nuclear power as a cost-optimal strategy to mitigate the nondomestic indirect emissions (Scott et al., 2016). Dandres et al. (2011) use a computable general equilibrium model together with LCA in order to address economy-wide consequences of bioenergy policy. The authors report the finding that bioenergy policy increases environmental impacts owing to effects of price changes, while also underlining that “more work is needed to evaluate” the approach used.

The aforementioned studies rely on economic input-output analysis (Daly et al., 2015; Scott et al., 2016) or a mapping between economic input-output sectors and detailed, bottom-up LCA activities (Dandres et al., 2011) to determine emission multipliers. All studies rely on price information to convert between monetary and mass units. Another study implements generic LCA-type indicators derived from theoretical considerations in a system dynamics model (Dale et al., 2012b). A general advantage of approaches that do not require detailed technology information is that, owing to relatively easy data compilation, extensive coverage of energy technology and fuel types can be achieved, as indeed is the case in the above-cited works. Another advantage of employing multiregional input-output (MRIO) analysis (Daly et al., 2015; Scott et al., 2016) is that international trade and geographical differences in production are generally better captured in MRIO than in LCA.

The current work adopts a different strategy, making use of physical, rather than monetary, accounting of product systems, and a bottom-up, rather than top-down, calculation technique for determining indirect energy use and environmental impact coefficients. The chief motivation for adopting this approach when analysing current and prospective technologies is to strive for high-precision projections, avoiding high uncertainty associated with aggregation in MRIO and conversion between monetary and mass units. In addition, owing to greater coverage of pollution types, bottom-up LCA facilitates meaningful assessment of a larger portfolio of impact categories (including effects of toxic pollution loads to soil and water) than contemporary MRIO. It also can account more explicitly for the effects of climate policies on the carbon intensity of the underlying energy system.

Another category of studies perform LCA of scenario results emanating from IAM or energy system model runs (Arvesen and Hertwich, 2011; Arvesen et al., 2014; Bergesen et al., 2016; Berrill et al., 2016; Gibon et al., 2017; Hertwich et al., 2015; Portugal-Pereira et al., 2016; Singh et al., 2012; Volkart et al., 2017), with or without consideration of future technological changes, and portraying snapshots of impacts in a given (future) year or evolution of impacts over time. With the exception of Volkart et al. (2017), these studies mainly focus on assessment results (as opposed to describing procedures or discussing methodological aspects), and they do not address the topic of deriving LCA-based coefficients for application in IAMs.

To our knowledge, no attempts have been made in the existing literature to develop formal procedures for how LCA, where activities are described bottom-up and in physical terms, can be incorporated into IAM while ensuring consistent use of IAM-specific data (e.g., emission factors) and attribution of life cycle effects to appropriate years, and avoiding the uncertainty associated with conversions between mass and monetary units.

2 Overview of study

As stated in the introduction section, this study has a twofold aim: to develop a general method for deriving LCA coefficients for use in IAMs, and to demonstrate the application of the method for the case of future global electricity supply. Before presenting the method in Section 3 and results for the case study of electricity in Section 4, the current section provides an overview of the study in terms of data sources and modelling framework used, and connections to other, related studies. In the following Subsection 2.1, we explain the selection of electricity supply as a case study and provide an account of main assumptions and data sources. We then, in Subsection 2.2, introduce the THEMIS LCA analytic model framework used in this work. Subsection 3.2 further details the study design and clarifies connections to related studies.

2.1 Case description: electricity supply

In 2010, one quarter of global GHG emissions was caused by fossil fuel combustion in power plants (Edenhofer et al., 2014). Electricity generation is important for climate change mitigation (Luderer et al., 2014; Rogelj et al., 2015; Wiebe, 2016; Williams et al., 2012), because it is relatively easy to decarbonize (compared to, e.g., transport), as many low-carbon energy sources by their nature generate electricity (e.g., wind, nuclear and solar power). From an LCA point of view, electricity generation makes an interesting case study because various different types of power plants, while serving the same function, operate by very different mechanisms and exhibit very different supply chains.

We adopt multiregional and prospective life cycle inventory data for photovoltaic power, concentrating solar power, hydropower, wind power, coal power and natural gas power from Hertwich et al. (2015), with some incremental improvements to the data. The data incorporates regional variations and future technological improvements of electricity production through changes in basic parameters such as photovoltaic module efficiency, fossil fuel power plant efficiency, insolation and wind load factors, as well as through shifts towards higher-performance technology generations (e.g., from crystalline silicon photovoltaic to thin-film photovoltaic).

Nuclear power and biomass power are not addressed in Hertwich et al. (2015). In the current work, we adopt life cycle inventory data from the Ecoinvent LCA database to cover nuclear power (Dones, 2007; Ecoinvent, 2010), assuming that these data are representative for all regions and over time. In addition, we establish life cycle inventories for electricity from biomass, modelling two different biomass feedstocks (or sources). One biomass feedstock is boreal forest residue, modelled using data from Singh et al. (2014). The other feedstock is lignocellulosic (second generation) bioenergy crops. Data for modelling this feedstock are obtained largely from scenario results produced by the global land use model MAgPIE (Bodirsky et al., 2012; Klein et al., 2014; Lotze-Campen et al., 2008). The MAgPIE results describe crop yields, land requirements, carbon dioxide emissions from land use, irrigation water demand, nitrogen and phosphorus fertilizer use, and nitrous oxide emissions related to fertilization across world regions and years, under nine policy scenarios representing different assumptions about carbon pricing, the type of bioenergy crops available and whether irrigation is allowed or not. Further, the MAgPIE results are supplemented by data gathered or derived from other sources, notably Nemecek and Kägi (2007), Njakou Djomo et al. (2013) and Njakou Djomo et al. (2015). A full account of data and assumptions used to model bioenergy crops is provided in the supplementary material.

Table 1 lists the electricity generation technology types modelled using LCA, and their classification into aggregated technology categories. Also shown are assumed market shares (Hertwich et al., 2015) for detailed technology types (e.g., ground-installed polycrystalline silicon solar photovoltaics) that we use to aggregate results into main technology categories (e.g., solar photovoltaics). The market shares are not a necessary element of our general method to derive LCA coefficients for use in IA modelling, but are introduced here for our case study of electricity because the aggregation into main technology types may be practical for results interpretation and application in IA modelling. The assumed market shares are constant across regions modelled using LCA.

Table 1

Overview of the 27 individual power generation technology types modelled using LCA, classified into 14 main technology types, with information on assumed market shares by year (2010, 2030 and 2050). Market share values give the assumed relative percentage shares of detailed technology types within the main technology type category to which they belong. In cases where there is only one detailed technology type per main technology category, the market share is 100%. The market share values are based on own assumptions or adopted from Hertwich et al. (2015). As explained in the main text, for biomass from crops, we present LCA results for nine scenarios reflecting different policy assumptions, but this is not reflected in this table.

Main technology type	Detailed technology type or attribute	Assumed market share		
		2010	2030	2050
Solar photovoltaics	Polycrystalline silicon (poly-Si), ground	67%	25%	15%
Solar photovoltaics	Polycrystalline silicon (poly-Si), rooftop	22 %	8.3%	5.0%
Solar photovoltaics	Cadmium-telluride (CdTe), ground	1.1%	25%	30%
Solar photovoltaics	Cadmium-telluride (CdTe), rooftop	0.4%	8.3%	10%
Solar photovoltaics	Copper indium gallium selenide, ground	6.5%	25%	30%
Solar photovoltaics	Copper indium gallium selenide, rooftop	2.2%	8.3%	10%
Concentrating solar	Parabolic trough	50%	50%	50%
Concentrating solar	Central tower	50%	50%	50%
Hydropower	Reservoir 660 MW (remote)	20%	20%	20%
Hydropower	Reservoir 360 MW (near)	80%	80%	80%
Wind, onshore	Wind farm 150 MW	100%	100%	100%
Wind, offshore	Wind farm 350 MW, concrete foundations	50%	50%	50%
Wind, offshore	Wind farm 350 MW, steel foundations	50%	50%	50%
Coal without CCS	Subcritical	72%	66%	66%
Coal without CCS	Supercritical	0%	0%	0%
Coal without CCS	Integrated gasification combined cycle	28%	34%	34%
Coal with CCS	Subcritical	100%	11%	11%
Coal with CCS	Supercritical	0%	19%	19%
Coal with CCS	Integrated gasification combined cycle	0%	70%	70%
Natural gas without CCS	Natural gas combined cycle (NGCC)	100%	100%	100%
Natural gas with CCS	Natural gas combined cycle (NGCC)	100%	100%	100%
Nuclear	Boiling water reactor (BWR)	30%	30%	30%
Nuclear	Pressurized water reactor (PWR)	70%	70%	70%
Crop-based biomass without CCS	Crops for growing lignocellolusic biomass	100%	100%	100%
Residue biomass without CCS	Forest residues	100%	100%	100%
Crop-based biomass with CCS	Crops for growing lignocellolusic biomass	100%	100%	100%
Residue biomass with CCS	Forest residues	100%	100%	100%

A special note is required for hydro. As is evident from Table 1, two hydropower facilities are modelled, one of which is situated in a remote location and the other not. The life cycle inventory data for both of these cases are based on two planned projects in Chile. Owing to comparatively large transport and infrastructure requirements for the remotely situated plant, life cycle impacts for this plant are up to one order of magnitude higher than that of the other, non-remote plant (Hertwich et al., 2015; Hertwich et al., 2016b). Ideally, a larger population of power plants should serve as a basis of the modelling, but such assessments are currently not available. As a result of this big difference in impacts between the two cases, aggregated results for hydropower are highly sensitive to the market shares assigned to each case.

