ZORAN STEINMANN

Reducing uncertainty and redundancy in environmental footprinting

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'Isn't it enough to see that a garden is beautiful without having to believe that there are fairies at the bottom of it too?'

DOUGLAS ADAMS

'In science there are no authorities;
at most, there are experts.'

CARL SAGAN

Contents

CHAPTER 1
Introduction 9

CHAPTER 2
A methodology for separating uncertainty and variability in the life cycle greenhouse gas emissions of coal-fueled power generation in the USA 19

CHAPTER 3
How To Address Data Gaps in Life Cycle Inventories: A Case Study on Estimating CO_2 Emissions from Coal-Fired Electricity Plants on a Global Scale 39

CHAPTER 4
Estimating the greenhouse gas balance of individual gas-fired and oil-fired electricity plants on a global scale 57

CHAPTER 5
How Many Environmental Impact Indicators Are Needed in the Evaluation of Product Life Cycles? 73

CHAPTER 6
Headline environmental indicators revisited with the global multi-regional input-output database EXIOBASE 89

CHAPTER 7
Resource Footprints are Good Proxies of Environmental Damage 103

CHAPTER 8
Synthesis 117

References 127

Appendices 1-7 140

Samenvatting 197

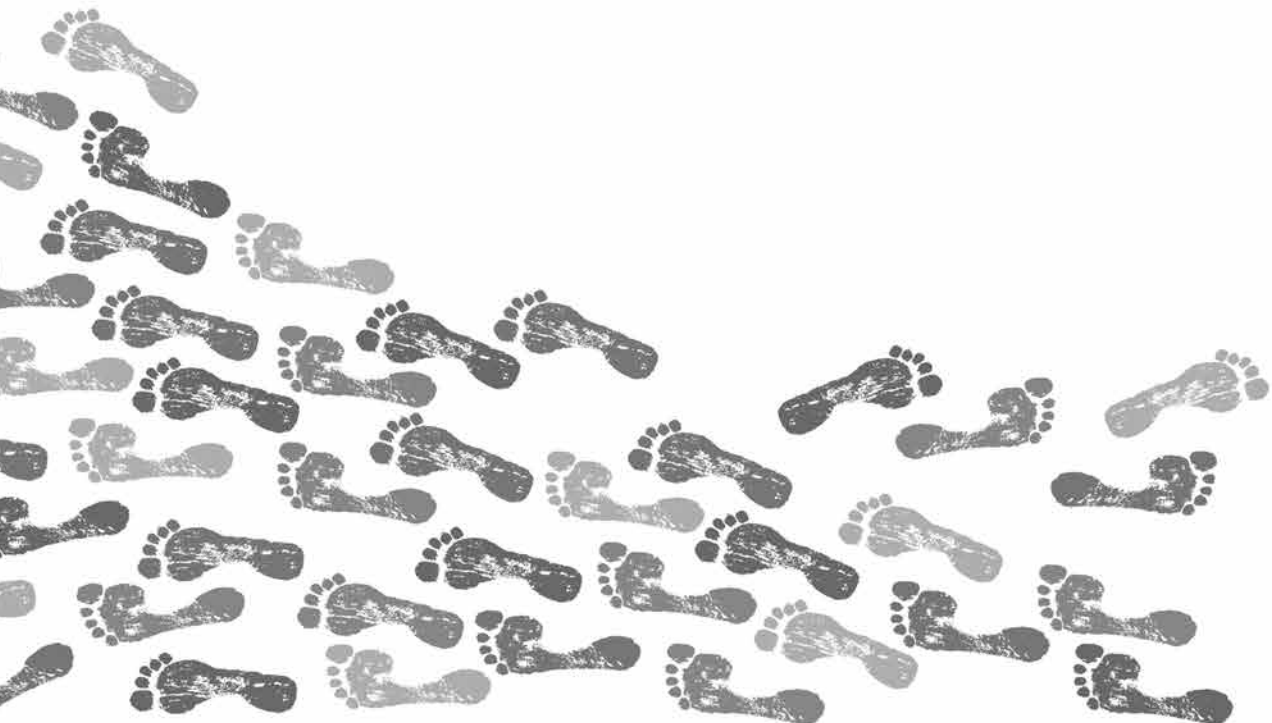
Summary 201

Acknowledgements (Dankwoord) 205

About the author 209

CHAPTER 1

Introduction



Environmental footprints

LIFE CYCLE PERSPECTIVE

Fulfilling and maintaining our needs and welfare in the modern industrialized society have brought unintended environmental and social impacts, for example on biodiversity and human health. In order to quantify our society's impacts on the world's biodiversity, integrated assessments such as the Millennium Ecosystem Assessment (MEA, 2005) and the Global Biodiversity Outlooks (Secretariat of the Convention on Biological Diversity, 2014) have been established. Impacts on human health are assessed by the Global Burden of Disease Studies (GBD collaborators, 2015). While these large-scale assessments estimate the total anthropogenic impact on the environment, they cannot be used directly to attribute these impacts to specific entities, like production processes, products, services or geographical entities like cities, regions or countries. The environmental impact caused by a given entity is called a footprint. These footprints can be used for comparisons aimed at impact reductions, for example through (production) process optimization and eco-labeling. There are numerous studies focusing on widely differing footprints and entities, ranging from the carbon footprints of British households (Druckman & Jackson, 2009) to the water footprint of jeans manufacturing (Chico et al., 2013). Environmental footprints are calculated over the full life cycle of these entities, from extraction of raw materials to manufacture, use and eventually waste disposal, whereby the required transport and infrastructure in any of the stages are also taken into account. It is crucial to consider the full life cycle, because the relative impact of each life cycle stage can vary depending on the process, product, service or geographical entity under consideration. For instance, for fossil energy technologies the use phase is most relevant (Jaramillo et al., 2007) while the production phase is highly relevant in the case of greenhouse gas emissions caused by solar energy technologies (Nugent & Sovacool, 2014). By taking into account the full life cycle, burden shifts from one stage to the other are avoided (ISO, 2006).

There are two main ways of calculating environmental footprints, i.e., process-based Life Cycle Assessment (LCA) and Environmentally Extended Multi-Regional Input-Output modelling (EEMRIO) (Suh & Huppes, 2005). Both approaches consist of two parts: the inventory and the impact assessment. The emissions and resource extractions (collectively referred to as interventions) that take place over the life cycle of a product or service are listed as completely as possible during the inventory part. The impact caused by these interventions is then quantified during the impact assessment step. In process-based LCA the life cycle inventory of a product or service is compiled by identifying all relevant processes that are required to manufacture and use a product. This is a bottom-up approach that can provide great spatial and technological detail, but also requires a large data-gathering effort if the supply chain of the product is complex. Using a cut-off to limit the number of included processes is needed, because otherwise the tracing of process to process could go on indefinitely (Suh & Huppes, 2002). EEMRIO on the other hand employs

a top-down strategy, whereby the economic Input-Output tables of multiple countries are used to trace the flow of money through the different sectors of an economy. For each sector the interventions, called environmental extensions in EEMRIO modelling, are provided per monetary unit. The EEMRIO approach is more comprehensive than the LCA approach in the sense that it covers the majority of the world's economy and avoids arbitrary cut-offs, making it relatively simple to cover the entire life cycle. However, this goes on the expense of detail. Since the economic sectors in Input-Output models are broad, there is limited detail on a product level. For example the steel sector, which produces numerous different kinds (e.g. plate steel, steel bars, nails, screws etc.) and qualities of steel is treated as one homogeneous sector with only one output product. Only a limited number of economic sectors (less than 200) can be included, meaning that numerous different products are modelled as one homogenous economic sector. The LCA approach is typically used to calculate footprints of specific products and processes, whereas the EEMRIO approach is more suited to calculate footprints of geographical entities. Both ways are sometimes used in conjunction in the assessment of products. In these so-called hybrid LCAs, process-based data is used for the most important foreground processes and Input-Output models are used to calculate the background system for which detailed data gathering is unfeasible (Williams et al., 2009; Majeau-Bettez et al., 2013).

In both approaches, processes or sectors do not only depend on external input, but they may also depend on their own output directly (for example if a fuel producing sector/process also consumes some of the fuel it produces) or indirectly via another sector (if there are mutual exchanges between two or more processes or sectors, for example the electricity sector buying coal from the coal mining sector while the coal mining sector at the same time requires electricity from the electricity sector). In order to calculate a comprehensive footprint, all these transactions within and between processes or sectors need to be taken into account. This can be achieved by calculating a footprint matrix (FP) as Leontief (1966) proposed:

$$FP = C * E * (I-A)^{-1} * y \qquad \textbf{Equation 1}$$

The emissions matrix (E) lists all interventions per economic sector (for EEMRIO) or process (for process-based LCA). The Leontief inverse of the activity matrix is given by $(I-A)^{-1}$, in which the activity matrix (A) contains all transactions between and within sectors or processes and I is an identity matrix of the same size. The Leontief inverse multiplied by the final demand vector (y) shows how much additional production is required to fulfil the final demand (i.e. the entity for which the footprint is to be assessed). The product of the emissions matrix, the Leontief inverse of the activity matrix and the final demand vector ($E*(I-A)^{-1}*y$) forms the life cycle inventory, a list of interventions belonging to the life cycle of a product, service or sector. To determine the environmental impact caused by these interventions, the inventory is multiplied by a characterization matrix (C), which lists the environmental impact per intervention (see next section for further explanation on characterization of impacts). This yields the environmental footprint (FP) for the entity under analysis (equation 1).

IMPACT INDICATORS

As mentioned in the previous section, the environmental impact caused by each intervention is given in the characterization matrix. Indicators for midpoint, endpoint and resource footprints can be included in the characterization matrix. The simplest type of footprint indicators are the resource footprints. These footprints are calculated by an unweighted summation of the life cycle resource use, without the need for any further calculation steps (Fig. 1.1). Examples are the land, energy, water and material footprints which express the life cycle land use (in m^2yr), energy use (in MJ) water consumption (in m^3) and raw material extraction (in kg), respectively. The rationale behind using these simple indicators is that limiting the use of these resources can have merit by itself (for example reducing the water consumption in water scarce countries). These resource footprints may also be representative of a more broad range of impacts because resource use can either directly (through water scarcity or land use) or indirectly cause environmental damage (for example through emissions released during the burning of fossil fuels).

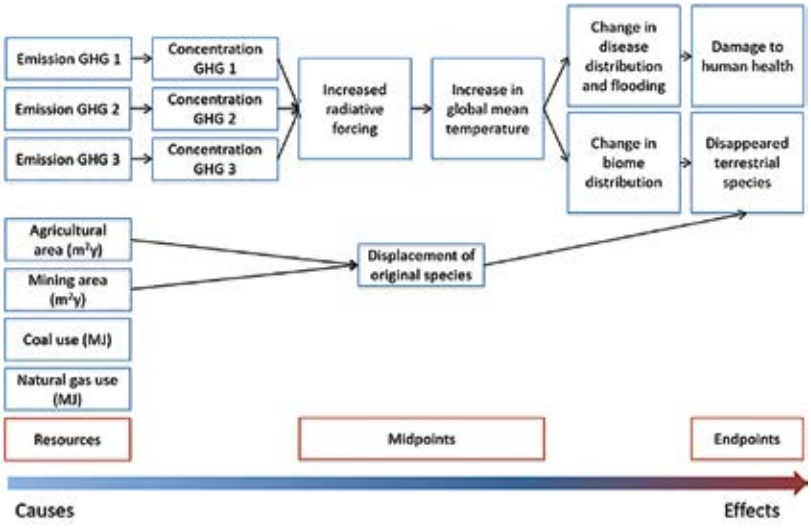


FIGURE 1.1 Cause-and-effect chain for climate change, caused by greenhouse gas (GHG) emissions (top part). Midpoint indicators can be derived on the point where the mechanism between different greenhouse gases is the same. Endpoint indicators quantify damage to the areas of protection we ultimately care about. Resource footprints (bottom part) are derived at the very beginning of the cause-and-effect chain and are simply calculated by summing several interventions from the inventory. These interventions may or may not have a direct connection to environmental damage, e.g. land use leads to disappeared terrestrial species whereas coal or natural gas use by itself is not harmful to the environment, but the emissions resulting from this use (which are listed separately in the inventory) may be.

The resource footprints are easy to calculate and communicate, but their representativeness (or lack thereof) of the environmental impact is unclear. More modeling steps are required to quantify how human health or biodiversity is ultimately impacted by the interventions generated during a product or service life cycle. Life cycle impact

assessment (LCIA) methods were developed to quantify the environmental impact of hundreds of potentially impactful interventions. LCIA translates interventions on the one hand (causes) to environmental impacts (effects) on the other hand (Figure 1.1). The interventions are grouped in so-called impact categories, which are defined in such a way that different interventions with the same mode of impact can be combined and aggregated. Midpoint indicators can be derived along different parts of the cause-and-effect chain, as long as the mechanism leading towards environmental impact is shared among the different interventions present in that impact category. An example of a midpoint impact category is climate change, which is caused by different greenhouse gases (GHGs) (Figure 1.1). The emissions and atmospheric fate of the different GHGs are different, but once their time-integrated radiative forcing effect is known they can be compared directly and combined into one metric. The factors that express the impact per intervention are called characterization factors.

The most used impact assessment methods provide up to 59 different midpoint indicators per method (Bare, 2011; Guinee et al., 2002; Hauschild & Potting, 2005; Huijbregts et al. 2016; Jolliet et al. 2003). To compare across all these different impact categories a further modelling step is required. This step translates multiple indicators at the midpoint level, each with their own unit, to a limited number of damage indicators on an endpoint level, with a single unit per so-called area of protection. It is common to include at least human health and ecosystems as areas of protection, while some methods also identify resource scarcity as area of protection (Frischknecht & Büsser Knöpfel, 2013; Goedkoop & Spriensma, 2001; Huijbregts et al. 2016; Jolliet et al. 2003; Steen, 1999a-b).