In the current study, all the life cycle inventory data sets are incorporated into the multi-regional and prospective model framework THEMIS that will be described in Subsection 2.2. The impact indicator categories considered in the case study of electricity supply are the ReCiPe version 1.08 categories freshwater ecotoxicity, freshwater eutrophication, human toxicity, ionizing radiation, land occupation, marine eutrophication and mineral resource depletion (Goedkoop et al., 2014; ReCiPe, 2012)[3], as well as four categories representing requirements for individual materials, namely aluminium, cement, copper and iron (Singh et al., 2015). Climate change impacts and impacts related to local air pollution are excluded from this list, as such impacts are preferably addressed by IA analysts by utilizing LCA energy coefficients in combination with IAM-specific emission factors for fuel combustion.

2.2 LCA modelling framework

THEMIS (Technology Hybridized Environmental-economic Model with Integrated Scenarios) is a multi-regional and prospective LCA modelling framework. THEMIS was formally introduced and described by Gibon et al. (2015); published applications of THEMIS include Hertwich et al. (2015), Bergesen et al. (2016) and Berrill et al. (2016). In this study, we employ THEMIS to produce results for each of the power generation technologies listed in Table 1, and for three years (2010, 2030, 2050), two policy scenarios (baseline scenario and the BLUE Map climate change mitigation scenario of IEA (2010)) and nine world regions (following the region classification of IEA (2010)).

The current version of THEMIS combines life cycle descriptions of individual power generation technologies developed by Hertwich et al. (2016), a process-based life-cycle assessment database (Ecoinvent, 2010)[4], and adapts the data so as to represent important regional differences and changes over time towards 2050. The adaptations include changing the electricity mix depending on region and year, following either the baseline or climate change mitigation scenario. Furthermore, THEMIS takes into account scenarios for future improvements in performance parameters for selected industrial processes (i.e., aluminium; copper; nickel; iron and steel; metallurgical grade silicon; flat glass; zinc; and clinker production). For example, in THEMIS, steel production in 2050 benefits from lower hard coal coke input to blast furnace reduction per unit of iron, as well as lower energy fuel requirements, cleaner electricity (in particular when the climate change mitigation scenario is analysed) and reduced emission intensities, compared with steel production in 2010. For a full description of

[3] ReCiPe is a prominent and widely applied method for life cycle impact assessment.

[4] Ecoinvent is a database providing life cycle inventory data sets for a large number of processes, for example minerals extraction and materials production.

the treatment of technological change in THEMIS, see the supplementary material to Gibon et al. (2015).

One limitation of the current version of THEMIS is that it does not include any changes in the characteristics of transport activities over time. Potential future decreases (due to technological innovations) or increases (due to a shift towards less accessible or lower quality resources) in the energy required to extract energy fuels (Hall et al., 2014) or metals (Norgate and Haque, 2010; Norgate et al., 2014) from the ground are also not considered. In general, selected technology representations are adapted to different years in THEMIS.

2.3 Study design and links to other studies

Fig. 1 illustrates connections between elements (data, procedures, results) of the current study as well as other, related studies. Also included in the figure are references to relevant sections in the present article. The figure reiterates the information from Subsections 2.1 and 2.2 that life cycle inventory data sets for a suite of electricity supply options were compiled for Hertwich et al. (2015) and integrated into the multi-regional and prospective LCA model framework THEMIS. THEMIS additionally takes into account future projected technological progress in selected industrial processes (Subsection 2.2 and Gibon et al. (2015)). The current article presents a general method to derive LCA coefficients for use in IA modelling (Section 3), and uses THEMIS to apply the method for the case of electricity supply (Section 4 and supplementary material).

As the figure also indicates, two related studies apply the derived LCA coefficients in IA modelling. Pehl et al. (2017) integrate the LCA energy coefficients in the REMIND IAM in order to explore life cycle greenhouse gas emissions associated with future global electricity systems, and to investigate the degree to which endogenizing life cycle emissions impact the computed optimal technology selection. In the second related study, Luderer et al. (under review) make use of both the LCA energy and impact indicator results to compare climate mitigation strategies for the power sector in terms of their performance by a range of environmental impact and natural resource use criteria.

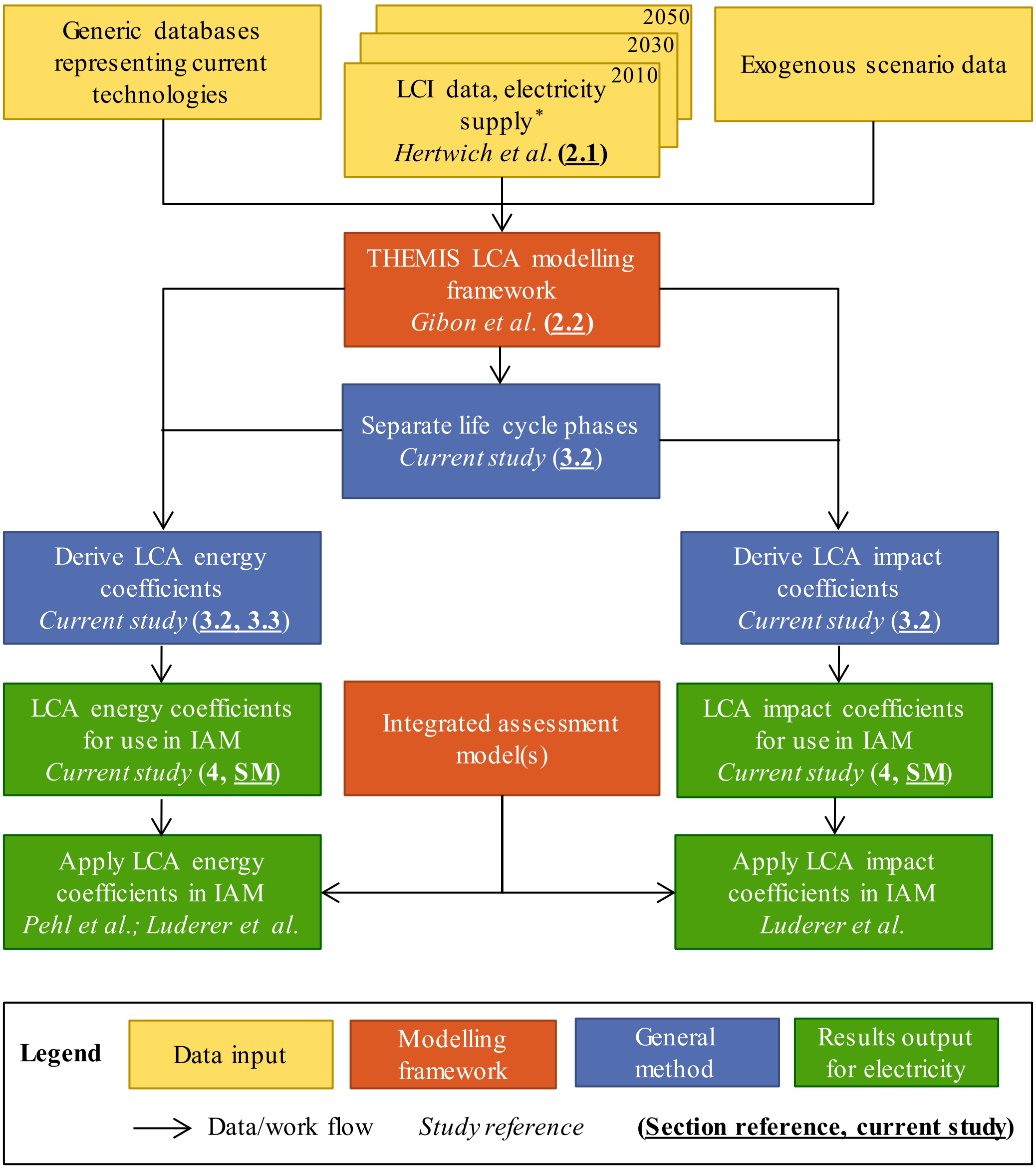

Fig. 1. Schematic illustration of the connections between data, procedures and results presented in the present study as well as in other, related studies. References cited in figure: Hertwich et al. (2015); Gibon et al. (2015); Pehl et al. (2017); Luderer et al. (under review). Numbers in parentheses refer to sections in current study in which relevant descriptions or data are available. SM = Supplementary material of current study. LCI = Life cycle inventory. *Biopower and nuclear power are not addressed in Hertwich et al. (2015) and Gibon et al. (2015) but are included in the current work (see Subsection 2.1).

3 Method to derive LCA coefficients

This section presents the method for calculating and organizing results obtained from LCA in such a way that the results can form a suitable interface with IA modelling. As remarked in the introduction section, the interface may be made up of two types of LCA results, energy results or impact indicator results. The former option allows IA analysts to use IAM-specific emission factors for carbon dioxide and air pollutants to determine energy-related emissions on a life cycle basis. The latter option involves characterization and aggregation of different types of pollutants or natural resource use into a set of impact categories defined in the LCA, and may be particularly useful for IA analysts seeking to address types of impacts not already addressed in the IAM (e.g., impacts caused by releases of toxic or eutrophying substances to water in connection with mining or agricultural activities). The computations of LCA energy and impact indicator results both involve a separate treatment of life cycle stages, as will be described in subsection 3.2. Additional procedures are described in subsection 3.3 for the computation of LCA energy results to identify individual energy carriers, industries and energy services, hence allowing IA analysts to take advantage of available IAM-specific emission factors.

It should be noted that while the LCA energy results can be used to address greenhouse gas emissions and air pollution associated with combustion, industrial process-based emissions (Müller et al., 2013), methane leakages from fossil fuel supply (Brandt et al., 2014; Gernaat et al., 2015), land use-related emissions (Bodirsky et al., 2012; Popp et al., 2013), methane emissions from hydropower reservoirs (Hertwich, 2013), sulphur hexafluoride leakages from electric equipment (Arvesen et al., 2015; Turconi et al., 2014) and other non-combustion emissions may constitute significant sources of greenhouse gas emissions or environmental impact. Some remarks on non-combustion greenhouse gas emission sources and an explanation of how they are dealt with in the present work are offered in the supplementary material.

3.1 Mathematical representation and notation

We follow the general terminology of LCA (JRC, 2010; Matthews et al., 2015) and its mathematical representation in terms of input-output algebra (Miller and Blair, 2009). LCA requires a systematic mapping of activities associated with production, use and waste handling of products. Any activity initially identified typically has both its own life cycle and its own supply chain, raising the need to map a further set of activities, again raising a need to map yet further activities. The complete set of activities that through such causal chains can be linked to the product being studied together make up a product system. Further, the activities targeted for special modelling attention, or for which data have been established specifically for the current work, comprise the foreground system. The remaining activities make up the background system (JRC, 2010; Wernet et al., 2016). Depending on the study, background activities could include minerals extraction, transport and manufacturing activities, and more.

Throughout Section 3, we use subscripts to indicate that a variable is dependent on or defined for a specific dimension (e.g., year, region), and superscripts to indicate a particular type of variable. We use the subscripts t, r, τ, s and p to denote technology under investigation (i.e., in our case study, one detailed power generation technology type shown in Table 1), region, year, scenario and life cycle phase, respectively. Vectors are denoted by lowercase boldface (e.g., $\boldsymbol{y}_{t,r,\tau,s}^{fd}$) and matrices by uppercase boldface (e.g., $\boldsymbol{A}_{\tau,s}$).

We denote the demand that is imposed on the system (e.g., to deliver one unit of electricity from onshore wind power for a given technology, region, year and scenario) by the column vector $\boldsymbol{y}_{t,r,\tau,s}^{fd}$. This demand vector has only one non-zero entry: The demand for the product being studied (e.g., onshore wind power for a given technology, region, year and scenario) is set to one and all others are set to zero, so that the impacts of the one product can be isolated. The superscript 'fd' denotes 'final demand' and is used to distinguish $\boldsymbol{y}_{t,r,\tau,s}^{fd}$ from $\boldsymbol{y}_{t,r,\tau,s,p}$, which we introduce next. Further, the direct requirements matrix $\boldsymbol{A}_{\tau,s}$ holds information on all interrelationships between the activities that make up a product system. In $\boldsymbol{A}_{\tau,s}$, the entry in row i and column j represents the direct input from activity i to activity j per unit of output j. In the approach and exposition of this paper, we assume that all modelled technologies (i.e., in our case study of electricity, the full set of technologies shown in Table 1) are described in the matrix $\boldsymbol{A}_{\tau,s}$. This is the reason why, in our definition, $\boldsymbol{A}_{\tau,s}$ is not technology- and region-specific.

We let the total number of foreground processes, covering all technologies and regions defined for year τ, be $n_{\tau,s}^{f}$, $n_{\tau,s}^{b}$ be the total number of background processes and $n_{\tau,s}^{fb} = n_{\tau,s}^{f} + n_{\tau,s}^{b}$ the combined foreground and background total. We define the following sets: T is the set consisting of all technologies; R the set of regions; T the set of years; S the set of scenarios; and P the set of life cycle phases.

Table 2 provides a list of key intermediate and final calculated variables, and numbers, sets and indices used throughout Section 3.

Table 2
Overview of key sets and indices, numbers, predetermined variables, and intermediate and final calculated variables defined throughout Section 3. Right column lists the section number (SN) in which the symbols are first introduced.

Symbol	Description	SN
Sets and indices:		
T, R, T, S, P	Sets of all technologies, all regions, all years, all scenarios and all phases.	3.1
t, r, τ, s, p	Indices representing specific technology, region, year, scenario and phase.	3.1
CEC	Set of characterized energy carriers ('cec'). We use $CEC = \{liquids,\ gases,\ solids,\ electricity\}$.	3.3.1

IND	Set of industry ('ind') sectors analysed separately. We use $IND = \{electricity,\ \ transport,\ \ iron/steel,\ \ cement\}$.	3.3.2
$FB^{ec}_{\tau,s}$	Set of foreground and background processes delivering energy carriers ('ec').	3.3.2
Numbers:		
$n^{f}_{\tau,s}, n^{b}_{\tau,s}$	Numbers of foreground ('f') and background ('b') processes, respectively.	3.1
$n^{fb}_{\tau,s} = n^{f}_{\tau,s} + n^{b}_{\tau,s}$	Total number of foreground and background processes.	3.1
n^{p}	Number of life cycle phases. We use $n^{p} = 3$.	3.1
n^{cec}	Number of characterized energy carriers. We use $n^{cec} = 4$.	3.3.2
n^{ind}	Number of industries analysed separately . We use $n^{ind} = 4$.	3.3.2
$n^{ec}_{\tau,s}$	Number of processes in the set $FB^{ec}_{\tau,s}$.	3.3.2
n^{str}	Number of environmental load types defined.	3.2
n^{imp}	Number of impact categories considered. We use $n^{imp} = 13$.	3.2
Predetermined variables:		
$\boldsymbol{y}^{fd}_{t,r,\tau,s}$	Final demand ('fd') vector ($n^{fb}_{\tau,s} \times 1$), representing demand imposed on system.	3.1
$\boldsymbol{A}_{\tau,s}$	Direct requirements matrix ($n^{fb}_{\tau,s} \times n^{fb}_{\tau,s}$).	3.1
$\boldsymbol{b}^{phase}_{\tau,s,p}$	Binary correspondence vector ($n^{fb}_{\tau,s} \times 1$) assigning processes to phase p .	3.2
$\varphi_{t,r,\tau,s,p}$	Multiplication factor for unit conversion.	3.2
$\boldsymbol{C}^{cec,tot}_{\tau,s}$	Matrix of characterization factors ($n^{cec} \times n^{fb}_{\tau,s}$), used to determine total ('tot') characterized energy carrier ('cec') values for the set CEC .	3.3.2
$\boldsymbol{B}^{ind}_{\tau,s}$	Binary correspondence matrix ($n^{fb}_{\tau,s} \times n^{ind}$) assigning processes to industries represented by the set IND .	3.3.2
$\boldsymbol{C}^{cec,dir}_{\tau,s}$	Similar as $\boldsymbol{C}^{cec,tot}_{\tau,s}$, but used to determine direct ('dir') energy use.	3.3.2
$\boldsymbol{F}_{\tau,s}$	Matrix of environmental load intensities ($n^{str} \times n^{fb}_{\tau,s}$), defined as in standard LCA.	3.2
$\boldsymbol{C}^{imp}$	Matrix of impact characterization factors ($n^{imp} \times n^{str}$), defined as in standard LCA.	3.2
Intermediate calculated variables:		
$\boldsymbol{y}_{t,r,\tau,s,p}$	Vector ($n^{fb}_{\tau,s} \times 1$) representing first round of activities in phase p after imposing demand $\boldsymbol{y}^{fd}_{t,r,\tau,s}$ on the system.	3.2
$\boldsymbol{x}_{t,r,\tau,s,p}$	Total output vector ($n^{fb}_{\tau,s} \times 1$).	3.2
$\boldsymbol{d}^{cec,tot}_{t,r,\tau,s,p}$	Matrix ($n^{cec} \times 1$) containing total ('tot') characterized energy carrier ('cec') values for the set CEC .	3.2
$\boldsymbol{A}^{ec}_{r,\tau,s}$	Direct requirements matrix ($n^{ec}_{\tau,s} \times n^{fb}_{\tau,s}$) containing only the rows of $\boldsymbol{A}_{\tau,s}$ corresponding to the set $FB^{ec}_{\tau,s}$.	3.2
$\boldsymbol{E}^{ec,dir}_{t,r,\tau,s,p}$	Matrix ($n^{ec}_{\tau,s} \times n^{ind}$) representing the direct use of energy carriers in industries represented by the set IND .	3.2
$\tilde{\boldsymbol{D}}^{cec,dir}_{t,r,\tau,s,p}$	Similar to $\boldsymbol{D}^{cec,dir}_{t,r,\tau,s,p}$ (see final calculated variables below), but normalized to total output levels for respective industries..	3.3
Final calculated variables:		
$\boldsymbol{D}^{cec,dir}_{t,r,\tau,s,p}$	Matrix ($n^{cec} \times n^{ind}$) representing the direct use of characterized energy carriers in industries represented by the set IND .	3.2

$\boldsymbol{d}^{cec,res}_{t,r,\tau,s,p}$	Vector ($n^{cec} \times 1$) representing the residual ('res') use of characterized energy carriers (i.e., energy use not captured by $\boldsymbol{D}^{cec,dir}_{t,r,\tau,s,p}$).	3.2
$\boldsymbol{x}^{ind}_{t,r,\tau,s,p}$	Vector recording total output values for industries represented by the set IND . Size: $1 \times n^{ind}$.	3.3
$\tilde{\boldsymbol{D}}^{cec,dir,med}_{t,r,\tau,s,p}$	Similar to $\tilde{\boldsymbol{D}}^{cec,dir}_{t,r,\tau,s,p}$, but contains median values across technologies and phases in $\tilde{\boldsymbol{D}}^{cec,dir}_{t,r,\tau,s,p}$.	3.3
$\boldsymbol{d}^{imp,tot}_{t,r,\tau,s,p}$	Vector ($n^{imp} \times 1$) containing total impact indicator values.	3.1

3.2 Separate treatment of life cycle phases

It is a principle purpose of IA modelling to address impacts of future scenarios on large scales. In order to best serve this purpose, coefficients derived from LCA for use in IAMs should distinguish the construction, operation and end-of-life phases. This is to ensure that IA users can attribute construction, operation and end-of-life coefficients to appropriate years and combine them with IAM-specific data on technology performance (e.g., emission factors) and technology deployment (e.g., new installed capacities, operating capacities) pertaining to the same years. Moreover, separating the life cycle phases is necessary if one wants to capture basic transition dynamics stemming from the different timing of infrastructure and operational inputs, which may be important during periods of rapid transformation (Arvesen and Hertwich, 2011; Gonçalves da Silva, 2010; Usubiaga et al., 2017). This subsection describes a generic procedure for separating out individual life cycle phases in LCA, taking as a starting point a standard LCA set-up with a demand vector containing only one non-zero element. In addition, and the procedure allows for construction phase effects to scale in proportion to installation size (capacity), and operation phase effects in proportion to utilization.