Problem setting

UNCERTAINTY

A large amount of life cycle data is required to compile the inventory and even more data is necessary to calculate the midpoint and endpoint environmental footprints. The more comprehensive the indicator of impact, the more input data is required and therefore the more statistical uncertainty in the final outcome of the assessment is to be expected. Similarly, a growing number of uncertain processes needs to be modelled as one progresses along the cause-and-effect chain. Three different types of uncertainty can be distinguished: (1) uncertainty due to lack of knowledge of the "true" value of a model parameter (parameter uncertainty), (2) uncertainty caused by arbitrary choices in a model (decision rule uncertainty), and (3) uncertainty caused by the loss of information resulting from the simplification of reality inherent in modeling (model uncertainty) (Huijbregts, 1998a,b). Apart from uncertainty, life cycle data also comes with variability. The main distinction between the two is that uncertainty may be reduced by additional research,

whereas variability cannot be reduced by additional research. Variability may need to be incorporated in footprint assessments in order to arrive at more representative impact estimates. This is because variability reflects real world differences among life cycles of alternative entities with an equal function, caused by systematic differences between for example individuals which differ in their product use, technological processes, location or time. Variability can only be reduced by making real-world changes, such as phasing out the most electricity-consuming lightbulbs or marketing campaigns to promote laundry at lower temperatures.

Even though uncertainty and variability are often mentioned as one of the most important challenges in environmental footprinting studies, quantifying these is still not commonplace (Lloyd & Ries, 2007; Hellweg & Milà y Canals, 2014). The separation of uncertainty and variability in LCA is even rarer. Separating uncertainty from variability has been successfully applied in the field of toxicology with the aim to inform decision makers whether they should focus on identification of sensitive individuals or on additional research to obtain more accurate parameter estimates (e.g. Huizer et al., 2012). In the field of LCA similar advantages can be expected from the separate quantification of uncertainty and variability. More specifically, if variability is ignored and treated as uncertainty, real-world differences in environmental footprints can be obscured. If variability and uncertainty can be quantified separately on the other hand, the remaining uncertainty will be lowered and real-world differences in footprints that were hitherto not visible can be shown and used to inform environmental policy.

Getting measured data for every individual entity in a life cycle can in practice be unfeasible, this may become especially problematic if a lot of variability between entities is to be expected. In these cases, models that take into account the key drivers of variability can be used to obtain an estimate of the variability at the expense of introducing some uncertainty through the modeling procedure (Basset-Mens, 2006). For instance, regression-based models have been used to estimate missing food processing inventory data (Sanjuán et al., 2014) and life cycle impacts of wind turbines (Caduff et al., 2012). Another area where the available data is limited and a relatively large amount of variability can be expected, is fossil energy generation. Since fossil electricity generation has a large contribution to the environmental impact of products (Huijbregts et al., 2010) it is crucial to estimate its impacts as accurately as possible. Using the average emissions of fossil power plants can lead to uncertain results as individual power plants may vary widely in their power generation efficiencies, depending on the type, size and age of the power plants. Power-plant specific data about fossil electricity generation is limited to a few well-studied regions, and without a facility-based separation between uncertainty and variability (Weber et al., 2010; Burnham et al., 2011). Therefore an approach is needed to quantify both variability and uncertainty in the environmental footprints of individual fossil-fueled power plants across the world.

REDUNDANCY

The growing number of available impact categories and LCIA methods has led to a myriad of available life cycle indicators of impact, both in number of impact assessment methods and in number of impact categories included per method. There may be overlap between methods as well as between indicators within a method. Because it is unfeasible to base decisions on all available indicators (even within one method) simultaneously, there is a strong need to reduce the number of indicators to be taken into account, as illustrated by a collaborative search for a recommended set of indicators (Hauschild et al. 2013). The number of indicators can be reduced in different ways. One approach is to calculate correlations between different indicators within and across methods to quantify the numerical/statistical redundancy in indicator sets. By removing the strongly correlated indicators one can obtain a set of indicators that is as small as possible but is still able to rank entities according to their environmental impact (Cadima & Jolliffe 2001, Peres-Neto et al. 2005). Systematic searches for an optimal set of indicators based on mutual correlations were performed by Gutiérrez and coworkers (2010) for impacts caused by a set of household appliances, by Berger and Finkbeiner (2011) for indicators of resource scarcity and by Lasvaux et al. (2016) for a large number of indicators used to quantify environmental impacts of the building sector. Another option is to start with a predefined set of key indicators, also called dashboard indicators, and assess whether that set is representative of the full set of environmental indicators. Some studies suggest, for instance, that energy use or the carbon footprint can be reasonable indicators of overall environmental impact for most, but not all, products (Huijbregts et al. 2010, Röös et al., 2013, Kalbar et al., 2017) while others argue that focusing on a single indicator results in problem shifting (Laurent et al., 2013). The latter authors warn that the carbon footprint does not correlate well with toxic impacts, resource depletion and land use. Therefore it seems unlikely that just one indicator can be seen as truly representative of the broad range of environmental impact pathways.

Studies focused on finding an optimal set of indicators have been limited in size and scope, including only a limited number of indicators (less than twenty), a small set of products within one product category or both. To provide a more comprehensive assessment of numerical/statistical redundancy in life cycle impact indicators, a much larger scope is necessary, in terms of both the number of products and the number of indicators. Additionally, it is useful to evaluate the extent to which small sets of key indicators, which can be either predefined or found via a correlation-based reduction procedure, are representative of endpoint damage. To do this, the relationships between small sets of key indicators and endpoint environmental damage need to be quantified for a broad range of products.

Thesis goal and outline

Summarizing, the field of environmental footprinting faces issues with unresolved uncertainty in key contributors of environmental impact as well as possible redundancy in terms of impact indicators. Therefore the goal of this thesis was to reduce uncertainty and redundancy in environmental footprinting. More specifically the following two research questions were addressed:

1 **To what extent can uncertainty in environmental footprints be quantified and reduced, with a focus on the carbon footprint of fossil-fired power plants?**

2 **What is the optimal representative set of impact indicators to be used for environmental footprinting?**

In chapter 2, parametric and decision rule uncertainty were quantified separately from spatial and technological variability in the carbon footprint of coal fueled power plants in the United States. This was done by modelling the individual supply chains and combustion of 364 coal fueled power plants, thereby covering the mining, transport and use phases specific to each power plant. Parameter uncertainty in the carbon footprint of individual power plants was calculated by using Monte Carlo simulation, while the differences between the power plants reflect spatial and technological variability. Scenario analysis was used to assess the influence of the choice of a specific time horizon (20, 100 or 500 years) on the carbon footprints. Only little information is available about technological variability in power plant-specific carbon footprints at the global scale. To fill this data gap, global regression models were developed to estimate the greenhouse gas emissions of power plants fueled by coal (chapter 3) and gas or oil (chapter 4), thereby including the uncertainty associated with these estimates.

Data reduction procedures based on principal component analysis (PCA) have been successfully applied for impact indicator reduction, yet on small sets of indicators and products only. In chapter 5 a PCA-based data reduction procedure was applied to find a non-redundant set of impact indicators from an original set of 135 indicators for 976 products. In chapter 6 the representativeness of a set of 4 key indicators (the material, land, water and carbon footprints) was determined for an EEMRIO model, by quantifying the redundancy among 119 impact indicators for 6982 product-region combinations. In chapter 7, multiple linear regression was used to evaluate the potential of a set of four simple resource-based indicators (water, land, energy and material use) to cover the more complicated endpoint indicators of damage to human health and ecosystems. This was done for the same set of products as used in chapter 5. The results of these studies are discussed in chapter 8.

CHAPTER 2

A methodology for separating uncertainty and variability in the life cycle greenhouse gas emissions of coal-fueled power generation in the USA

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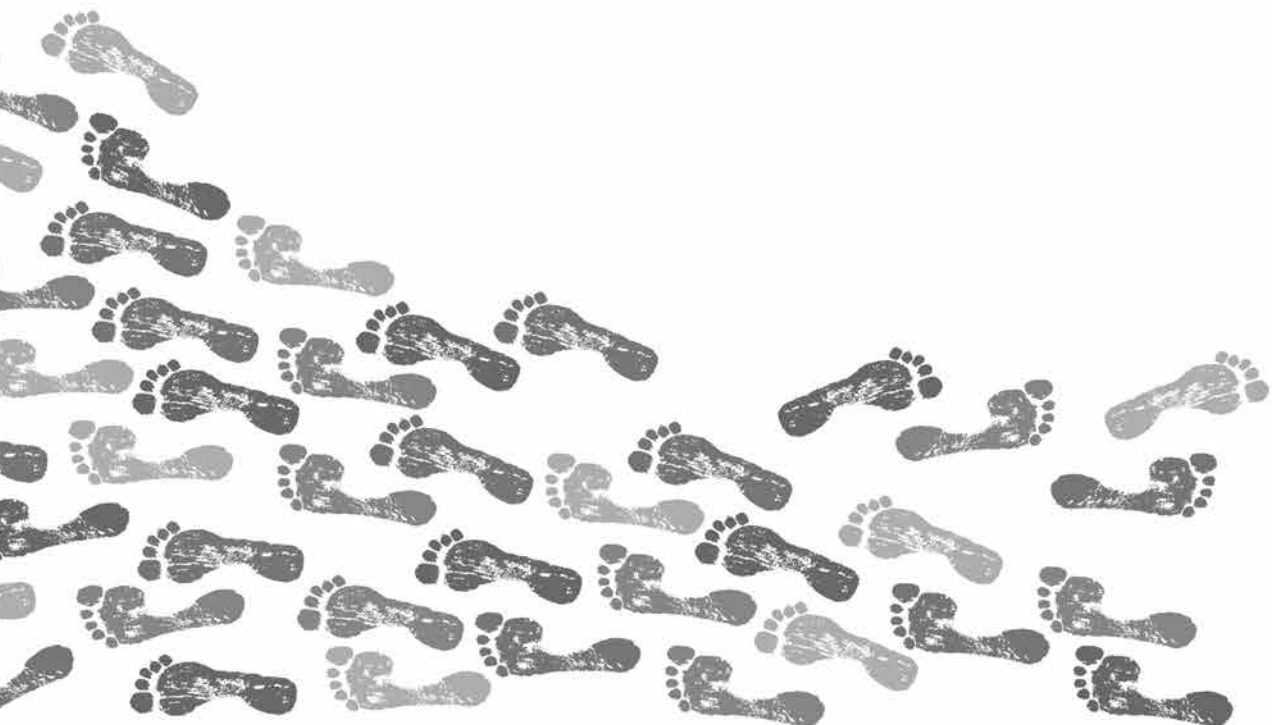

Abstract

PURPOSE Results of life cycle assessments (LCAs) of power generation technologies are increasingly reported in terms of typical values and possible ranges. Extents of these ranges result from both variability and uncertainty. Uncertainty may be reduced via additional research. However, variability is a characteristic of supply chains as they exist; as such, it cannot be reduced without modifying existing systems. The goal of this study is to separately quantify uncertainty and variability in LCA.

METHODS In this paper, we present a novel method for differentiating uncertainty from variability in life cycle assessments of coal-fueled power generation, with a specific focus on greenhouse gas emissions. Individual coal supply chains were analyzed for 364 US coal power plants. Uncertainty in CO_2 and CH_4 emissions throughout these supply chains was quantified via Monte Carlo simulation. The method may be used to identify key factors that drive the range of life cycle emissions as well as the limits of precision of an LCA.

RESULTS AND DISCUSSION Using this method, we statistically characterized the carbon footprint of coal power in the USA in 2009. Our method reveals that the average carbon footprint of coal power (100 year time horizon) ranges from 0.97 to 1.69 kg CO_2eq/kWh of generated electricity (95 % confidence interval), primarily due to variability in plant efficiency. Uncertainty in the carbon footprints of individual plants spans a factor of 1.04 for the least uncertain plant footprint to a factor of 1.2 for the most uncertain plant footprint (95 % uncertainty intervals). The uncertainty in the total carbon footprint of all US coal power plants spans a factor of 1.05.

CONCLUSIONS We have developed and successfully implemented a framework for separating uncertainty and variability in the carbon footprint of coal-fired power plants. Reduction of uncertainty will not substantially reduce the range of predicted emissions. The range can only be reduced via substantial changes to the US coal power infrastructure. The finding that variability is larger than uncertainty can obviously not be generalized to other product systems and impact categories. Our framework can, however, be used to assess the relative influence of uncertainty and variability for a whole range of product systems and environmental impacts.

Introduction

Typically, life cycle assessments (LCAs) are conducted by constructing models of each stage and connecting them via material or energy balances. Alternatively, LCAs may be developed top-down using input-output modeling or in a hybrid way combining the two approaches (Williams et al. 2009). Any type of modeling, however, introduces uncertainties. However, not all LCA practitioners take uncertainty into account (Lloyd and Ries 2007). Furthermore, Williams et al. (2009) argue that those who do account for uncertainty do so inconsistently or incompletely. Part of this may be caused by confusion about the definition and the appropriate way to deal with uncertainty.

Over the years, different classifications of uncertainty and variability in LCA have been developed (EPA 1989; Huijbregts 1998a; Paté-Cornell 1996). An examination of the different frameworks conducted by Heijungs and Huijbregts (2004) showed a large overlap among them. Perhaps the most important distinction is that uncertainty may be reduced by additional research whereas variability may not be reduced. This is because variability reflects real-world differences among alternative life cycles of equivalent products. Variability is caused by systematic differences between individuals (interindividual), processes (technological), and location (spatial), or in time (temporal). This definition of variability is employed by the US EPA (1989) and has been adapted for use in LCA by Huijbregts (1998a). Other authors, e.g., Paté-Cornell (1996), use the term "epistemic" uncertainty to refer to uncertainty caused by incomplete knowledge and "aleatory" uncertainty for true variation that cannot be reduced by additional research. Ergo, aleatory uncertainty is similar to the concept of variability used by the EPA and Huijbregts. In the remainder of this paper, we will use the definition of uncertainty and variability and the further subdivision of these two concepts as used by Huijbregts and the EPA (Huijbregts 1998a, b; Huijbregts et al. 2003).

The implications of variability and uncertainty are different, and thus, it is important to distinguish these two factors (EPA 1989; Huijbregts 1998a). If the range of LCA results is dominated by uncertainty, then more reliable data, more precise emission factors, etc., may be needed before one can robustly conclude that a product has a significantly different environmental impact from another. By contrast, results of LCAs exhibiting a high degree of variability demonstrate true differences among alternative production processes, supply chains, etc. This information can further guide system optimization, product development, or policy.

Three different types of uncertainty are distinguished in this framework for LCA: (1) uncertainty due to lack of knowledge of the "true" value of a model parameter (parameter uncertainty), (2) uncertainty caused by arbitrary choices in a model (decision rule uncertainty), and (3) uncertainty caused by the loss of information resulting from the simplification of reality via models (model uncertainty) (Huijbregts 1998b). Accounting for

uncertainty, e.g., via Monte Carlo (MC) simulation, yields multiple output or a distribution of life cycle impacts instead of a single estimate. In addition to these uncertainties, several types of variability may be distinguished for environmental footprinting. For example, differences in the performances of power plants are consequences of variability, as these plants may have different designs, utilize different types of furnaces, get fuel from different sources, or have different types of cooling systems. If an LCA accounts for this variability, many life cycle impacts will result, each corresponding to a unique systematic implementation of the technology.

Electricity plays a vital role in the life cycle of many products. Therefore, it is important to be able to estimate the extent of greenhouse gas (GHG) emissions over the life cycle of electricity generation with as much accuracy and precision (i.e., as close to the actual value and with the smallest range, respectively) as possible. In the USA, GHG emissions from electricity generation accounted for 33 % of total GHG emissions in the year 2009, making electricity generation the single largest American source of greenhouse gas emissions (EPA 2011a). Most of these emissions come from coal-fired power plants. The US EIA reports that in 2009, 44.5 % of the electricity in the USA was produced by coal-fueled power plants, constituting the largest fossil source of electricity, and the corresponding greenhouse gas emissions make up approximately 80 % of the total greenhouse gas emissions from electricity generation in this year (EIA 2011a).

In recent years, a number of LCAs of US coal power have reported ranges of possible life cycle emissions (Jaramillo et al. 2007; Venkatesh et al. 2012b; Burnham et al. 2011; Littlefield et al. 2010; Weber et al. 2010). However, the drivers of these ranges are unclear, as the underlying analyses took into account both variable and uncertain parameters without separating the two. Moreover, these ranges were calculated via different methods. Therefore, one cannot compare these ranges with each other in a statistically meaningful way, nor identify possible ways, if any, to reduce them.

In this paper, we present a novel approach that allows for the characterization of both uncertainty and variability separately. This separate assessment allows the researcher to identify ways to improve the precision of assessments of power generation technology as well as changes in practice that may reduce heterogeneity of actual life cycle emissions. In our approach, both spatial variability and technological variability were accounted for as well as decision rule uncertainty and parameter uncertainty; temporal variability in emissions was covered only to a limited extent. Influence of spatial variability among transport distances from mine to plant was quantified on an individual power plant level, as were spatial differences in coal characteristics (e.g., carbon content) at the level of the mines. Technological variability in (1) mine type (surface vs. underground), (2) mode of transport (e.g., truck or rail), and (3) power plant efficiency was also assessed. Decision rule uncertainty regarding the choice of time horizon in the global warming potential (GWP) of methane was quantified via discrete choice analysis in conjunction with our general approach. Lastly, parametric uncertainty associated with the mining, transport,

and use phases (e.g., electricity use during mining and fuel use during transport) was quantified via Monte Carlo simulation.

Methods

SYSTEM DESCRIPTION

The life cycle of coal from "mine to wire" is illustrated in Fig. 2.1. We divided the life cycle into three stages, following the convention of other LCAs (Burnham et al. 2011; Littlefield et al. 2010). In the extraction stage, coal is obtained via surface or underground mining. This phase includes activities such as methane venting, dewatering, mechanical transportation of coal to rail cars, etc. The transportation phase includes all operations associated with the transportation of coal from a mine to a power plant, including the operation of diesel locomotives and barges. The end of the coal life cycle is a power plant. There, coal is burned to yield carbon dioxide and water vapor, as well as the electricity that defines the functional unit of the LCA. We employed a functional unit of 1 kWh of electricity generated at a plant or plants in a particular calendar year. In the forthcoming example, we applied our methodology to the US coal power fleet in 2009.

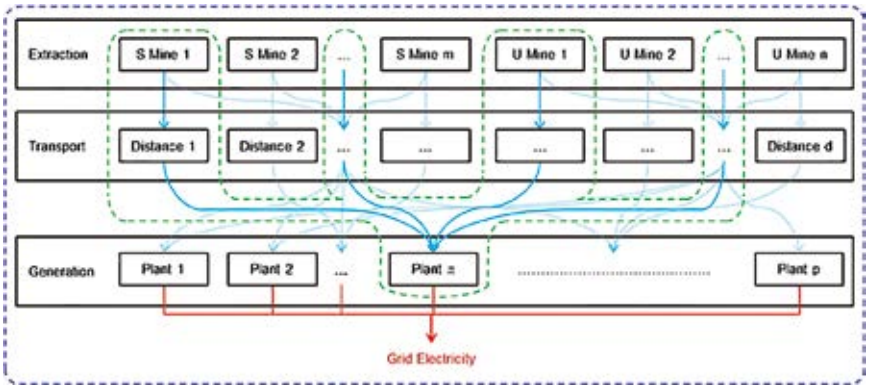

FIGURE. 2.1 Life cycle model for electricity generation from coal in the USA, including boundaries (dashed lines), flows of material (light blue arrows), and electrical output at the power plant (red). Variability by mine, transportation, and operation of power plants (surface (S) vs. underground (U) mining) is represented by horizontal boxes at each stage of the life cycle. A life cycle boundary corresponding to plant π is defined by the dashed green line: The plant is supplied by "surface mine 1," "underground mine 1," and several other mines

We utilized two types of system boundaries: one for each "individual plant" life cycle and a second for the "comprehensive" life cycle of coal-fired power plants in the USA. Each individual power plant life cycle was defined by a single power plant and all mines that

supply its coal, as illustrated by the dashed green line in Figure 2.1. Thus, there are as many of these life cycles as there are power plants. The "comprehensive" life cycle boundary includes all mines and plants and is illustrated by the dark blue line in Figure 2.1. Impacts associated with the two types of life cycles were used to define the uncertainty and variability associated with the carbon footprint of coal power.

DATA

A key input for our approach was the data set reported by the US EIA in its annual EIA-923 Time Series File (EIA 2011b). The file includes an extensive amount of actual data reported by power plant operators. Data include receipts of coal delivered from specific mines to each power plant throughout the calendar year, the locations of coal power plants and mines, and the heat input (higher heating value, HHV) and net power output of each plant. These data are broken down by each coal type (bituminous coal, sub-bituminous coal, and lignite). The extent of information published in the EIA data file may serve as the "backbone" of any LCA of coal power generation process in the USA as it provides the sources and amounts of all coal burned at a plant from "mine to wire."

In the implementation of our approach, we conducted an assessment of carbon dioxide and methane emissions associated with US coal power in 2009. These emissions were aggregated with the GWP reported by the IPCC AR4 (IPCC 2007). For the purposes of constraining our analysis to de facto base load power plants, we restricted our analysis to 364 coal power plants that generated at least 50 MW on average for nine or more months throughout 2009 (EIA 2011b) – a criterion similar to that employed by the EcoInvent database (Dones et al. 2007) (run time >8,000 h). To avoid errors caused by unclear allocation of emissions, all combined heat and power (CHP or "cogen") plants were left out of the analysis.

In 2009, approximately 5 % of all coal (on a mass basis) was extracted from mines that utilize both surface mining and underground mining. The EIA 923 data file does not report the mining type for an additional 5 % of the extracted coal. In such cases, we used the fractions of surface and underground production for the mine counties to approximate the relative amounts of coal extracted via the two techniques (EIA 2010).

Fuel use for underground and surface mining was estimated from data provided in the US economic census of 2002 (US Census Bureau 2011) (see Electronic Supplementary Material 1.1 for more detailed information). Electricity use during mining for both surface and underground mining was calculated from results published by Jaramillo et al. (2007). Emissions from provision of electricity in the mines were taken from the US EPA eGRID database at a US national level (EPA 2010). Fuel use per ton-kilometer of coal transport was adopted from the EcoInvent database (Spielmann et al. 2007) for transport of coal by diesel train, truck, barge, and freight ship.

We included uncertainty in many of the parameters associated with the models of individual power plant and "comprehensive" coal life cycles. Each such parameter was implemented with Crystal Ball as a distribution defined by statistics from the literature. Parameters are available as Electronic Supplementary Material. Foreground parameters on a national level are reported in Table S1, foreground parameters on a state- or coal basin-specific level are reported in Table S2, and background parameters (all on a national level) are reported in Table S3. Most parameters that exist on the range [0,∞) were modeled as log-normal random variables to prevent inadvertent MC selection of negative parameters. This skewed distribution is often appropriate for emission factors and other parameters employed in LCA (Huijbregts et al. 2003). Parameters existing within positive finite ranges, such as fractions, were modeled with the beta-pert distribution – a continuous distribution akin to the triangular distribution specified by minimum, maximum, and "most likely" values.

GENERAL MODEL

For each individual power plant life cycle, we calculated the carbon footprint as follows: First, we assessed the greenhouse gas emissions associated with the mining of each quantity of coal transported to the power plant. The EIA data file reports the type of mine (surface or underground) as well as the location. Using this information, we assessed mine methane emissions using additional information from the US EPA and US EIA (EPA 2011a; EIA 2011b), which is explicitly dependent upon the mine region and mine type (EPA 2011b). Uncertain parameters associated with the extraction phase (including methane emissions) were modeled as random numbers, with distributions conforming to data or engineering judgment. For instance, methane emissions (kilograms CH_4 per ton of mined coal) were modeled as lognormal distributions with means and standard deviations reported by EPA. All impacts associated with mining were calculated on the basis of the coal sent to a specific plant, including mine operations, commissioning, and decommissioning.

Next, we assessed the impacts associated with transportation. Most coal utilized for power generation in the USA is transported directly from the mine to the power generation plant via rail transport (McCollum 2007) although other types of transport include river barges, trucks, and interoceanic freight ships. In the modeling of rail transportation, we have supplemented the mine location information in the EIA 923 data file with the EIA 860 data file from 2009, which reports locations of most power plants (EIA 2011c); other power plant locations were identified via web search. EIA provides locations of mines and plants as ZIP codes, states (e.g., for collections of coal from small mining operations), and in some cases, nations (e.g., the locations of foreign mines). These were converted into geographical coordinates using information published by the US Census Bureau (2010), which includes the latitude and longitude of ZIP codes, states, and nations and their land areas. Rail distances between mines and plants are equivalent to road distances due to the historical evolution of road and rail transportation in the USA. Therefore, mine-plant

rail transportation distances in the USA were estimated via the Google Map API that calculates road distances. Uncertainty in these distances was also quantified according to the methodology described in Electronic Supplementary Material 2.3.

The power generation stage of the coal life cycle requires two key calculations: calculation of the GHG emissions and calculation of the energy output. Emissions were estimated via converting the amounts of coal arriving at the plant into heat inputs and multiplying these by the carbon intensities of bituminous coal, sub-bituminous coal, and lignite. For assessments of coal power in the USA at a state level, we recommend the use of the carbon contents reported by Hong (Hong and Slatick 1994). We refer the interested reader to the online supporting information for more detail regarding US states and their corresponding coal basins.

The power generated at the plant was directly taken from the EIA 923 data file (for all coals). The actual operating efficiency of each plant in the USA was calculated from data in the file from

$$\in_{\pi} = \frac{P_{\pi}}{Q_{\pi}} \tag{1}$$

where $\in_{\pi}$ is the net power generation efficiency of plant π [in megajoules of net electricity per megajoule heat, HHV basis], P_{π} is the net power generation from coal at plant π (in megajoules of electricity), and Q_{π} is the total coal consumption for plant π (in megajoules of heat, HHV basis). A valuable aspect of this approach is that it yields the actual operating efficiencies of operating plants.

We simultaneously calculated the carbon footprints for all individual power plants $\pi = 1 \ldots p$ as well as the comprehensive life cycle via MC. Each MC simulation is akin to an experiment wherein each uncertain parameter takes on a random value, in accordance with data or a known distribution. Calculations of the carbon footprints were conducted as follows: For each plant π, we conducted a mass balance on all supplied coal to determine impacts associated with its mining and transportation steps. Next, we calculated impacts and power output at the power plant. Finally, we summed the GHG emissions associated with all phases and normalize the sum by P_{π}, yielding the carbon footprint of an individual power plant life cycle in kilograms of CO_2eq per kilowatt hour. We denote this individual plant life cycle by the variable y_{π}.

The footprint of the "comprehensive" system (i.e., the dashed dark blue line of Figure 2.1) was calculated as follows:

$$Y = \frac{\sum_{\pi} y_{\pi} P_{\pi}}{\sum_{\pi} P_{\pi}} \tag{2}$$

where P_π is the power output of plant π (in kilowatt hour), and y_π is the carbon footprint of its corresponding life cycle (in kilograms of CO_2eq per kilowatt hour).

The MC selection procedure was repeated N times, generating p sets of N values representing each individual power plant footprint $\{y_{\pi n}\}$, $\pi = 1 \ldots p$; $n = 1 \ldots N$ as well as one set of N values for the comprehensive footprint $\{Y_n\}$, $n = 1 \ldots N$. The two sets are distinct in their interpretations: Statistics calculated from $\{y_{\pi n}\}$ are equivalent to those one would obtain from an analysis that considers variability as equivalent to uncertainty, e.g., an analysis that considers power plant efficiency as a random variable. Statistics calculated from $\{Y_n\}$ only capture the effects of uncertainty on the carbon footprint of all US coal-fired electricity.

The number of MC simulations required to generate these sets (N) depends upon features of the system including the number of uncertain parameters in a particular assessment, the extent of variability among power plant efficiencies, and other technological features of the supply chain. We used a sample size of $N = 1{,}000$ runs; the difference in uncertainty ratio for all 364 plants was <1 % from a test run with 10,000 iterations (data not shown).