We assume that for technology t, region r, year τ and scenario s, the demand that is imposed on the system (e.g., to deliver one unit of electricity by a distinctive technological option) is recorded in a demand vector with a single non-zero entry, $\boldsymbol{y}^{fd}_{t,r,\tau,s}$ (already introduced in subsection 3.1), of size $n^{fb}_{\tau,s} \times 1$ .We let $\boldsymbol{y}_{t,r,\tau,s,p}$ be an $n^{fb}_{\tau,s} \times 1$ vector representing the first round of activities in phase p after imposing the demand $\boldsymbol{y}^{fd}_{t,r,\tau,s}$ on the system. In other words, $\boldsymbol{y}_{t,r,\tau,s,p}$ contains any direct inputs for phase p to the demand being studied. $\boldsymbol{y}_{t,r,\tau,s,p}$ may be calculated as shown in equation (1), based on $\boldsymbol{y}^{fd}_{t,r,\tau,s}$, the direct requirements matrix $\boldsymbol{A}_{\tau,s}$, and a binary $n^{fb}_{\tau,s} \times 1$ correspondence vector, $\boldsymbol{b}^{phase}_{\tau,s,p}$, assigning foreground processes to life cycle phase p . In $\boldsymbol{b}^{phase}_{\tau,s,p}$, the entry in row j is 1 if foreground process j is associated with life cycle phase p , and zero otherwise. Because background processes are used generically and cannot necessarily be unambiguously assigned to a life cycle phase, rows in $\boldsymbol{b}_{\tau,s,p}^{phase}$ representing background processes should contain only zeros. We assume that there are three life cycle phases ($n^{p} = 3$), the construction phase, the operation phase and the end-of-life phase.

$$\boldsymbol{y}_{t,r,\tau,s,p} = \varphi_{t,r,\tau,s,p} \cdot \left(\widehat{\boldsymbol{A}_{\tau,s} \cdot \boldsymbol{y}_{t,r,\tau,s}^{fd}} \cdot \boldsymbol{b}_{\tau,s,p}^{phase} \right) \quad , \quad t \in T, \quad \mathrm{r} \in R, \quad \tau \in \mathrm{T}, \quad s \in S, \quad p \in P \qquad (1)$$

Here, the circumflex ($\widehat{\quad}$) represents diagonalization of a vector. The multiplication factor $\varphi_{t,r,\tau,s,p}$ (a scalar) is introduced for the purpose of unit conversion, as will be explained at the end of this section. The use of equation (1) presupposes that the data are organized in such a way that: *i)* there are no energy use or emissions directly associated with $\boldsymbol{y}_{t,r,\tau,s}^{fd}$; *ii)* the first round of activities after imposing the demand $\boldsymbol{y}_{t,r,\tau,s}^{fd}$ on the system concerns processes defined in the foreground system only (not the background system); and *iii)* all processes involved in first round activities can be unambiguously assigned to a life cycle phase. The two latter requirements are achieved through appropriate definition of $\boldsymbol{A}_{\tau,s}$, in the manner illustrated by Fig. 2 for the case study of electricity. In the figure, processes labelled 'Process to deliver 1 kWh' represent processes for which there can be a non-zero entry in $\boldsymbol{y}_{t,r,\tau,s}^{fd}$, while 'Immediate inputs to 1 kWh process' indicate the processes that must be uniquely assigned (using $\boldsymbol{b}_{\tau,s,p}^{phase}$) to either the construction ('C'), operation ('O) or end-of-life ('E') phases. Note that $\boldsymbol{A}_{\tau,s}$ covers both foreground and background systems, but because rows in $\boldsymbol{b}_{\tau,s,p}^{phase}$ representing background processes contain only zeros, equation (1) does not involve any actual modelling for the background.

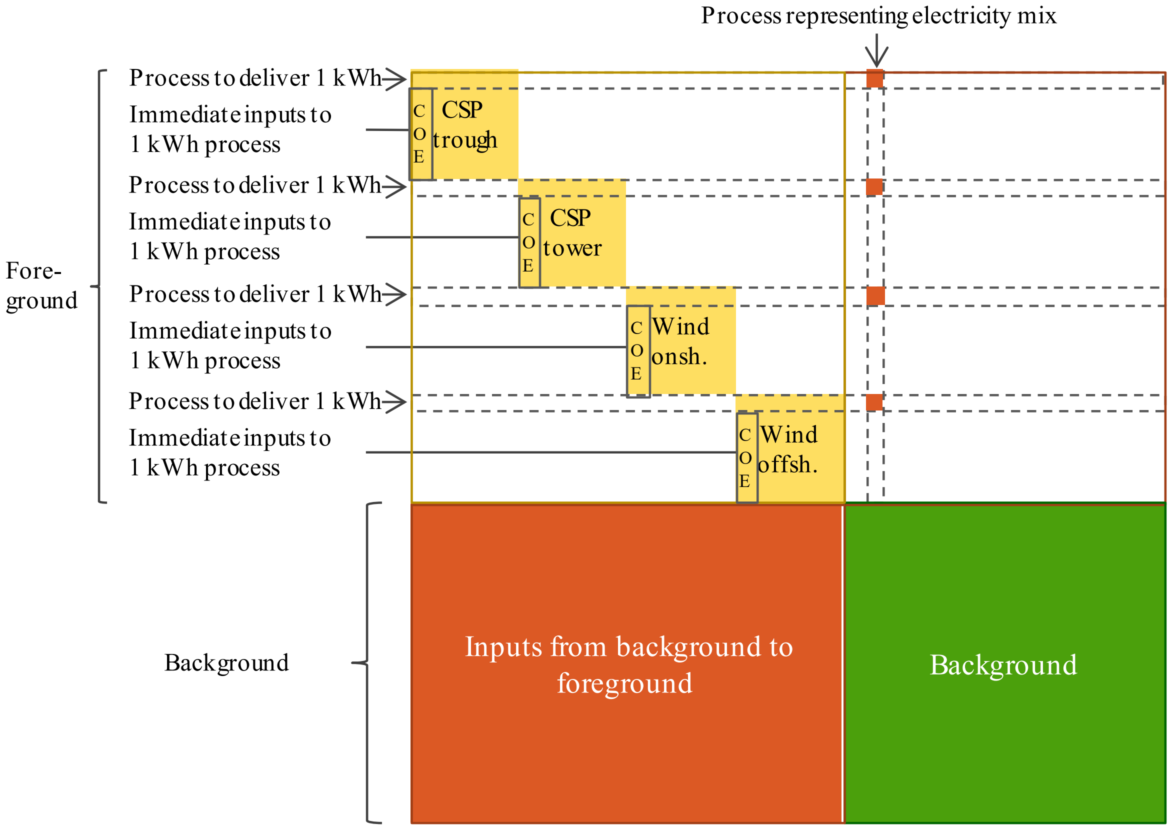

Fig. 2. Simplified illustration of the direct requirements matrix, $A_{\tau,s}$, in the case study of electricity supply, showing four technological options (cf. Table 1). Parts of the matrix that contain non-zero values are shown in colours (schematically). Elements labelled 'Immediate inputs to 1 kWh process' indicate the elements that must be uniquely assigned (using $\boldsymbol{b}^{phase}_{\tau,s,p}$) to one of the life cycle phases, where 'C' denotes construction, 'O' operation and 'E' end-of-life.

In equation (1), elements of the product $\widehat{\boldsymbol{A}_{\tau,s} \cdot \boldsymbol{y}^{fd}_{t,r,\tau,s}} \cdot \boldsymbol{b}^{phase}_{\tau,s,p}$ will be measured in relation to the single measurement unit used for the demand specified in $\boldsymbol{y}^{fd}_{t,r,\tau,s}$. An optional multiplication by a unit conversion factor $\varphi_{t,r,\tau,s,p}$ is introduced in equation (1) to make it possible to use different units for the construction, operation and end-of-life phases respectively. We anticipate that the value of $\varphi_{t,r,\tau,s,p}$ can be determined based on information already contained in the LCA foreground system data (e.g., information about the lifetime, efficiency and capacity factor of a thermal power station). One application of $\varphi_{t,r,\tau,s,p}$ can be to perform a unit conversion so that construction phase requirements are measured in relation to the size of installations, and operation phase requirements in relation to the utilization of installations. $\varphi_{t,r,\tau,s,p}$ can also be seen as a means to avoid imposing LCA-specific assumptions on the IA modelling: For example, by measuring requirements of power plant construction in relation to nominal capacity (as opposed to power generation), influence of LCA-specific assumptions about power plant lifetime and capacity factor on results can be avoided.

Table 3 summarizes our selection of measurement units in the case study of electricity supply. A further discussion on the use of is offered in the supplementary material.

Table 3
Overview of measurement units selected for main power generation technology types and life cycle phases in the electricity supply case study. Two technology types are distinguished: thermal power (i.e., power generated by combustion of fossil fuels or biomass, as well as power generation from nuclear fuels), and non-biomass renewable power (i.e., power generated from wind, solar or hydro resources). Unit symbols: MW = megawatt; kWh = kilowatt hour; yr = year. Asterisk (*) indicates any unit (e.g., gigajoule, tonne-kilometre).

Technology type	Life cycle phase	Unit	Remarks
Thermal	Construction	*/MW	Inputs scale in proportion to capacity
Thermal	Operation	*/kWh	Inputs scale in proportion to utilization
Thermal	End-of-life	*/MW	Inputs scale in proportion to capacity
Non-bio renewable	Construction	*/MW	Inputs scale in proportion to capacity
Non-bio renewable	Operation	*/MW/yr	Inputs scale in proportion to capacity, but measured per year to eliminate influence of lifetime assumption in the LCA
Non-bio renewable	End-of-life	*/MW	Inputs scale in proportion to capacity

Having established $\boldsymbol{y}_{t,r,\tau,s,p}$, it is straightforward to determine the total output vector, $\boldsymbol{x}_{t,r,\tau,s,p}$, for a given technology t, region r, year τ and scenario s and life cycle phase p:

$$\boldsymbol{x}_{t,r,\tau,s,p} = (\boldsymbol{I} - \boldsymbol{A}_{\tau,s})^{-1} \cdot \boldsymbol{y}_{t,r,\tau,s,p} \quad , \quad t \in T, \ \ \mathrm{r} \in R, \ \ \tau \in \mathrm{T}, \ \ s \in S, \ \ p \in P \qquad (2)$$

where $\boldsymbol{I}$ is the identity matrix of appropriate order.

We now turn to the computation of LCA impact indicator coefficients. We let n^{imp} be the number of impact categories considered. We let $\boldsymbol{d}_{t,r,\tau,s,p}^{imp,tot}$ be an $n^{imp} \times 1$ column vector containing total impact indicator scores for a given combination of the parameters t, r, τ, s and p. Having determined $\boldsymbol{x}_{t,r,\tau,s,p}$, it is straightforward to establish the elements of $\boldsymbol{d}_{t,r,\tau,s,p}^{imp,tot}$ using standard LCA procedure, as expressed in Equation (3).

$$\boldsymbol{d}_{t,r,\tau,s,p}^{imp,tot} = \boldsymbol{C}^{imp} \cdot \boldsymbol{F}_{\tau,s} \cdot \boldsymbol{x}_{t,r,\tau,s,p} \quad , \quad t \in T, \ \ \mathrm{r} \in R, \ \ \tau \in \mathrm{T}, \ \ s \in S, \ \ p \in P \qquad (3)$$

We let n^{str} be the number of environmental load types defined in the system (in THEMIS, $n^{str} = 1613$). In Equation (3), $\boldsymbol{F}_{\tau,s}$ is an $n^{str} \times n_{\tau,s}^{fb}$ matrix of environmental load intensities (e.g., phosphate leaching to ground water from disposal of spoil from coal mining), and $\boldsymbol{C}^{imp}$ an $n^{imp} \times n^{str}$ matrix of characterization factors (e.g., representing the potency of phosphate released to ground water for eutrophication impacts) (ReCiPe, 2012).

3.3 Detailed treatment of energy use

In addition to distinguishing the three main life cycle phases (Subsection 3.2), our method decomposes energy requirements into energy carrier use by industries, and selected energy service types. While the method is valid for an arbitrary number of energy carriers, industries and energy service types, we select default options and use them in our case study of electricity supply: The selected energy carriers comprise liquid, gaseous and solid fuels, and electricity; and the selected energy services are freight transport, iron and steel production, and cement production. The selection of industries needs to correspond to the energy service types (freight transport, iron and steel, and cement), plus electricity, as electricity is a secondary energy form. One motivation for separating out key energy carriers, industries and energy services, is to avoid imposing LCA-specific assumptions on the IA modelling as far as possible. By this we mean that electricity mixes, transport and industry fuel mixes and fuel characteristics (including the emission intensities of fuels) should not be predetermined from the LCA side; rather, the IA analyst should be given the opportunity to represent such mixes and characteristics consistently using IAM-specific representation of these processes. By doing this, one can achieve unprecedented coverage of technology change in future-oriented analyses of life cycle impacts[5], as is demonstrated in the accompanying study by Pehl et al. (2017). Another motivation for separating out energy carriers by industries is that it may help to address potential problems of double-counting when LCA coefficients are introduced in IAMs[6].

In the following, we first describe an approach for achieving sound treatment of energy flows when deriving LCA energy coefficients for use in IAMs (subsection 3.3.1). This is a prerequisite for the decompositions of energy requirements into energy carriers, industries and energy service types, which are described next (subsections 3.3.2 and 3.3.3).

3.3.1 Consistent energy accounting

The Ecoinvent LCA database (and hence THEMIS, which relies extensively on Ecoinvent) does not support systematic energy accounting at the point of energy use. The energy content of losses in fuel supply chains (notably, such losses can be methane leakages from natural gas extraction sites or pipelines, or losses of coal during transport and storage) is not easily identifiable and distinguishable from fuel burning. Furthermore, heating value assumptions are not necessarily consistent across fossil fuel supply chains, due to internal inconsistencies in energy statistics used as data input to describe different parts of fuel supply chains in Ecoinvent

[5] Consider, for example, that because the LCA coefficients separate out solid fuels by industries, one can capture the life cycle effects of biomass replacing coal in IA scenarios; and because freight transport is separated out, one can capture the effects of shifts to low-carbon transport fuels (e.g., biofuels, hydrogen) in IA scenarios.

[6] Such double-counting issues are discussed in Daly et al. (2015) and Volkart et al. (2017).

(Arvesen and Hertwich, 2015). The established LCA practice for measuring energy is to consistently track energy streams to the point of resource extraction from nature, including energy losses along the chain linking energy carrier use and primary energy withdrawal from nature (e.g., fugitive methane emissions, loss in energy content of coal during transport and storage) (Arvesen and Hertwich, 2015; Frischknecht et al., 2015). The resulting energy quantity is often referred to as cumulative energy demand.

Consistency is ensured when using the cumulative energy demand method in Ecoinvent to perform standard LCA-type calculations. However, consistency is not necessarily achieved in calculations involving breaking up supply chains into disaggregated segments; in such cases a failure to properly handle heating value variations can lead to errors (Arvesen and Hertwich, 2015). In the context of deriving LCA energy coefficients for use in IAMs, it is also important to consider that state-of-the-art IAMs explicitly account for leakages (or losses) of methane in fossil fuel production and supply; hence, such methane leaks should be excluded from the LCA energy coefficients, in a similar manner as energy loss in thermal electricity production should be excluded. Our method to derive LCA energy coefficients resolves both these issues (heating value variations, and the need to exclude losses already represented in IAMs) by adopting the cumulative energy demand accounting practice in a uniform manner when calculating quantities of combustible energy (i.e., liquid, gaseous and solid fuels)[7]. This is also the case when measuring flows representing direct energy use in industrial activities. A further note of clarification is included in the supplementary material.

We refer to combustible energy flows determined in accordance with the cumulative energy demand method as characterized energy carriers, denoted as 'cec'. For the sake of convenience, we let electricity be included in the set of characterized energy carriers, and express the set as $CEC = \{liquids,\ \ gases,\ \ solids,\ \ electricity\}$. $n^{cec} = 4$ is the number of characterized energy carriers.

3.3.2 Energy carrier use by industries

We let $\boldsymbol{d}^{cec,tot}_{t,r,\tau,s,p}$ be an $n^{cec} \times 1$ column vector containing total characterized energy carrier values for the set CEC . An expression for determining $\boldsymbol{d}^{cec,tot}_{t,r,\tau,s,p}$ is given in Equation (4).

$$\boldsymbol{d}^{cec,tot}_{t,r,\tau,s,p} = \boldsymbol{C}^{cec,tot}_{\tau,s} \cdot \boldsymbol{x}_{t,r,\tau,s,p} \quad , \quad t \in T,\ \ \mathrm{r} \in R,\ \ \tau \in \mathrm{T},\ \ s \in S,\ \ p \in P \tag{4}$$

[7] Appendix A in Arvesen and Hertwich (2015) offers an example illustrating the basic procedure.

The analyst should define $\mathbf{C}_{\tau,s}^{cec,tot}$ such that the values for the combustible energy carriers included in the set CEC are calculated in accordance with the cumulative energy demand method, and that electricity requirements are captured as well. Electricity requirements may be calculated by a simple summation of appropriate entries in $\boldsymbol{x}_{t,r,\tau,s,p}$, while making sure that electricity represented at different voltage levels in the LCA database is not double-counted (this can achieved through Equation (4) and by defining $\boldsymbol{C}_{\tau,s}^{cec,tot}$ appropriately).

We let IND be the complete set of industries ($IND = \{electricity, \quad transport, \quad iron/steel, \quad cement\}$) and $n^{ind} = 4$ the number of industries for which we need to identify direct energy carrier use. We define $FB_{\tau,s}^{ec}$ as a subset of the set of all foreground and background processes which represents processes delivering energy carriers (e.g., coal, electricity), and $n_{\tau,s}^{ec}$ the number of processes included in $FB_{\tau,s}^{ec}$. At a minimum, $FB_{\tau,s}^{ec}$ must include the processes delivering energy carriers to processes that are part of the set IND (activities by any additional processes included in $FB_{\tau,s}^{ec}$ will be zeroed out in the calculations that follow). We let $\boldsymbol{A}_{\tau,s}^{ec}$ be an $n_{\tau,s}^{ec} \times n_{\tau,s}^{fb}$ matrix containing only the rows of $\boldsymbol{A}_{\tau,s}$ corresponding to the set $FB_{\tau,s}^{ec}$. Next, we let $\boldsymbol{B}_{\tau,s}^{ind}$ be a binary $n_{\tau,s}^{fb} \times n^{ind}$ correspondence matrix assigning foreground and background processes to the industry sectors included in IND. In $\boldsymbol{B}_{\tau,s}^{ind}$, a non-zero entry indicates that a process belongs to one of the selected industries. Rows representing processes that do not match with any of the selected industries contain only zeros. Finally, we let $\boldsymbol{E}_{t,r,\tau,s,p}^{ec,dir}$ be an $n_{\tau,s}^{ec} \times n^{ind}$ matrix representing the direct use of $n_{\tau,s}^{ec}$ energy carriers by n^{ind} industries (the superscript 'dir' denotes 'direct'). $\boldsymbol{E}_{t,r,\tau,s,p}^{ec,dir}$ may be calculated according to equation (5).

$$\boldsymbol{E}_{t,r,\tau,s,p}^{ec,dir} = \boldsymbol{A}_{\tau,s}^{ec} \cdot \widehat{\boldsymbol{x}_{t,r,\tau,s,p}} \cdot \boldsymbol{B}_{\tau,s}^{ind} \quad , \ t \in T, \ \mathrm{r} \in R, \ \tau \in \mathrm{T}, \ s \in S, \ p \in P \tag{5}$$