QUANTIFICATION OF VARIABILITY

The expectation value of each set of MC simulations corresponding to an individual power plant's life cycle π (i.e., the arithmetic mean $E(y_\pi) = N^{-1}\sum_n y_{\pi n}$) estimates the actual life cycle GHG emissions. In the absence of parametric uncertainty, it would be the true value. Hence, variability was expressed in terms of the set of average GHG emissions $E(y_\pi)$, $\pi = 1 \ldots p$. We express variability in terms of a "variability ratio," which can be interpreted as a metric for interplant variation.

$$r = \frac{q_{0.975}(\{E(y)\})}{q_{0.025}(\{E(y)\})} \tag{3}$$

where the numerator is the 97.5th percentile of $\{E(y_\pi)\}$ (set of $\pi = 1 \ldots p$), and the denominator is the 2.5th percentile. Because our set included 364 power plants, the 2.5th and 97.5th percentiles do not refer to two specific plants. The percentiles were calculated with the Excel function PERCENTILE.INC.

QUANTIFICATION OF UNCERTAINTY

We considered two types of uncertainty in our method: parametric uncertainty and decision rule uncertainty. Each of these "uncertainties" must be addressed differently. Decision rule uncertainty is conceptually a matter of "uncertainty" in the value choices of individual researchers. In the framework by Huijbregts (1998b), it differs from model uncertainty in that it does not reflect incomplete knowledge of the workings of nature, but rather incomplete knowledge about the values of the intended user of the knowledge. Therefore, different values may therefore be assessed via scenario analysis.

In the carbon footprinting of coal power, a key value choice is that of the time horizon for the GWPs: 20, 100, or 500 years. Recently, there has been considerable debate regarding the appropriate choice of the "time horizon" for GHG emission studies (MIT 2011). GWP is defined as the quotient of the absolute global warming potential (AGWP) of a GHG and the AGWP of carbon dioxide (IPCC 2007), where each AGWP is a measure of radiative forcing associated with these molecules. Therefore, the GWP of CO_2 is 1 for any time horizon and has no uncertainty, but the GWP of methane depends upon the time horizon and also exhibits parametric uncertainty due to uncertainties in the AGWPs of methane and CO_2. To analyze the decision rule uncertainty, we calculated our LCA results for three different time horizons of 20, 100, and 500 years.

Parametric uncertainty may result from the statistical summarization of variability, e.g., estimation of emission factors from different mines within a geographical region. Alternately, it may result from imprecision in measurement. In practice, it is introduced to LCA by way of using non-site-specific or non-process-specific parameters in models of process stages.

Differences among the MC-generated values of y_π result from parametric uncertainty. Uncertainty in the carbon footprint of an individual coal-fired power plant was quantified as

$$\rho = \frac{q_{0.975}(\{Y\})}{q_{0.025}(\{Y\})} \tag{4}$$

where the numerator is the 97.5th percentile of the MC simulation results (set of $n = 1 \ldots N$) for power plant π, and the denominator is the 2.5th percentile. The percentiles were calculated with the Excel function PERCENTILE.INC.

An uncertainty ratio for the carbon footprint of US coal-fired electricity, which we denote by ρ, may be calculated by substituting $\{y_{\pi n}\}$ (the set of MC results for the life cycle emissions for power plant π) for $\{Y_n\}$ (the set of MC results for the life cycle emissions for all coal power in the USA) in Eq. (4).

DISTINGUISHING UNCERTAINTY FROM VARIABILITY

The parameters r and ρ share certain features that assist in the interpretation of their values: If $r = 1$, then there is no effect of variability upon the results of the LCA; if $\rho = 1$, then there is no effect of uncertainty upon the results of the LCA. The two statistics are analogous to the sums of squares compared in ANOVA. Insofar as $\{y\}$, $\{Y\}$, and $\{E(y)\}$ are different types of sets with different sizes and statistical properties, no statistical hypothesis test for the comparison of r and ρ can be formulated in terms of commonly utilized distributions employed by statisticians. For the practitioner, it will often be

sufficient to note the relative magnitudes of these quantities: If $r > \rho_{\pi}$ for all power plants (π), then variability is the primary cause of the range of life cycle emissions: Further research will not reduce the range substantially; rather, physical changes must occur to reduce the range. If $r < \rho_{\pi}$ for all power plants (π), then uncertainty is the primary cause of the range of life cycle emissions. In this case, additional research may reduce the range of life cycle GHG emissions, e.g., improvement in the precision of emission factors.

IDENTIFICATION OF KEY PARAMETRIC UNCERTAINTIES

If one wishes to reduce the range of the carbon footprint of coal power via reduction of uncertainty, one must evaluate the sensitivity of the final results with respect to the uncertain parameters. This was accomplished via sequential perturbation of each uncertain parameter, e.g., variation of its value between its 2.5^{th} and 97.5^{th} percentiles and observing the effect upon the comprehensive footprint Y. The effect of each uncertain parameter may be visualized by way of a tornado diagram, which reports both the upper and lower values of Y corresponding to perturbation of each uncertain parameter. This process is automated by software packages such as @RISK and Crystal Ball; we employed the latter of these for our analysis. Uncertain parameters yielding the largest ranges in variation of Y are those that contribute the greatest uncertainty in the LCA, for the case that all other parameters are at a constant value.

An underlying assumption of this approach is that uncertainties in parameters are uncorrelated. In the case of the LCA of coal power, parameters may generally describe unrelated processes, e.g., methane release fractions and fuel use for rail transportation. Therefore, we believe this assumption is reasonable.

SCENARIO ANALYSIS

Our method for carbon footprint estimations considering individual plants can be used to assess the effects of emission reduction measures on the carbon footprint of coal-fired electricity generation. Because the emissions and efficiencies of every single plant are modeled separately, it is possible to assess the influence of improving individual plant efficiencies or changing fuel type on the overall carbon footprint. Uncertainty is also propagated throughout the life cycles of the individual power plants; therefore, it is also possible to quantify the effect of changing the parameters of *any subset* of the plants on the total uncertainty, which would not be possible without separate plant life cycles. We performed three scenario analyses to illustrate how our approach can be used to assess the potential for reduction of the carbon footprint.

Results and discussion

DIFFERENTIATION OF UNCERTAINTY FROM VARIABILITY

In Fig. 2.2, we present the results of MC simulations of all individual power plant life cycles of coal in the USA. Please keep in mind that our data are representative for the 2009 fleet. Temporal variability is only addressed on the level of power plant efficiencies and is discussed in Electronic Supplementary Material 5.3. We illustrate the medians and 95 % confidence intervals, sorted via the medians of the GHG emissions of the particular life cycles. By contrast, medians (and 95 % confidence intervals) of the GHG emissions of the comprehensive life cycle were 1.12 (1.08–1.19), 1.06 (1.04–1.08), and 1.03 (1.02–1.05) kg CO_2eq/kWh for the 20-, 100-, and 500-year time horizons, respectively. At a 100-year time horizon, our results are comparable to the results of Littlefield et al. (2010) (1.1 kg CO_2eq/kWh) and Dones et al. (2007) (1.2 kg CO_2eq/kWh), among others.

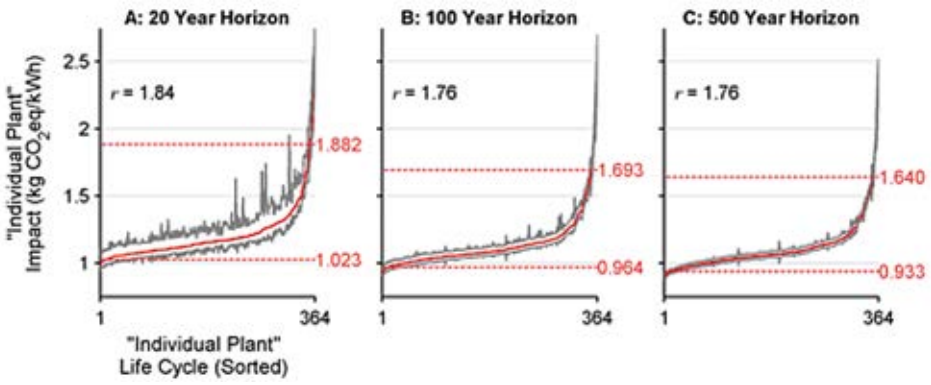

FIGURE 2.2 Life cycle GHG emissions (in kilograms of CO_2eq per kilowatt hour of electricity generated) for life cycles defined by individual power plants and the mines that supply them. The width of each plant's uncertainty distribution (95 % interval) is delineated by black points, whereas the median is highlighted in red. Horizontal red dashed lines represent the 95 % variability intervals

At a 100-year time horizon, the lowest average life cycle GHG emission was 0.92 kg CO_2eq/kWh, whereas the highest average life cycle GHG emission was 2.57 kg CO_2eq/kWh. Average emissions for the 2.5th and 97.5th percentile power plants (the *x*-axis range) were 0.97 and 1.69 kg CO_2eq/kWh, respectively, yielding a variability ratio of $r = 1.76$. By contrast, the uncertainty ranges from individual power plants (ρ_{IT}) varied from 1.04 to 1.2 (100-year time horizon). The life cycles with higher uncertainty ratios are those that utilize fuel sourced from outside of the USA – transportation contributes a larger fraction of the total GHG emissions for these life cycles due to longer transportation distances. Moreover, those distances have greater uncertainties than intracontinental rail distances. The uncertainty ratio for the comprehensive life cycle was $\rho = 1.05$. An advantage of our plant-level-based method is that any subset of plants may be readily analyzed, e.g., plants

residing in different regions. We report the carbon footprints for coal power generated in the North American Electric Reliability Corporation (NERC) regions in Electronic Supplementary Material 5.2.

In Fig. 2.3, we illustrate the relationship between the average life cycle GHG emissions of individual power plants (100-year time horizon) and their net generation (in megawatt hours). As a trend, life cycle GHG emissions decrease with respect to increasing net generation. Moreover, the variability for a given annual generation also decreases with generation. These trends are primarily explained by power plant efficiency: Plants with high net generation tend to have relatively high power plant efficiencies. Differences among coal types are also evident. Plants that run exclusively on lignite tend to have higher GHG emissions than those that exclusively utilize bituminous coal. The difference in GHG emissions can be attributed to differences in weighted average net efficiencies between the fuel types, which were 30.2, 32.6, and 33.4 % for lignite, sub-bituminous plants, and bituminous plants, respectively. In addition to this, lignite also has higher carbon content (in kilograms of CO_2 per megajoule of heat, HHV basis) than other fuel types from the same state (Electronic Supplementary Material, Table S3). The maximum difference in carbon content between lignite and bituminous coals mined in Montana is 5.2 %. Life cycles employing bituminous and sub-bituminous coals are less easily differentiated, owing to the fact that the average net efficiencies of their plants and carbon contents are similar (Electronic Supplementary Material, Table S3).

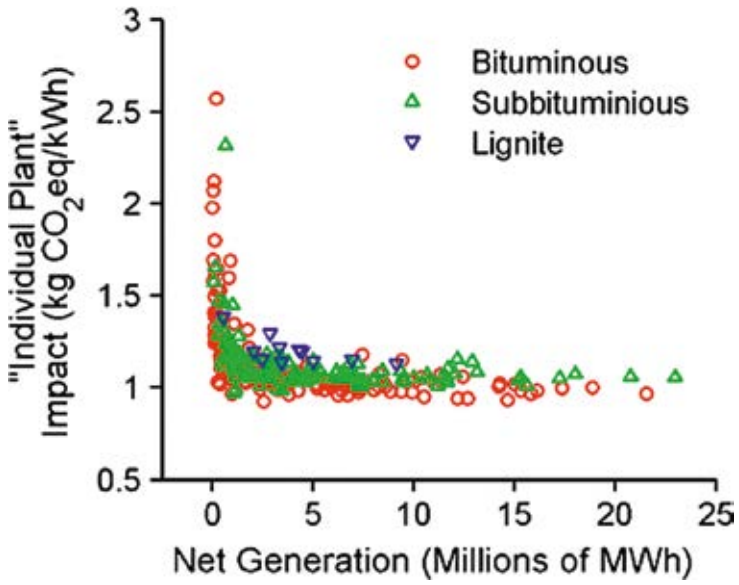

FIGURE 2.3 Effect of coal type and power plant output upon the average life cycle GHG emissions (100-year time horizon). Increased plant capacity and generation tend to result in the reduction of emissions, largely as a consequence of improved power plant efficiency: Results of 11 lignite, 169 bituminous coal, and 127 sub-bituminous coal life cycles are illustrated

In Fig. 2.4, we illustrate the relative contributions of uncertainty and variability to the coal power footprint. In Fig. 2.4a, we show the complete distribution of the life cycle GHG emissions from coal power ($\{y\}$), which includes both uncertainty and variability. When uncertainty is removed, the resulting set of life cycle emissions ($\{E(y)\}$) has a very similar distribution; indeed, the 10th and 90th percentiles of the data constituting Figs. 2.4a, b are indistinguishable. By contrast, when variability is removed from $\{y\}$, the relatively small impact of uncertainty is evident. From these results, we may conclude that life cycle variability is the key driver of the range of life cycle GHG emissions from coal power.

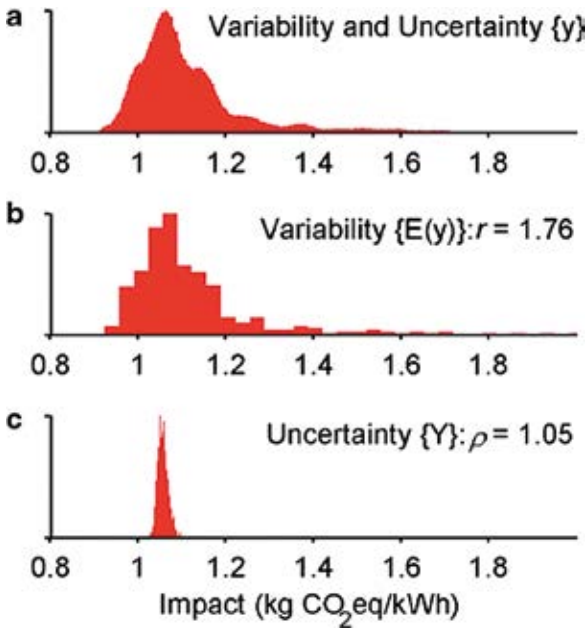

FIGURE 2.4 Variability is the primary cause of the range of life cycle emissions associated with coal power in the USA. a Histogram illustrating 1,000 MC simulations of 364 coal life cycles defined by coal plants in 2009 and the mines that provided their fuel. b Histogram illustrating average life cycle emissions of the aforementioned systems. c Histogram illustrating 1,000 MC simulations of the US coal footprint

KEY PARAMETRIC UNCERTAINTIES

In Fig. 2.5, we illustrate the sensitivity of the comprehensive footprint with respect to uncertain variables. The comprehensive coal footprint was sensitive to the uncertainty in the absolute GWPs of methane and CO_2: their ratio constitutes the GWP of methane, which is a significant GHG emission source in the upstream phase of the coal life cycle.