$\boldsymbol{E}_{t,r,\tau,s,p}^{ec,dir}$ will typically represent a large number of energy flows individually (e.g., various inputs of electricity of different geographical origin, fuel oil burned in various machines or devices). There is a need to classify these energy flows into the main energy carrier types comprising the set CEC, and to characterize the combustible energy flows using the cumulative energy demand method in order to achieve consistent accounting (cf. subsection 3.3.1). This implies that entries representing non-electricity energy carriers in $\boldsymbol{E}_{t,r,\tau,s,p}^{ec,dir}$

need to be multiplied by appropriate factors to convert to cumulative energy demand equivalence. In order to achieve this, we introduce $\boldsymbol{C}_{\tau,s}^{cec,dir}$ as an $n^{cec} \times n_{\tau,s}^{ec}$ matrix collecting coefficients to convert non-electricity entries in $\boldsymbol{E}_{t,r,\tau,s,p}^{ec,dir}$ to cumulative energy demand equivalence, as well as coefficients allowing for entries representing electricity to be summed together. $\boldsymbol{C}_{\tau,s}^{cec,dir}$ should be defined such that left-multiplying $\boldsymbol{E}_{t,r,\tau,s,p}^{ec,dir}$ by $\boldsymbol{C}_{\tau,s}^{cec,dir}$ (Equation (6)) yields an $n^{cec} \times n^{ind}$ matrix, $\boldsymbol{D}_{t,r,\tau,s,p}^{cec,dir}$, representing direct non-electricity and electricity use in the selected industries.

$$\boldsymbol{D}_{t,r,\tau,s,p}^{cec,dir} = \boldsymbol{C}_{\tau,s}^{cec,dir} \cdot \boldsymbol{E}_{t,r,\tau,s,p}^{ec,dir} \quad , \quad t \in T, \ \ \mathrm{r} \in R, \ \ \tau \in \mathrm{T}, \ \ s \in S, \ \ p \in P \tag{6}$$

The characterized energy carrier values in $\boldsymbol{d}_{t,r,\tau,s,p}^{cec,tot}$ and $\boldsymbol{D}_{t,r,\tau,s,p}^{ec,dir}$ are partially overlapping, as the direct energy use in the selected industries are accounted for in both variables. We now subtract values in $\boldsymbol{D}_{t,r,\tau,s,p}^{cec,dir}$ from values in $\boldsymbol{d}_{t,r,\tau,s,p}^{cec,tot}$ to obtain residual energy requirements (i.e., the energy use occurring in other industries than those comprising the set IND), as expressed in Equation (7). $\boldsymbol{d}_{t,r,\tau,s,p}^{cec,res}$ refers to an $n^{cec} \times 1$ column vector containing the residual energy requirement values.

$$\boldsymbol{d}_{t,r,\tau,s,p}^{cec,res} = \boldsymbol{d}_{t,r,\tau,s,p}^{cec,tot} - \boldsymbol{D}_{t,r,\tau,s,p}^{ec,dir} \cdot \boldsymbol{1} \quad , \quad t \in T, \ \ \mathrm{r} \in R, \ \ \tau \in \mathrm{T}, \ \ s \in S, \ \ p \in P \tag{7}$$

where 1 is a $n^{ind} \times 1$ column vector of ones.

3.3.3 Energy service requirements

We measure energy service requirements in terms of total output of the industries delivering the energy services, in units of tonne-kilometres (for transport) or tonnes (for material production). As different industries are represented in different ways in the LCA database, it is not possible to provide a general recipe for how to establish numbers on total industry outputs. We establish transport requirements by simple summation of freight transport outputs (including different types of road, rail and water transport outputs) represented in $\boldsymbol{x}_{t,r,\tau,s,p}$. Life cycle accounting of material outputs is less simple and cannot generally be achieved by summation of entries in $\boldsymbol{x}_{t,r,\tau,s,p}$. This is because $\boldsymbol{x}_{t,r,\tau,s,p}$ defines outputs from various material processing steps that partially form linear chains of processes and partially looped systems (i.e., output from one process becomes the input to another process). In this study, we employ the algorithm presented by Singh et al. (2015) to determine material requirements. We let $\boldsymbol{x}_{t,r,\tau,s,p}^{ind}$

be an $1 \times n^{ind}$ row vector collecting all industry output levels (here understood as analogous to energy service requirements) for the industries represented by the set IND.

A data set consisting of $\boldsymbol{d}_{t,r,\tau,s,p}^{ec,res}$ and $\boldsymbol{x}_{t,r,\tau,s,p}^{ind}$ together with IAM-specific energy intensity and emission intensity factors will contain sufficient information for IA analysts to determine life cycle emission estimates. Meanwhile, IAMs differ in their resolution and not all IAMs resolve transport and material producing industries explicitly. Hence, we provide energy multiplication factors for the industries represented by the set IND as well, based on LCA model-specific data. IA analysts may choose to use these data in lieu of IAM-specific data. We let $\tilde{\boldsymbol{D}}_{t,r,\tau,s,p}^{cec,dir}$ be an $n_{\tau,s}^{cec} \times n^{ind}$ matrix representing the use of $n_{\tau,s}^{cec}$ energy carriers by n^{ind} industries, normalized to the total output levels of the respective industries. $\tilde{\boldsymbol{D}}_{t,r,\tau,s,p}^{cec,dir}$ may be determined from equation (8).

$$\tilde{\boldsymbol{D}}_{t,r,\tau,s,p}^{cec,dir} = \boldsymbol{D}_{t,r,\tau,s,p}^{cec,dir} \ \bigcirc \ \boldsymbol{x}_{t,r,\tau,s,p}^{ind} \tag{8}$$

Here, the empty circle ($\bigcirc$) indicates division of all entries in column number j of $\boldsymbol{D}_{t,r,\tau,s,p}^{cec,dir}$ by entry number j in $\boldsymbol{x}_{t,r,\tau,s,p}^{ind}$.

In the case study of electricity supply, the numerical values in $\tilde{\boldsymbol{D}}_{t,r,\tau,s,p}^{cec,dir}$ are approximately the same irrespective of technology and phase. For this reason and in order to simplify data exchange, we compute median values across technologies and phases, and let $\tilde{\boldsymbol{D}}_{r,\tau,s}^{cec,dir,med}$ be an $n_{\tau,s}^{cec} \times n^{ind}$ matrix recording the median values.

4 LCA coefficient results for illustration

Table 4 shows, as an illustrative example, LCA energy and impact indicator results obtained for solar photovoltaic electricity for year 2010, 2030 and 2050. Results for China are shown as an example. The table also clarifies how the numerical results relate to variables defined in the exposition of the approach. The rationale for including Table 4 is not to present quantitative results per se, but rather the table is included for the purposes of illustration. For the same purposes, Figs. 3 and 4 offer illustrative energy results. The complete set of energy and impact indicator results is available as electronic supplementary material, and is utilized in the related studies Pehl et al. (2017) and Luderer et al. (under review).

Table 4
Illustrative LCA energy and impact indicator coefficients. Results are shown for solar photovoltaic (PV) electricity, Baseline scenario and China region, as an example. The end-of-life phase is omitted here for the sake of brevity, but is included in the numerical results provided as supplementary material. GJ = gigajoule; MW = megawatt; tkm = tonne-kilometres; t = tonne; yr = year.

Scenario	Region	Unit	Variable name	Value by year		
				2010	2030	2030
Residual energy requirements (general symbol: $\boldsymbol{d}^{cec,res}_{t,r,\tau,s,p}$):						
Baseline	China	GJ/MW	Residual energy requirements|PV|Construction|Electricity	8.8E+03	2.7E+03	1.8E+03
Baseline	China	GJ/MW	Residual energy requirements|PV|Construction|Liquids	6.1E+03	2.7E+03	2.2E+03
Baseline	China	GJ/MW	Residual energy requirements|PV|Construction|Gases	6.1E+03	2.5E+03	1.9E+03
Baseline	China	GJ/MW	Residual energy requirements|PV|Construction|Solids	1.0E+03	7.8E+02	6.9E+02
Baseline	China	GJ/MW	Residual energy requirements|PV|Operation|Electricity	5.8E-01	4.1E-01	3.4E-01
Baseline	China	GJ/MW	Residual energy requirements|PV|Operation|Liquids	5.2E-02	3.5E-02	2.9E-02
Baseline	China	GJ/MW	Residual energy requirements|PV|Operation|Gases	1.7E+00	1.2E+00	9.7E-01
Baseline	China	GJ/MW	Residual energy requirements|PV|Operation|Solids	1.5E-02	1.0E-02	8.1E-03
Energy service requirements (general symbol: $\boldsymbol{x}^{ind}_{t,r,\tau,s,p}$):						
Baseline	China	tkm/MW	Energy service requirements|PV|Construction|Freight transport	3.93E+06	1.56E+06	1.07E+06
Baseline	China	t iron/MW	Energy service requirements|PV|Construction|Iron and steel	8.44E+01	6.45E+01	5.49E+01
Baseline	China	t cement/MW	Energy service requirements|PV|Construction|Cement	2.60E+01	1.65E+01	1.34E+01
Baseline	China	tkm/MW/yr	Energy service requirements|PV|Operation|Freight transport	1.47E+02	9.53E+01	7.49E+01
Baseline	China	t iron/MW/yr	Energy service requirements|PV|Operation|Iron and steel	9.51E-04	6.66E-04	5.44E-04
Baseline	China	t cement/MW/yr	Energy service requirements|PV|Operation|Cement	1.83E-04	1.27E-04	1.04E-04
Industry direct energy requirements (general symbol: $\tilde{\boldsymbol{D}}^{cec,dir,med}_{r,\tau,s}$):						
Baseline	China	GJ/tkm	Industry direct energy requirements|Freight transport|Electricity	1.6E-05	1.6E-05	1.7E-05
Baseline	China	GJ/tkm	Industry direct energy requirements|Freight transport|Liquids	1.0E-04	1.0E-04	1.0E-04
Baseline	China	GJ/tkm	Industry direct energy requirements|Freight transport|Gases	0.0E+00	0.0E+00	0.0E+00
Baseline	China	GJ/tkm	Industry direct energy requirements|Freight transport|Solids	8.9E-13	2.4E-12	3.1E-12
Baseline	China	GJ/t iron	Industry direct energy requirements|Iron and steel|Electricity	5.1E-01	5.1E-01	5.1E-01
Baseline	China	GJ/t iron	Industry direct energy requirements|Iron and steel|Liquids	4.3E-02	4.3E-02	4.3E-02
Baseline	China	GJ/t iron	Industry direct energy requirements|Iron and steel|Gases	3.9E-01	3.9E-01	3.9E-01
Baseline	China	GJ/t iron	Industry direct energy requirements|Iron and steel|Solids	8.5E+00	8.5E+00	8.5E+00
Baseline	China	GJ/t cement	Industry direct energy requirements|Cement|Electricity	4.6E-01	4.5E-01	4.5E-01
Baseline	China	GJ/t cement	Industry direct energy requirements|Cement|Liquids	1.4E+00	1.4E+00	1.4E+00
Baseline	China	GJ/t cement	Industry direct energy requirements|Cement|Gases	1.0E-02	1.0E-02	1.0E-02

Baseline	China	GJ/t cement	Industry direct energy requirements|Cement|Solids	9.2E-01	9.2E-01	9.2E-01
Impact indicator results (general symbol: $\boldsymbol{d}_{t,r,\tau,s,p}^{imp,tot}$):						
Baseline	China	kg 1,4-DCB-Eq/MW	Freshwater ecotoxicity|PV|Construction	1.44E+05	4.27E+04	2.93E+04
Baseline	China	kg P-Eq/MW	Freshwater eutrophication|PV|Construction	1.67E+03	7.66E+02	5.89E+02
Baseline	China	kg 1,4-DCB-Eq/MW	Human toxicity|PV|Construction	1.89E+06	6.75E+05	4.60E+05
Baseline	China	kg U235-Eq/MW	Ionising radiation|PV|Construction	4.98E+04	2.71E+04	2.28E+04
Baseline	China	m2a/MW	Land occupation|PV|Construction	9.11E+04	3.45E+04	2.45E+04
Baseline	China	kg N-Eq/MW	Marine eutrophication|PV|Construction	5.90E+02	2.22E+02	1.54E+02
Baseline	China	kg Fe-Eq/MW	Mineral resource depletion|PV|Construction	8.53E+05	7.13E+05	6.56E+05
Baseline	China	t Al/MW	Aluminium|PV|Construction	2.05E+01	1.06E+01	8.14E+00
Baseline	China	t Cu/MW	Copper|PV|Construction	9.47E+00	8.15E+00	7.28E+00
Baseline	China	t Fe/MW	Iron|PV|Construction	8.63E+01	6.74E+01	5.77E+01
Baseline	China	t cement/MW	Cement|PV|Construction	2.61E+01	1.66E+01	1.35E+01
Baseline	China	kg 1,4-DCB-Eq/MW/yr	Freshwater ecotoxicity|PV|Operation	1.19E+00	7.92E-01	6.42E-01
Baseline	China	kg P-Eq/MW/yr	Freshwater eutrophication|PV|Operation	6.60E-02	4.34E-02	3.50E-02
Baseline	China	kg 1,4-DCB-Eq/MW/yr	Human toxicity|PV|Operation	1.97E+01	1.28E+01	1.01E+01
Baseline	China	kg U235-Eq/MW/yr	Ionising radiation|PV|Operation	3.36E+00	2.66E+00	2.30E+00
Baseline	China	m2a/MW/yr	Land occupation|PV|Operation	1.34E+04	9.47E+03	7.74E+03
Baseline	China	kg N-Eq/MW/yr	Marine eutrophication|PV|Operation	2.14E-02	1.40E-02	1.12E-02
Baseline	China	kg Fe-Eq/MW/yr	Mineral resource depletion|PV|Operation	4.31E+00	3.03E+00	2.47E+00
Baseline	China	t Al/MW/yr	Aluminium|PV|Operation	3.82E-05	2.64E-05	2.15E-05
Baseline	China	t Cu/MW/yr	Copper|PV|Operation	9.39E-05	6.61E-05	5.41E-05
Baseline	China	t Fe/MW/yr	Iron|PV|Operation	1.02E-03	7.14E-04	5.83E-04
Baseline	China	t cement/MW/yr	Cement|PV|Operation	1.86E-04	1.29E-04	1.05E-04

Fig. 3 displays life cycle indirect energy requirements for a series of power generation options. As IAMs already cover all direct energy use (i.e., energy fuel combustion occurring at the power plants being studied) and our current aim is to provide coefficients for indirect energy use, direct energy use is not treated in our method and not included in Fig. 3[8]. Results for Europe and year 2010 are shown here, as an example. For the sake of simplicity, and because contributions from the end-of-life phase are uniformly small (< 2% of totals), in this graphical representation the construction and end-of-life phases are aggregated into one single category. For similar reasons, energy use occurring in iron and steel production, and in cement production are aggregated in the figure. Another factor to note is that the results shown in Fig. 3 are produced using capacity factor and lifetime assumptions in THEMIS. However, these assumptions will effectively be replaced by IAM-specific assumptions when IA analysts utilize the numerical results as they are presented in the electronic supplement.

[8] It may also be noted that besides application in IAMs, the indirect energy use of supplying energy has relevance for discussions on the importance of energy for economic growth (Ayres and Voudouris 2014; Carbajales-Dale et al. 2014; Hall et al. 2014).

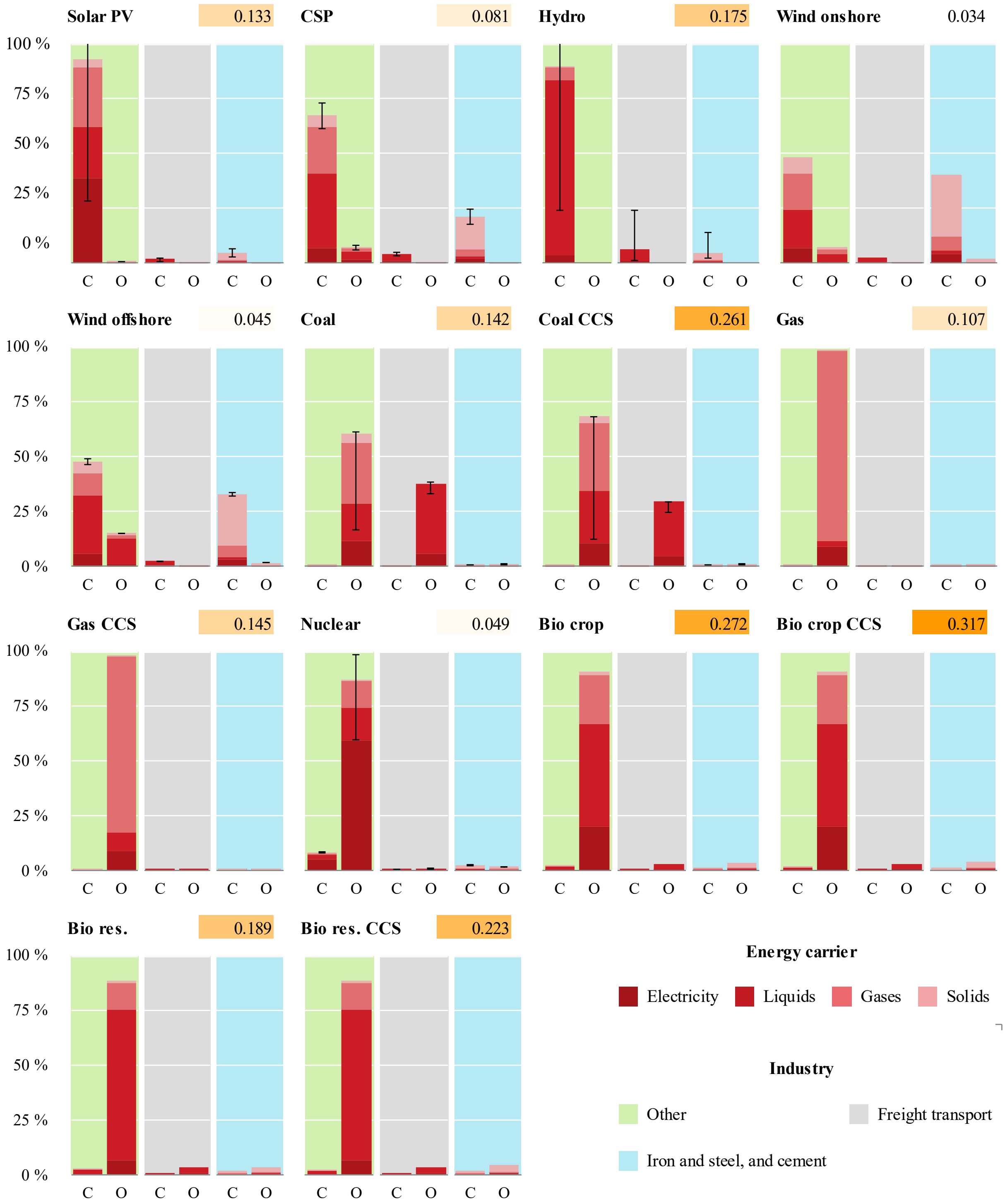

Fig. 3. Life cycle indirect energy requirements for 14 main types of power generation for Europe and year 2010, broken down into phase (construction and end-of-life total, denoted by C; operational, denoted by O), energy carrier used (electricity; liquid, gaseous and solid fuels) and industry in which the use occurs (iron and steel; cement; freight transport; and other). Stacked columns represent relative contributions to total indirect energy (i.e., sum across all columns and stacked categories within columns equals 100% for each plot). For bio crop, results for a scenario assuming no restriction on types of cellulosic biomass crop available and where irrigation is allowed are shown as an example (the 'TAX30_begr_betr_ir' scenario'; see electronic supplement). Error bars indicate extrema totals across technology subcategories relative to the mean across technology type (cf. Table 1). Vertical axes are cut at 100%, but some maxima lie above 100%: slightly >100% for solar PV, C, other; and 350% for hydro, C, other. Numerical values above plots give total indirect energy requirements in units of megajoule (MJ) energy input per MJ electricity output and exclude losses in the power production process itself. The values are shaded according to their relative magnitude (in reference to the whole set of values), with light

(heavy) shading denoting small (big) magnitude. PV = photovoltaic; CSP = concentrating solar power; CCS = carbon capture and storage; Bio crop = cellulosic biomass from crops; Bio res. = biomass from forest residues.