FIGURE 2.5 Sensitivity of comprehensive coal power footprint to uncertain parameters. Blue bars indicate higher than average values of the parameters, and red bars indicate values that are below the average

Sensitivity of the carbon footprint to uncertainties in factors associated with the mining of sub-bituminous coal from Wyoming reflects the significance of this coal in the US supply (about 20 % by mass). Even though the uncertainty in the carbon content is relatively small, the large share of this coal source to the total supply made the influence of this parameter on the footprint relatively large.

DECISION RULE UNCERTAINTY

Decision rule uncertainty was analyzed over three different time horizons, revealing that the ratio between the median footprints at the 20- and 500-year time horizons is 1.09: a slight decrease in the life cycle GHG emissions of coal power generation was observed with increasing length of the time horizon. The decrease was a consequence of the fact that the GWP of methane decreases with time. The small effect of decision rule uncertainty is due to the fact that the vast majority of the GHG emissions originate from the power generation and transportation stages of the coal power life cycle where mainly CO_2 is emitted – methane emissions constitute a small fraction of the total emissions. Parameter uncertainty and variability in the life cycle GHG emissions at time horizons of 20 and 500 years were similar to those of the 100-year time horizon.

UPSTREAM CONTRIBUTIONS TO LIFE CYCLE GHG EMISSIONS

For a 100-year time horizon, upstream emissions (mining and transport phase combined) accounted for 6 % of the total life cycle GHG emissions for US power generation with the 95 % uncertainty interval ranging from 5 to 9 % The upstream contribution of 8 % reported by the NETL LCA of coal power (Littlefield et al. 2010) is well within this range. The relative contribution of upstream emissions was larger for the 20-year time horizon with an average value of 12 % (95 % interval, 8–17 %) and smaller for the 500-year time horizon average of 4 % (95 % interval, 3–6 %). Additional information is provided in Electronic Supplementary Material 5.1 (Fig. S1 A–C). The difference between results at these time horizons reflects the relative importance of methane emissions, already discussed. The

relatively large uncertainty intervals reflect the larger uncertainty in input data for the upstream phases, compared to the uncertainty in use phase parameters. The 97.5th and 2.5th percentiles of average upstream contributions of individual power plant life cycles differed by a factor of four: evidence of relatively large variability in upstream emissions compared to the variability in the total life cycle GHG emissions. The relatively large variability in GHG emissions in upstream processes, such as coal transport, contributes little to the variability in the overall carbon footprint. This can be explained by the fact that GHG emissions of upstream processes are relatively small compared to the GHG emissions during the use phase per functional unit.

COMPARISON WITH OTHER STUDIES

Our study is the first to delineate uncertainty from variability, but other studies do report ranges of emissions. "Range ratios" akin to r or ρ calculated from previously reported studies (Jaramillo et al. 2007; Burnham et al. 2011; Dones et al. 2007) vary from 1.4 to 1.1 and include both uncertainty and variability. The difference is primarily attributable to the larger overall range of power plant efficiencies predicted from the EIA 923 data set: 13.5 to 36.8 % HHV (minimum–maximum). By contrast, the Argonne GREET model (Burnham et al. 2011) uses a *theoretical* power plant efficiency range of 33.5–34.4 % for conventional coal plants, and the 2007 study of Jaramillo et al. (2007) used a range of 30–37 %. Venkatesh et al. (2011) have recently updated the Jaramillo study and considered power plant efficiency as a random variable ranging from 24 to 37 % (90 % interval) based on the EPA eGRID data set from 2006. This range is similar to the 90 % interval in our data (24–35 %). It should be noted that the efficiency to be selected also depends on the goal of the study. If the average carbon footprint of coal power in the USA is of primary interest, then the average efficiency may be suitable. By contrast, if the prediction of GHG emissions of new coal-fired power plants is the point of inquiry, then a relatively high plant efficiency may be more suitable. For the analysis of the total variability in plant emissions, however, our approach of using the actual plant efficiencies (rather than a theoretical estimate) is preferred. As the range of efficiencies increases, one expects a larger value of r. As our results show, the variability of the emissions is tantamount to the range owing to the relative disparity between uncertainty and variability.

SCENARIO ANALYSIS

Our results indicate that a reduction of the range of the coal power footprint requires a reduction in variability. The two most important sources of variability are in coal type and power plant efficiency. The average efficiency for coal-fueled power plants in the USA was 32.9 %. If all US plants had this efficiency, then r would decrease from 1.76 to 1.2. The remainder of the variability is due to differences in transportation and mining type. Changes in these types of variability require large changes in the fuel market as well as large technological changes in power plant operations. Without considering *how* such changes might be implemented, we considered the following scenarios:

A All coal power plants operating below 32.9 % HHV (the 2009 average) in 2009 operate at 32.9 % HHV.
B All coal power plants operating below 35 % HHV (95th percentile in 2009) in 2009 operate at 35 % HHV.
C Total power production allocated to plants that utilize bituminous coal only.

Scenarios A and B were chosen to investigate the effects of raising the efficiencies of poorer performing plants. Scenario C was chosen to investigate the effect of excluding the least efficient fuel type. We evaluated these effects in the context of a 100-year time horizon.

In scenarios A and B, the total life cycle GHG emissions were reduced by approximately $3.8 \cdot 10^{10}$ and $1.1 \cdot 10^{11}$ kg CO_2eq/year, respectively. Scenario C reduced the emissions by $4.3 \cdot 10^{10}$ kg CO_2eq/year. In scenarios A, B, and C, the base case total GHG emissions were reduced by 2.1, 6.0, and 2.4 %, respectively. The maximum achievable reduction of 6 % in the most ambitious scenario does not take into account the feasibility of this scenario. Venkatesh et al. (2012a), who have analyzed the practical aspects of implementing coal plant retirement scenarios in more detail, found a maximum feasible emission reduction of about 4 %.

MODEL LIMITATIONS AND ALTERNATIVES

While we put much effort in disentangling uncertainty and variability, it is not always feasible to completely do so. In our modeling approach, we specified parameters as uncertain, even though the influence of variability could not be fully excluded. An example is the diesel use in coal-transporting trains, which is modeled as an uncertain parameter. The fuel use per ton-kilometer may, however, also depend on spatially (or temporally) variable parameters such as whether the route from mine to plant is uphill, downhill, or flat and the average wind speed.

In our study, we observed that the uncertainty ratios are much smaller than the variability ratios. We therefore conclude that the influence of possibly overestimating uncertainty ranges of input parameters on our results is most likely limited. This may, however, not always be the case in LCA and should be studied on a case-by-case basis.

In our approach, we applied Monte Carlo simulation to quantify the uncertainty. Another approach to analyze the simultaneous influence of several uncertain parameters throughout the entire life cycle is analytical error propagation. The analytical error propagation approach may require less computational power than Monte Carlo (Ciroth et al. 2004), especially for less complex systems. This approach might be used in our model framework as well.

Conclusions and recommendations

We have demonstrated that the variability in the carbon footprint of US coal-fueled electricity generation is much larger than the uncertainty found for any of the 364 examined power plants. An important implication of this result is that obtaining more accurate estimations of uncertain parameters will do little to improve the accuracy of a deterministic LCA. Instead, we advise LCA practitioners to consider incorporating variability in their LCAs as a range of possible emissions and/or plant efficiencies. It is particularly important to account for variability in GHG emissions from coal-fired power plants in LCA studies when electricity is sourced from one or a few known coal-fired power plants; this may be the case for some large industrial consumers. In such cases, estimates of the carbon footprints of products manufactured with this coal-generated electricity may be substantially under- or overestimated if an average value is used for the carbon footprint of coal-fired electricity. Furthermore, we have also shown that the potential for reduction in total coal GHG emissions in the USA is about 6 %, even under the very optimistic assumption that all plants can obtain a net efficiency of 35 % or higher.

Acknowledgments

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CHAPTER 3

How To Address Data Gaps in Life Cycle Inventories: A Case Study on Estimating CO_2 Emissions from Coal-Fired Electricity Plants on a Global Scale

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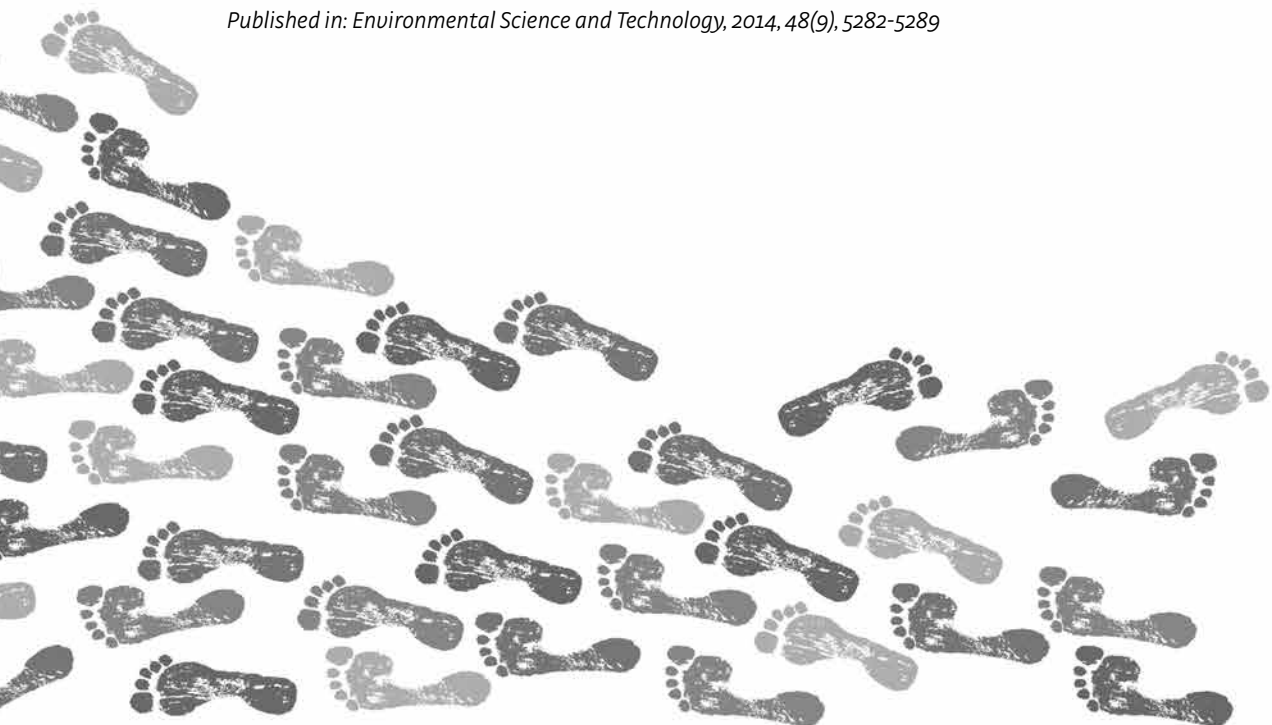
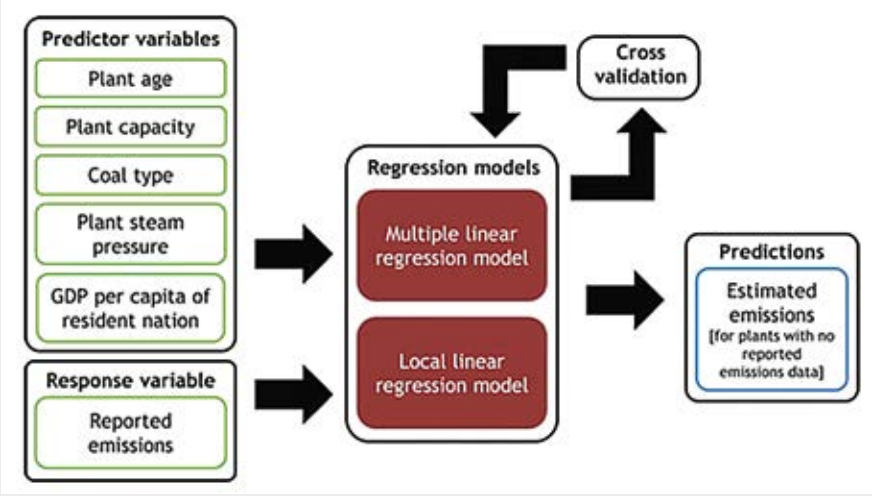


Abstract



One of the major challenges in life cycle assessment (LCA) is the availability and quality of data used to develop models and to make appropriate recommendations. Approximations and assumptions are often made if appropriate data are not readily available. However, these proxies may introduce uncertainty into the results. A regression model framework may be employed to assess missing data in LCAs of products and processes. In this study, we develop such a regression-based framework to estimate CO_2 emission factors associated with coal power plants in the absence of reported data. Our framework hypothesizes that emissions from coal power plants can be explained by plant-specific factors (predictors) that include steam pressure, total capacity, plant age, fuel type, and gross domestic product (GDP) per capita of the resident nations of those plants. Using reported emission data for 444 plants worldwide, plant level CO_2 emission factors were fitted to the selected predictors by a multiple linear regression model and a local linear regression model. The validated models were then applied to 764 coal power plants worldwide, for which no reported data were available. Cumulatively, available reported data and our predictions together account for 74% of the total world's coal-fired power generation capacity.