It is evident from Fig. 3 that fossil and biomass fuel-based power generation options generally exhibit the highest total indirect energy requirements. This is, in different ways for the different options, attributable to extraction or collection, processing and distribution of fuel energy sources and carriers. All power plants utilizing carbon capture and storage (CCS) have lower efficiencies and additional process inputs compared to their non-CCS counterparts, which lead to higher indirect energy per unit of electricity output for CCS cases. Among non-biomass renewable alternatives, hydropower and solar photovoltaic power show the highest total indirect energy requirements (Fig. 3). For hydro, the comparatively large energy requirements are a result of considerable transport requirements for one of the two hydro power facilities modelled, namely the facility situated in a remote area. As for solar photovoltaic power, energy-intensive material processing and manufacturing activities, in particular connected to solar-grade silicon production, give rise to considerable indirect energy requirements. While Fig. 3 only shows results for the year 2010, results for 2030 and 2050 reflect substantial technological improvements for solar photovoltaic power, as is illustrated by Fig. 4 and discussed later in this subsection. A more detailed discussion of Fig. 3, including comparisons with results in literature (Raugei and Leccisi, 2016; Warner and Heath, 2012), is presented in the supplementary material.

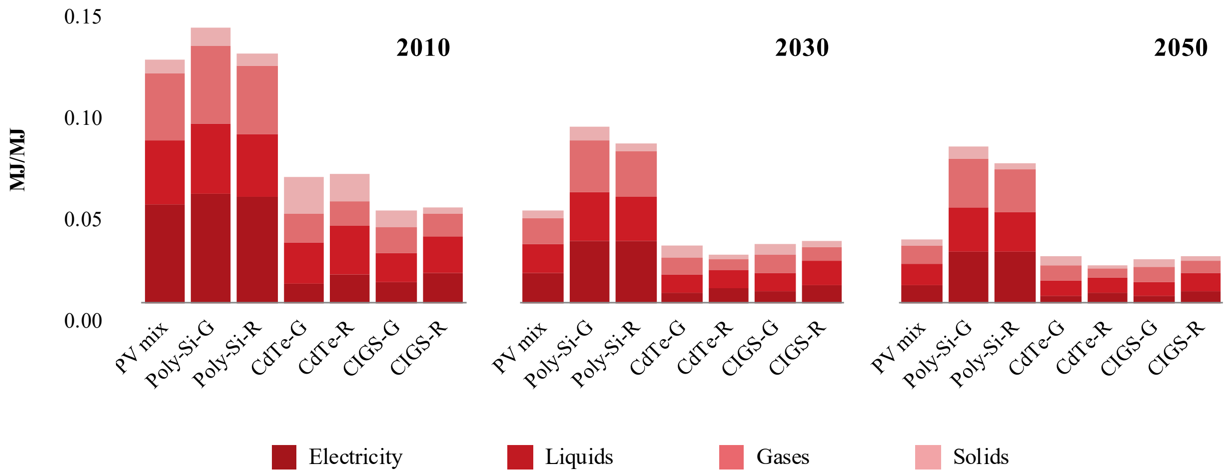

Fig. 4. Total life cycle indirect energy requirements (measured in megajoule (MJ) energy input per MJ electricity output) associated with solar photovoltaic (PV) power in China for year 2010, 2030 and 2050, for six individual types of PV technologies as well as for the mix of individual types ('PV mix', leftmost column in each panel; given the assumed market shares of individual technologies displayed in Table 1). Energy requirements are broken down into energy carrier (electricity; liquid, gaseous and solid fuels) contributions, correspondingly as in Fig. 3, but the current Fig. 4 does not make the separation into life cycle phases. Energy requirements are measured as indirect energy input per electricity output. PV technology abbreviations: Poly-Si-G: polycrystalline silicon, ground; Poly-Si-R: polycrystalline silicon, rooftop; CdTe-G: cadmium-telluride, ground; CdTe-R: cadmium-telluride, rooftop; CIGS-G: copper indium gallium selenide, ground CIGS-R: copper indium gallium selenide, rooftop.

While Fig. 3 displays results for year 2010 only, we also produce results for the years 2030 and 2050. Fig. 4 details prospective indirect energy requirements results for solar photovoltaic (PV) electricity, showing results for both the aggregate mix of PV technology types (leftmost column in each panel) and for each individual type (the six rightmost columns in each panel). Solar PV electricity is chosen here as an example because it is a technology for which considerable future technological improvements are anticipated (as opposed to, for example, hydropower, which is based on relatively mature technology). As is evident from Fig. 4, thin-film PV, here represented by cadmium-telluride and copper indium gallium selenide technologies, exhibit much lower indirect energy requirements than conventional, poly-crystalline silicon PV. Moreover, the indirect requirements of the thin-film technologies decline noticeably over time, mainly owing to projected rises in conversion efficiencies[9]. In our results, the combination of *i*) a shift away from polycrystalline silicon and towards thin-film technologies (cf. Table 1) and *ii*) thin-film technologies becoming more efficient over time, entails a reduction in the energy requirements of the average PV electricity mix of 70% from 2010 to 2050. Electricity is an important energy carrier in relative terms for PV (compare the relative importance of electricity for PV versus other power generation options, evident from Fig. 3), which implies further reductions in the life cycle greenhouse gas emissions of PV in scenarios where electricity becomes cleaner.

5 Final remarks

We believe that potentials exist for the IAM and LCA fields to interact in beneficial ways. The IAM community has a strong tradition in analysing transformation pathways on the macro level, while for LCA – which traditionally has been micro- and static-minded – this is an emerging research interest. The LCA community has decades of experience in developing formal procedures for assessing impact types as diverse as, among others, air pollution and toxic contamination of soil and water, while IA analysts in recent years have made major strides in incorporating various air pollutants as well as aspects of land use and water demand in their models. The life cycle perspective is unique for LCA, but LCA lacks the optimization perspective of IAM.

In this article, we present a novel method for deriving LCA-based coefficients suitable for application in IAMs. The method decomposes LCA coefficients into life cycle phases and energy carrier use by industries, thus facilitating attribution of life cycle effects to appropriate years, and consistent and comprehensive use of IA model-specific scenario data (e.g., emission factors, lifetime and utilization rates of equipment) when the LCA coefficients are applied in IA scenario modelling. The method is flexible with respect to possible use (i.e., it can be applied to study any kind of product) and resolution levels of input data (i.e., the life cycle inventory

[9] A related discussion is available in Bergesen et al. (2014).

data can have any degree of resolution) and output data (i.e., the final LCA coefficients can represent any number of energy carriers or industries separately).

The method is devised for LCA analytic frameworks where activities are described bottom-up and in physical terms, as opposed to multiregional input-output (MRIO) frameworks as employed in other work (Daly et al., 2015; Scott et al., 2016). Bottom-up LCA and MRIO analysis both have their merits and demerits (Subsection 1.2), and we anticipate that both techniques will be used in future research addressing the role of life cycle effects in climate change mitigation scenarios. In the version of THEMIS used to derive LCA coefficients for electricity supply, scenario data inputs to THEMIS itself come from exogenous sources, as described in Gibon et al. (2015). A possible future improvement when THEMIS is used in conjunction with an IAM, however, would be to obtain scenario data inputs to THEMIS specifically from the IAM in question, thus enhancing harmonization of scenario data across the LCA and IAM modelling.

We regard the method presented in this article as a generally applicable and useful method to derive LCA coefficients for use in IA modelling, when core structures and data organization principles in LCA and IAM are given. The energy accounting based on cumulative energy demand (subsection 3.3.1) may usefully be replaced by a simpler procedure if LCA databases adopt a more practical and consistent inventory of secondary and final energy (i.e., an inventory distinguishing supply chain energy losses and energy use, based on consistent heating value assumptions). In the future, parts of the method may be integrated into new and more advanced methods – or be replaced by them, – for example if IAMs should be re-structured to consider indirect energy use and emissions in a systematic fashion and with internal consistency. Strategies and priorities for taking into account life cycle effects in evaluations of vast-scale transformation pathways need to be evaluated continuously, considering the moving frontiers of LCA and IAM research and available evidence on the importance of life cycle effects in the context of climate change mitigation and sustainability assessment, as well as practical concerns such as the need to limit model complexity. With exceptions (Daly et al., 2015; Pehl et al., 2017; Scott et al., 2016), to date it remains largely unexplored whether, or under what circumstances, the types of causality relationships that form the heart of LCA (e.g., wind turbines require steel, steel producers require fossil fuels and fossil fuel use causes emissions) can have significant influences on optimized global energy and climate mitigation strategies (Arvesen et al., 2011; Dale et al., 2012a).

Finally, it is worth noting that this article is written largely from the standpoint of LCA, and to a much lesser degree from the standpoint of IAM. Accompanying articles currently in preparation address this imbalance by applying LCA coefficients for electricity supply in integrated assessment (Luderer et al., under review; Pehl et al., 2017).

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Supplementary material

Supplementary material related to this article can be found at http://...

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