Introduction

Life cycle assessment (LCA) is a tool that is often used to quantify the environmental impact of products and services (ISO, 2006). One of the major challenges in LCA is the availability and quality of life cycle inventory (LCI) data, i.e., the emissions of substances and use of resources during a product's life cycle. LCI databases, such as Ecoinvent (Frichknecht et al., 2007), GaBi (PE International, 2012) and the U.S. Life Cycle Inventory Database (NREL, 2012), provide information for a large number of processes but are at the same time far from complete. Approximations and assumptions are often made if appropriate data are not readily available. For instance, a common approach used to address data gaps in LCA is to derive estimates from similar processes in other regions of the world, as done in the Ecoinvent database (Frischknecht et al., 2007). These proxies introduce uncertainty into LCA results by neglecting regional differences. An alternative approach is to derive inventory data from more readily available information on process characteristics. For example, Wernet et al. (2008) used neural networks to estimate the cumulative energy demand (CED) of chemicals based on their molecular properties. Caduff et al. (2011, 2012) used scaling laws to estimate the fuel use of different size generators and the environmental impact of energy generation from wind. Venkatesh et al. (2011) and Karras (2010) used linear regression models based on characteristics of crude oil to estimate emissions associated with its refining. While these approaches take into account regional or process-specific differences, which are often not well-characterized in LCA, uncertainties in the model predictions need to be quantified.

Regression models can be developed using parametric or non-parametric approaches (Everitt & Dunn 2010). Non-parametric regression techniques, such as local linear regression, allow for the fitting of local models around a particular query point without assuming a global model structure that is valid for the entire data set, thus allowing for some flexibility in modeling the structure of functional relationships (Schaal & Atkeson, 1994; Hastie et al., 2009). A drawback of the non-parametric models is that all data have to be stored in the model, so that it can be accessed for each new query. Parametric models, such as multiple linear regression models, on the other hand, assume an existing global data structure and use all data points to fit the model. These models have the advantage of being able to determine the most influential parameters easily, and they are easily transferred to other applications (only the model parameters need to be known).

Fossil energy demand constitutes one of largest sources of environmental impacts for many products and processes (Huijbregts et al. 2006, 2010). In particular, coal power plants are among the highest emitters of greenhouse gases (GHGs) per kWh of electricity compared to other sources of electricity (Frischknecht et al. 2007b). Coal is also the dominant source of electricity generation; i.e., 42% of all electricity generated in the world in 2011 was produced by coal plants (Worldcoal, 2012). Coal power plant efficiencies and, therefore, their CO_2 emissions vary greatly across the world. For example, the average

thermal efficiency of Japanese plants is around 42%, while plants from India have an average efficiency of about 30% (Graus et al., 2007). Hence, approximations of power generation models using "typical" values from other contexts (for example, assuming Indian power plants have impacts similar to U.S. power plants) may significantly influence an assessment of environmental impacts over a product's life cycle. Quantifying emission factors of coal-fired electricity as accurately as possible could therefore significantly improve the performance of life cycle models that include electricity generation as a major component. A considerable effort has been made by Dones et al. (2007) who developed coal power plant emission factors for China, the United States, and 19 different European countries/regions based on reported data for coal use and electricity generation. However, coal-fired electricity generation is widespread, and emission data are not reported for many other countries in the world. Moreover, Steinmann et al. (2014) demonstrated that there is considerable variability in life cycle GHG emissions between individual power plants, implying that there is added value in plant-based emission models compared to country-based approaches.

We are aware of one study by the Center for Global Development (Wheeler & Ummel 2008; Ummel, 2012) called Carbon Monitoring in Action (CARMA), where combustion-phase CO_2 emissions from thermal power plants across the world were estimated with a global regression model based solely on the design characteristics of the plants. As far as we know, no other efforts have been made to estimate power plant emissions on a global scale. We predict CO_2 combustion emissions per kWh (from here onward referred to as emission factors) from coal power plants on a global scale and quantify uncertainty in the predictions. We employ two predictive regression models: a parametric and a non-parametric model. After fitting and validating both models, we use these to predict CO_2 emission factors for 764 coal-fired power plants worldwide. These predictions can be used to supplement information in life cycle modeling efforts wherever the required data are unavailable.

Similar to the Center for Global Development approach, we include power plant design characteristics as explanatory variables within the regression models. There are, however, some notable differences between the two approaches. The quantification of statistical uncertainty is one of the advantages of our model framework. Quantifying the uncertainty that arises from using a predictive model is important because it can be propagated to the final output of any LCA that uses electricity from one of these coal plants as input. Another difference is that our model can distinguish between lignite and non-lignite plants, whereas the CARMA model cannot. Also, the differences between countries were made explicit in our model by including per capita gross domestic product (GDP) as a predictor. Finally, we explored various types of parametric and non-parametric model approaches and settings to find optimal model predictions.

Methods

Regression models using reported emission data were developed and validated to predict CO_2 emission factors from coal-fired power plants across the world. In this section, we describe the data used to develop the regression models, model structures, metrics to evaluate the performance of the models, and application of the models.

EMISSION DATA

Reported CO_2 emissions from individual power plants were obtained from databases published by governmental agencies, such as the U.S. Energy Information Administration (EIA), or from reports by private power companies. A more extensive discussion on how the CO_2 emissions per kWh were derived from reported data can be found in SI1 of the Supporting Information.

If emission data were available for multiple years, the most recent year was used. Only plants with a capacity greater than 100 MW were included in the analysis to ensure that the data set was not confounded by very small autonomous producers (for example, a power plant belonging to a paper mill). In total, emissions were reported for 444 plants with a total capacity of 494 GW (Table 3.1).

TABLE 3.1 Characteristics of individual coal fired power plants by country used for model validation

Country	Number of plants	Sum capacity (MW)	Year	Source
United States	310	288,689	2010	Steinmann et al. (2014), based on EIA (2012)
India	59	64,623	2010-2011	Central Electric Authority (2012)
Australia	24	27,494	2010	AEMO (2012)
South Africa	13	37,678	2011	ESKOM (2012)
China (incl. Hong Kong)	2	5,368	2011	CLP group (2012)
Canada	4	4,221	2010	OPG (2011)
Bulgaria	1	908	2010	ENEL (2011)
Greece	4	3,977	2006	Kavouridis (2008)
WWF (2007)				
England & Wales	8	17,884	2006	WWF (2007)
Germany	10	22,324	2006	WWF (2007)
Poland	4	10,905	2006	WWF (2007)
Czech Republic	1	1490	2006	WWF (2007)
Italy	1	2,640	2006	WWF (2007)
Spain	1	140	2006	WWF (2007)
Portugal	1	1,250	2006	WWF (2007)
Scotland	1	2,400	2006	WWF (2007)
Total	**444**	**493,586**		

PREDICTOR VARIABLES AND DATA

To estimate power-plant-specific CO_2 emission factors, a number of potentially important predictor variables were identified (Table 3.2). For our models to be applicable to coal-fired plants throughout the world, we selected predictors that were available from public data sources. Plant age, total capacity, steam pressure, and coal type were all expected to influence CO_2 emissions and were derived from the World Electric Power Plant (WEPP) database (Platts, 2012). The plant age was calculated by taking the capacity-weighted average of the age of all active generators at a plant. The GDP per capita of the resident nations of the power plants was also chosen as a predictor because we hypothesized that it correlates with the GHG emission policies and/or power plant maintenance in those nations, which, in turn, affects the efficiency (and therefore the CO_2 emissions) of the plants. The 2011 GDP per capita [in purchasing power parity (PPP)] for each country was obtained from the International Monetary Fund's World Economic Outlook (2012). Figure S1 of the Supporting Information shows how the emission factors and predictor variables relate to each other.

TABLE 3.2 Range of Predictor Variables

Variable	Range used in model fitting	Total range in WEPP database and IMF	Notes
Plant age	0-60 years	0-70 years	In case of multiple generators, a weighted average age is used. The ages of the generators were calculated by subtracting the operation year from the year for which the data was reported. The weights were based on the generator capacity as a proportion of the total plant capacity.
Coal type	Lignite or non-Lignite[a]	Lignite or non-Lignite	Plants that did not report their fuel type or that report a combination of fuel types such as lignite/bituminous were excluded from the analysis
Steam pressure	35-293 Bar	17-286 Bar	The average steam pressure of all operational generators per plant
Total capacity	100 MW – 4440 MW	100 MW-5500 MW	Total capacity of all operational generators per plant. Only plants >100 MW were included.
GDP per capita	$3694-$48387	$487-$48387	GDP per capita in $ of Purchasing Power Parity (PPP)

[a] Non-lignite plants are modeled as 0, while Lignite plants were assigned a value of 1

MODEL FITTING

Two different modeling approaches were employed, i.e., a multiple linear regression model and a local linear regression. Because the models derived in this study were used to predict CO_2 emission factors for a large number of unknown plants, a thorough

assessment of the predictive power of the model is required. Therefore, prior to model fitting, the data set (444 plants) was split into a training set and a test set. The training set consisted of 311 of 444 plants (approximately 70%), while the remaining 133 plants in the test set were used for validation of the models.

Multiple Linear Regression

A multiple linear regression model can be used to predict the value of a response variable based on a linear relation to any number of predictor variables. The CO_2 emission factor associated with a power plant is inversely related to its generation efficiency. We hypothesize that the selected predictors are linearly related to the efficiency of the power plant and, therefore, inversely related to its CO_2 emission factor (eq 1)

$$\hat{z} = \frac{1}{\hat{y}} = \beta_0 + \beta X \qquad \textbf{Equation 1}$$

where $\hat{y}$ is a vector representing an estimate of the emission factor for all plants, X is the matrix where each column corresponds to individual predictor variables (Table 3.2), β is a vector of coefficients, and β_0 represents the intercept of the model.

Ordinary least-squares (OLS) fitting was used to calculate the model coefficients. The need for log transformation (with 10 as a base) of the predictor variables, total capacity, plant age, steam pressure, and GDP per capita, was assessed, given the skewed distribution of the predictor variables (see SI2 of the Supporting Information). Prior to the log transformation, 1 year was added to the plant age because some plants that were less than 1 year old were assigned a plant age of 0. We used the package MuMIn in the statistical program R (R Core team, 2012) to generate all possible models using any combination of the predictor variables (both log-transformed and non-transformed). To find the optimum between model complexity and the accuracy of the predictions, we calculated Akaike's Information Criterion (AIC) for all 162 possible combinations. AIC gives a bonus for the goodness of fit [the log likelihood function, ln(L)] and a penalty for the number of predictors k (eq 2). The model with the lowest AIC value was considered to be the best model.

$$AIC = 2k - \ln(L) \qquad \textbf{Equation 2}$$

The best model was subsequently checked for multicollinearity in its predictor variables by calculating variance inflation factors (VIFs). Typically, predictors with a VIF > 10 indicate multicollinearity in the inputs and need to be excluded from the model (Field, 2009). No predictor variables were excluded from our model based on this threshold because the highest observed VIF was below 2 (see Table S1 of the Supporting Information). Furthermore, 95% prediction intervals (as a function of the standard error in the model fit and the deviation of each predictor from its mean value) were calculated by the R function predict.lm.

Furthermore, leave-one-out cross-validation (LOOCV) was performed, which is a procedure in which a model is fitted with all power plants but one. The fitted model is then used to predict the emission factor of the power plant that was left out, and this procedure is repeated until a prediction is obtained for every single power plant. These estimates were used to assess the predictive power of the model.

To determine the relative importance of each of the predictor variables for the best model (that is, the model with the lowest AIC), we performed a separate analysis based on standardized predictor variables. Because all of the input variables are measured in different units (e.g., age in years, capacity in MW, etc.), they were first standardized to *z* scores. Regression coefficients resulting from the standardized fit directly reflect the relative importance of each predictor variable.

Local Linear Regression Model

In locally weighted polynomial regression, a low-degree polynomial is fitted locally around a query point using a weighted least-squares approach, where observations near the query point are assigned higher weights (Cleveland, 1979). In this study, we used an implementation of a local first-order (linear) regression by Kalnins et al. (2008) developed by Jekabsons (2010) detailed as follows.

Assume that y^p is a vector that represents emission factors and X^p represents a matrix of d columns corresponding to the individual predictor variables; these represent the training set. The training set includes n observations (X_i^p, y_i^p); $i = 1, \ldots, n$. The predicted emission factor of a particular (query) plant j, with characteristics described by X_j^q, is estimated by performing a linear regression locally in the neighborhood of query plant j.

The linear model to be used locally can be represented as shown in eq 3.

$$F(X_i) = a_0 + \sum_{m=1}^{d} a_m X_{i_m} \qquad \textbf{Equation 3}$$

The coefficients a in eq 3 are calculated using a weighted least-squares method, as shown in eq 4. In this method, the neighbors nearest to query point X_j^q are assigned higher weights.

$$\boldsymbol{a} = \arg\min \sum_{i=1}^{n} w(X_j^q, X_i^p)\,(F(X_i^p) - y_i^p)^2 \qquad \textbf{Equation 4}$$

The weighting function w used in eq 4 is a function of the distance between observations X^p and query point X_j^q. While a number of different weighting functions, such as the Epanechnikov quadratic weighting, tri-cube, and Gaussian weighting can be used, it has been shown that the choice of the weighting function does not significantly affect the results (Chu & Marron, 1991). We used the Gaussian weighting function, implemented by

Kalnins et al. (2008), as follows. In this implementation, μ_i refers to the scaled distance from the query point *j* to the i^{th} plant in the training set, as shown in eq 5.

$$\mu_i^j = \frac{||X_j^q - X_i^p||}{||X_j^q - X_{farthest}^p||} \qquad \textbf{Equation 5}$$

The Gaussian weight function is then calculated as a function of the scaled distance μ_i and coefficient α, as shown in eq 6. This coefficient controls the linear approximation, by defining the extent of the neighborhood around a query point that is weighted strongly in the approximation.

$$w(X_j^q, X_i^p) = \exp(-\alpha \mu_i^j) \qquad \textbf{Equation 6}$$

Before being used to estimate weights, all predictors in the training set (without log transformation) were first transformed to *z* scores. Furthermore, Gower's dissimilarity metric was used to transform the binary coal-type variable (by multiplying the *z* scores of the binary coal-type variable by a factor of $1/\sqrt{2}$, as suggested by Sigovini (2001)). The coefficient α was tuned using LOOCV, suggested as a widely accepted method to measure the goodness of fit of the local model (Schaal & Atkeson, 1994b). In this approach, for a specific value of α, a prediction was made for a single power plant based on a fitted model that included all other power plants in the training set. This was performed for each power plant in the training data set, resulting in emission factor estimates for every single plant that was used to evaluate the model mean square error for that specific value of α. The optimal value of the coefficient α was determined using a simple stepwise search algorithm presented by Kalnins et al. (2008) which resulted in the lowest LOOCV mean square error.

The optimal coefficient α, thus determined, was then used in conjunction with the training set data to estimate the emission factors of all plants in the test set.

Finally, bootstrap sampling was used to develop pointwise prediction interval estimates for all power plants, as shown by Aneiros-Pérez et al. (2010). The training data residuals, calculated using the local linear regression model, were used to estimate 1000 bootstrapped residuals for each data point in the test set. The 95% prediction intervals for new plants were based on these 1000 bootstrapped residuals.

MODEL EVALUATION

We analyzed the R^2 for the cross-validated training set (311 plants) and the R^2 for the 133 plants in the test set to obtain an indication of the predictive power of the models (Schüürman et al., 2008). These R^2 metrics have values that are between $-\infty$ and 1. A value of 1 reflects a perfect prediction, while any model with a R2 value below 0 has no added value compared to using the average of the data set (Legates & McCabe, 1999; Todeschini, 2012).

In addition to the R^2 metrics for the training and test sets, we calculated relative prediction errors for each power plant, as the difference between the reported and predicted emission factors, represented as a fraction of the reported emission factor. We also plotted relative prediction errors for all plants against the individual predictors to identify predictor ranges for which the estimates are particularly uncertain. To check the influence of the relatively large number of U.S. plants in the training data set (223 of 311) on the global multiple linear regression model, an additional multiple regression fit was performed where 135 of the U.S. plants were removed from the training data set to obtain a data set with an equal number of U.S. and non-U.S. plants (88 each).

MODEL APPLICATION

The multiple linear regression model with the lowest AIC value and the local linear regression model were applied to coal-fired power plants in the WEPP database, for which all predictors listed in Table 3.2 were available and for which no reported emission data were available. In total, the WEPP database includes 1974 coal plants with a capacity of >100 MW (cumulative capacity of 1687 GW) in 72 countries, with at least one operational generator in the year 2012. Emissions were reported for 444 of these plants (494 GW), contributing to 29% of the total capacity of the world (see the Emission Data section). Of the remaining 1540 plants, all predictor data were available for 764 plants with a total capacity of 760 GW (45% of the total capacity of the world).

Results

MULTIPLE LINEAR REGRESSION MODEL

The AIC values of all possible multiple regression models (see Table S2 of the Supporting Information) showed that the model with the log-transformed values of the four continuous predictors and the categorical fuel type (lignite or non-lignite) was the best model. The coefficients for this model are shown in Table 3.3. The normalized model coefficients, indicating influence of each predictor, are shown in Table S3 of the Supporting Information. The log-transformed steam pressure has the highest normalized coefficient value, indicating that it is the most important predictor. The coefficients of the model that used an equal number of U.S. plants and non-U.S. plants are well within 50% of coefficients of the model fitted to the training data, for all predictors except for plant age, for which the coefficient almost doubles because of the removal of the U.S. plants (see Table S4 of the Supporting Information). The predictions from this model are consistent with the predictions from the model based on the entire training data set; on average, these differ by 1.5%.

TABLE 3.3 Coefficients of the best multiple linear regression model

Predictor name	Coefficient	p-value
intercept	-3.65E-01	9.7E-05
log [capacity (in MW)]	6.38E-02	9.8E-06
log [age + 1 (in years)]	-8.69E-02	2.7E-04
log [steam pressure (in bar)]	3.46E-01	8.8E-14
log [GDP (in $PPP) per capita]	1.20E-01	3.7E-17
fuel type (1=lignite, 0=non-lignite)	-1.49E-01	3.5E-17

The cross-validated R^2 value based on the training set fit is 0.53, while the R^2 based on the 30% test set is 0.49. Reported and predicted emission factors (with 95% prediction intervals) for the 133 power plants in the test set are displayed in Figure 3.1A. On average (over all 133 plants), the lower bound of the 95% prediction interval (2.5th percentile) is 14% lower than the mean value, while the upper bound (97.5th percentile) is 19% higher than the mean value.

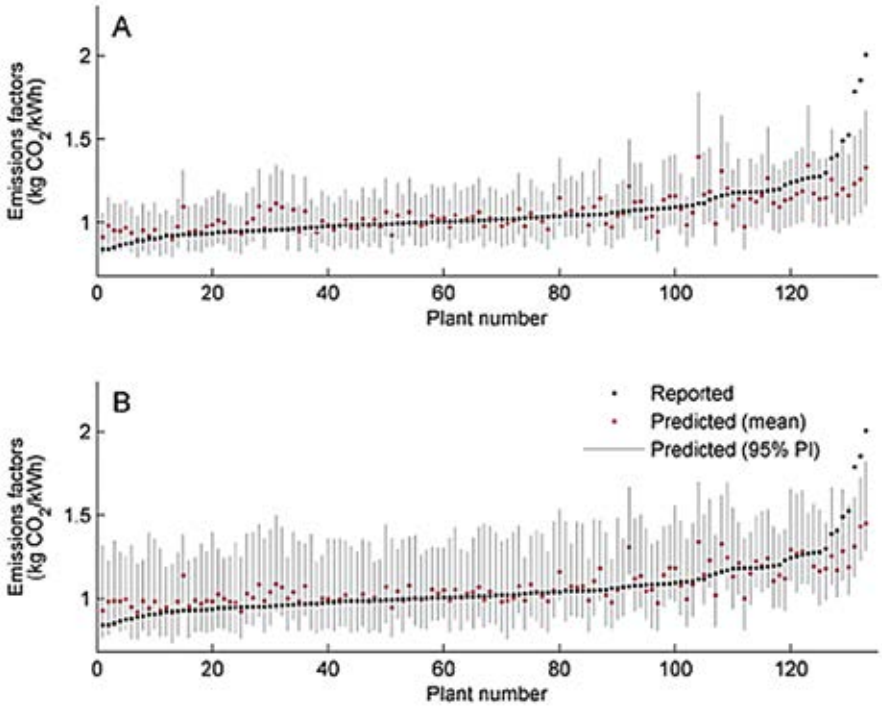


FIGURE 3.1 Reported and predicted CO_2 emission factors for the 133 plants in the test set with corresponding 95% prediction intervals (y axis) by an individual power plant (x axis) for the (A) multiple regression and (B) local linear regression models. Power plants are sorted from low to high by reported CO_2 emission factor.

The multiple regression model does not perform well for plants with emission factors exceeding 1.5 kg of CO_2/kWh (Figure 1A). Results of the relative errors plotted against the predictors (see SI3 of the Supporting Information and Figure S2) show that relative errors lower than −0.2 (i.e., plants for which the model underestimates emission factors by more than 20%) are mainly observed for plants that are older than 30 years, have a capacity <1000 MW, and/or a steam pressure below 125 bar.

LOCAL LINEAR REGRESSION MODEL

The optimal value of α, selected by minimizing the mean square error through LOOCV of the training set, was found to be 9.3. The R^2 value of the local linear model based on the training data set is 0.55, while this value based on the test set is 0.61. Reported and predicted emission factors (with 95% prediction intervals) for all 133 power plants in the test set are displayed in Figure 3.1B. On average (over all 133 plants), the lower bound of the 95% prediction interval (2.5th percentile) is 17% lower than the mean value, while the upper bound (97.5th percentile) is 31% higher than the mean value. The model performs slightly better than the global multiple regression model, as also observed from Figure 3.1.

MODEL APPLICATION

Both models were applied to predict the CO_2 emission factors of 764 coal-fired power plants worldwide. As an example, Figure 3.2 shows the predicted CO_2 emission factors for countries with >30 power plants, for which (almost) no reported emission data were available, Russia and China. For the Russian plants, the multiple regression model predicts an unweighted (i.e., with equal weight to every plant, regardless of the capacity of the plant) mean emission factor of 1.14 kg of CO_2/kWh (individual plant emission factors ranging between 0.95 and 1.48 kg of CO_2/kWh), while the local linear regression method predicts an unweighted mean emission factor of 1.25 kg of CO_2/kWh (0.97–1.57 kg of CO_2/kWh). The estimated emission factors of Chinese coal-fired power plants are typically lower than Russian plants, i.e., 1.03 kg of CO_2/kWh (0.90–1.49 kg of CO_2/kWh) for the multiple regression model and 1.04 kg of CO_2/kWh (0.88–1.46 kg of CO_2/kWh) for the local linear regression.

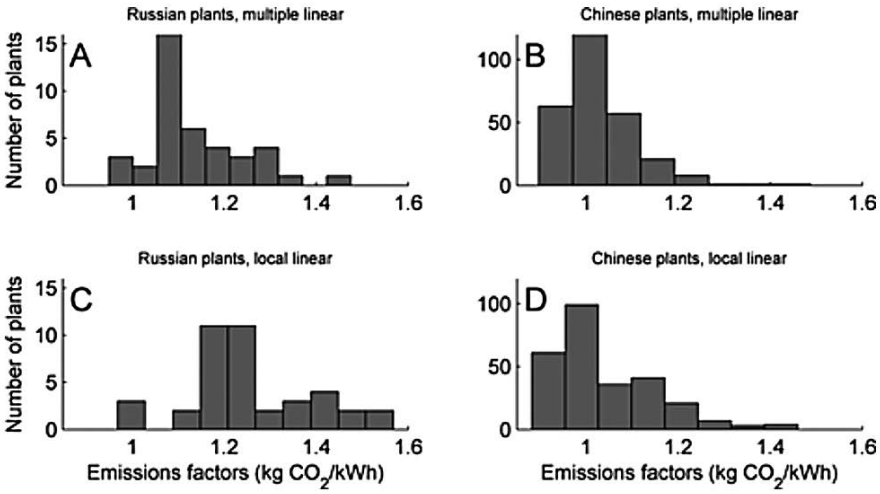


FIGURE 3.2 Histograms of predicted CO_2 emission factors (kg of CO_2/kWh) of coal plants in Russia and China for the (A and B) multiple regression model and (C and D) local linear regression model. The predicted emission factors (mean and 95% prediction intervals) for the corresponding individual plants are presented in Figure S4 of the Supporting Information.

Estimates and the corresponding 95% prediction intervals for each of the 764 plants can be found in Table S5 of the Supporting Information. Unweighted mean CO_2 emission factors over 764 plants were estimated to be 1.08 kg of CO_2/kWh by the multiple regression model and 1.12 kg of CO_2/kWh by the local linear regression model. The range of mean predictions per power plant obtained by the multiple regression model (0.84–2.34 kg of CO_2/kWh) is larger than the range for the local linear model (0.87–1.89 kg of CO_2/kWh). It should be noted, however, that the maximum value predicted by the multiple regression model refers to a plant with extreme characteristics (old plants with small capacity and low steam pressure) located in a country with low GDP per capita (Zimbabwe). The characteristics of this plant are outside the range of predictors used to train the model. When the 95% prediction intervals are considered, we observe a smaller range for the multiple regression model (0.90–1.42 kg of CO_2/kWh) compared to the range (0.90–1.57 kg of CO_2/kWh) found for the local linear regression.

Discussion

MODEL PERFORMANCE

We employed two regression techniques (multiple linear regression and local linear regression) to estimate the CO_2 emission factors of coal-fired power plants on a global scale. Predictions obtained by the local linear regression model show a slightly better

performance, as demonstrated by the higher R^2 of the test set (0.61 for local linear regression versus 0.49 for the multiple linear regression). We also tested a number of alternate non-parametric regression approaches, including k-nearest neighbors and kernel regression (see Table S6 of the Supporting Information). However, the local linear regression was found to perform better than these methods based on the training and test set R^2 values.

Both regression models have a relative error of less than 20% for more than 95% of the power plants based on the test set with 30% of the plants. A direct comparison of these values to the findings by Ummel (2012) in the CARMA model is impossible because the results were not provided separately for coal-fired plants; CO_2 emissions from all thermal power plants (including other generation types, such as natural gas plants) were estimated in that study. As noted, our multiple regression model, in particular, underestimates the highest reported emission factors (>1.5 kg of CO_2/kWh). A similar effect can be observed in the CARMA model (Ummel, 2012). The highest predictions (for any fuel type) from that study were approximately 1.5 kg of CO_2/kWh, while the highest reported emission factors were close to 2.0 kg of CO_2/kWh.

A possible limitation of our models is that they do not address temporal variability in the emission factors. Because of data limitations, it was not possible to obtain reported emissions and generation data for multiple years for all power plants in the data set. We did, however, assess the temporal variability in the emission factors of a subset of U.S. coal plants for which data were available (see SI4 of the Supporting Information). Even though the total annual CO_2 emissions and the net generation were found to fluctuate over the years (as presented in the CARMA report (Ummel, 2012)), our results show that emission factors appear to be relatively stable. For the 306 plants with an emission factor of <1.5 kg of CO_2/kWh, the difference between extreme values observed over a 3 year time period was, on average, 3.1% of the mean value. Additionally, the highest temporal variability was found for plants with high CO_2 emission factors. The four plants with an average emission factor of >1.5 kg of CO_2/kWh show an average difference of 33% between the extreme values. This finding indicates that the CO_2 emission factors of the plants with relatively high CO_2 emission factors are inherently variable over time. This finding may also help explain why our models make less accurate predictions for plants with high emission factors.

Analysis of the relative errors in the training set and the test set (see SI3 of the Supporting Information) shows that the model fit is not as good for plants that are over 30 years old, have a capacity below 1000 MW, or especially, have steam pressures below 125 bar. Therefore, we suggest caution when applying our model to plants with characteristics in this range, especially if a plant has all three characteristics in the critical range.

NUMBER OF PREDICTORS

A limited number of readily available predictors was included in our models, because the aim was to develop models to predict emission factors for a large number of power plants. On the basis of AIC, we found that the best model included all predictors, indicating that none of these predictors were redundant. However, several other predictors may influence plant efficiencies and, therefore, CO_2 emission factors, such as the cooling processes of the plant, the presence of SO_2 and NO_x control equipment, and plant capacity factor. Furthermore, the grid stability of a country may influence the performance of a power plant as well. If the grid lacks stability, plants have to stop and start relatively often, which lowers the average plant efficiency. We were, however, not able to add the regional grid stability as an extra predictor because of the lack of data.

Lam and Shiu (2001) found that the capacity factor strongly influences power plant efficiency. As part of a sensitivity analysis, we included the plant capacity factor as an additional predictor (see SI5 of the Supporting Information). The predictive power of both models increased as a result of including the capacity factor as an additional predictor. However, both models were not able to make accurate predictions for plants with high emission factors, even when including the capacity factor as a predictor variable. It was also found that estimates for plants with capacity factors higher than 50%, in general, have lower relative errors (as shown in SI5 of the Supporting Information). It should be noted, however, that for the external application of our models, the capacity factor has no added value because net electricity generation is typically not known for plants that do not report CO_2 emissions.

MODEL APPLICATION

The applicability domain of a model refers to the range of predictor values in which a model can be applied. The observed ranges of predictors in the application set were similar to or within the range of the model development set. From this, we conclude that the plants in the application set were within the applicability domain of our models. One exception is the per capita GDP, which ranges between $3700 and $48 000 per capita in the model training set. A total of 11 plants in the application set are situated in countries with GDP below $3700 per capita. Extrapolation outside the original range causes the predictions for these plants to be more uncertain, such as for the prediction for the coal plant in Zimbabwe, which should be interpreted with caution.

The uncertainties that are introduced by predictive modeling are around 8 times larger than the uncertainty that was found for measured emissions in the United States by Steinmann et al. (2014). Their study showed that it is possible to reduce uncertainty in the emissions from individual power plants to a much smaller range with full disclosure of power plant fuel use and electricity generation data. In the absence of more data, however, a modeling approach for calculating the CO_2 emission factors of

individual power plants could help address data gaps in life cycle inventories. With small adaptations to our model framework, it is possible to estimate power plant efficiencies directly. The estimated average efficiency of plants in a country could then be applied in a database, such as Ecoinvent, where the process of coal delivery to a plant is already coupled to the operational efficiency. To derive a country estimate from the individual power plants in that country, one needs to combine the estimates (and the uncertainty in the estimates) for every power plant. Uncertainty ranges may vary from plant to plant depending upon the number of predictors that are available for each plant. Monte Carlo simulations can be used to sample from the uncertainty range of each individual power plant. These samples can then be combined to generate an overall country estimate (with its own uncertainty interval).

The regression models presented here predict the combustion-phase CO_2 emission factors for coal-fired power plants. Although coal combustion typically contributes to 90% or more of the life cycle emissions from coal-fired electricity generation (see e.g. Steinmann et al., 2014 and Littlefield et al., 2010), upstream emission factors need to be assessed as well. The upstream emissions cannot be modeled easily, however, because they depend upon factors such as the type of coal mine, heat content of the fuel, transport type, and transport distance (as demonstrated by Steinmann et al., 2014). Except for the type of fuel, these data are not readily available for most power plants. Part of this information (country-specific transport distances and coal sources) is, however, already available in life cycle inventory databases. Coupling of our model estimates with this type of data can provide a better estimate (for data-scarce countries) of the total life cycle emissions of electricity generation.

Despite limitations in the regression models developed, we found that they provide an improvement compared to assigning averaged CO_2 emission factors to each power plant. Although we applied this methodology to a case study of coal-fired power plants, we expect that a similar approach can be used to estimate emission factors from biomass-, gas-, and oil-fired power plants.

Acknowledgment

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CHAPTER 4

Estimating the greenhouse gas balance of individual gas-fired and oil-fired electricity plants on a global scale

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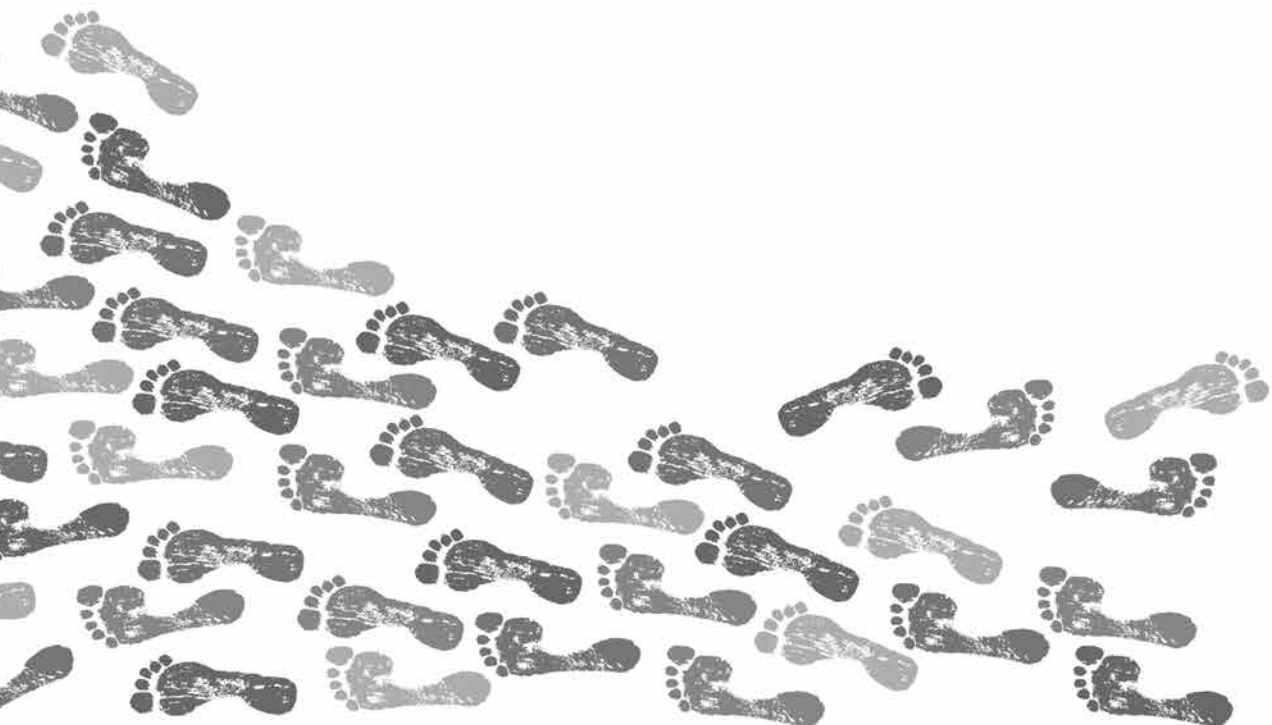

Abstract

Life cycle greenhouse gas (LC-GHG) emissions from electricity generated by a specific resource, such as gas and oil, are commonly reported on a country-by-country basis. Estimation of variability in LC-GHG emissions of individual power plants can, however, be particularly useful to evaluate or identify appropriate environmental policy measures. Here, we developed a regression model to predict LC-GHG emissions per kilowatt-hour (kWh) of electricity produced by individual gas- and oil-fired power plants across the world. The regression model uses power plant characteristics as predictors, including capacity, age, fuel type (fuel oil or natural gas), and technology type (single or combined cycle) of the plant. The predictive power of the model was relatively high (R^2 = 81% for predictions). Fuel and technology type were identified as the most important predictors. Estimated emission factors ranged from 0.45 to 1.16 kilograms carbon dioxide equivalents per kilowatt-hour (kg CO_2-eq/kWh) and were clearly different between natural gas combined cycle (0.45 to 0.57 kg CO_2-eq/kWh), natural gas single cycle (0.66 to 0.85 kg CO_2-eq/kWh), oil combined cycle power plants (0.63 to 0.79 kg CO_2-eq/kWh), and oil single cycle (0.94 to 1.16 kg CO_2-eq/kWh). Our results thus indicate that emission data averaged by fuel and technology type can be profitably used to estimate the emissions of individual plants.

Introduction

Fossil energy demand and related greenhouse gas (GHG) emissions constitute one of the largest sources of environmental impacts for many products, particularly by electricity generation throughout a product's life cycle (e.g., Huijbregts et al. 2006; De Schryver et al. 2013). It is therefore considered important to estimate the GHG emissions of electricity generation as accurately as possible. Generic data on electricity generation, for example, on a country level, is often used in GHG balance calculations (e.g., Dones et al. 2007; Faist Emmenegger et al. 2007). On an individual power plant level, these estimates, however, neglect differences in GHG emissions between these plants caused by differences in technology, efficiency, or location, the latter determining the distance to extraction of the energy sources (coal mines and oil, or gas fields). Steinmann and colleagues (2014) and Hauck and colleagues (2014) showed that the range in carbon footprints from electricity generation by coal and gas within the Unites States are primarily driven by technological differences between individual power plants using the same fossil energy source.

Various statistical estimation methods have been employed to quantify the effects of technological variability in energy generation on GHG emissions, including the development of power scaling laws (Caduff et al. 2011, 2012, 2014), kriging (Moreau et al. 2012a, 2012b), and regression models (Steinmann et al. 2014b; Ummel 2012). A generally applicable model to estimate life cycle GHG (LC-GHG) emissions specific to individual gas- and oil-fired power plants is, however, lacking.

The aim of this research is to develop a predictive regression model to estimate LC-GHG emissions per kilowatt-hour (kWh) of electricity generated by individual gas- and oil-fired power plants worldwide, using data available for a limited subset of power plants. The regression model includes the power plant characteristics age, capacity and technology, and fuel type as predictors. To show how the model can be applied, we predict LC-GHG emissions for all gas- and oil-fired power plants across the world.

Materials and Methods

We developed a regression model to predict LC-GHG emissions per kWh electricity production from gas- and oil-fired power plants across the world. Our approach is similar to Steinmann and colleagues (2014b) for coal-fired power plants. However, our modeling goes beyond their approach by applying a mixed-model structure that accounts for differences in prediction uncertainty according to technology and fuel types. The chosen model structure also allows for assessing the importance of regional differences in the model fit. In this section, we describe the data used to develop the regression models, the model structure, metrics to evaluate the performance of the model, and the application of the model.

DATA SELECTION

Most power plants consist of several units, which, in turn, consist of one or several turbines. Turbines may run stand-alone (single cycle; SC) or in combination with other turbines (combined cycle; CC). In a combined cycle, hot combustion products are reused to drive a second turbine. For our regression model, we selected and performed analysis on operational power plant units (hereafter called "plants"). Operational power plants were required to run at least 1 day a year. We selected power plants that run on gas or oil only and that were designed to produce only electricity. Cogeneration plants producing both electricity and heat and plants running on several fuels were excluded because we were not able to allocate GHG emissions to heat and electricity or the fuels used based on the plant-specific information available. To select for power plants that were designed to provide grid electricity, we only included power plants with a capacity above 100 megawatts (MW).

EMISSION DATA

Unit-specific emission data (observations) were obtained for 384 facilities situated in nine different countries. For the United States and Singapore, life cycle emissions were directly taken from Hauck and colleagues (2014) and Kannan and colleagues (2005), respectively. For the other plants, upstream emissions were taken from the ecoinvent 3.1 model (Faist Emmenegger et al. 2007). Emissions included carbon dioxide (CO_2) and, for the natural gas life cycle, methane (CH_4) emissions arising from losses of natural gas during extraction, processing, and transport. These GHG emissions were translated to CO_2-equivalents (CO_2-eq) using a global warming potential for CH_4 of 30 kilograms (kg) CO_2-eq/kg from the Fifth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC) (Myhre et al. 2013). Table 4.1 shows the sources of the unit-specific emission data.

PREDICTOR VARIABLES

We selected predictors that were available from public data sources with a world-wide coverage to enhance general model usability (see table S1 in the supporting information available on the Journal's website). Plant age and total capacity were included because these were expected to influence GHG emissions of power plants (Steinmann et al. 2014b). Total plant capacity was calculated as the sum of the capacities of all active turbines within a plant unit. Plant age was calculated as the capacity-weighted average of all active turbines within a unit. Combined cycle plants generally have a higher overall efficiency and lower GHG emissions per kWh electricity produced (Hauck et al. 2014). The distinction between SC and CC was therefore also included as predictor. Table 4.1 shows the data gathered for model development. Plant characteristics (age, fuel type, and technology type) were taken from Platts (2012) if not available in the original sources in table 4.1..

We also developed an alternate model including the capacity factor, the fraction of capacity actually used for power generation, as additional predictor, for a subset of power plants for which these data were available. The capacity factor has been stated as important factor for power plant efficiency (Lam and Shiu 2001). Capacity factors were derived as the ratio between net generation (from sources in table 1) and the maximum possible generation based on the plant's capacity (from sources in table 4.1 or UDI World Electric Power Plants Data Base [WEPP]).

TABLE 4.1 Overview of gas and oil fired power plants and data sources for emission factors employed in model development. With exception of the United States and Singapore, upstream emissions were taken from ecoinvent (Faist Emmenegger et al. 2007; Jungbluth 2007). Upstream emissions for natural gas refer to the Rest of the World region in ecoinvent, with exception of Italy where country-specific upstream emissions were reported, and upstream emissions for Mexico that were taken from the Region of North America. For oil, only upstream emissions for the Rest of the World were available. Plant characteristics age, fuel type and technology type were taken from Platts (2012).

Country	Number of observations	Capacity (MW)	LC-GHG emission factors (kg CO_2-eq/kWh)	Age (years)H	Fuel Type	Technology Type	Source
Natural gas fired power plants							
USA	274	120 – 3750	0.46 - 0.72	1 – 40	Natural gas	Combined Cycle	Hauck et al. (2014)
		148 - 2051	0.71 - 0.90	4 - 54	Natural gas	Single Cycle	
Italy	2	780 - 1030	0.51 - 0.60	7 - 8	Natural gas	Combined Cycle	Enipower[A]
Australia	24	140 – 630	0.46 – 0.68	3 - 15	Natural gas	Combined Cycle	AEMO[B]
		156 - 800	0.71 – 1.16	1 - 45	Natural gas	Single Cycle	
Hong Kong	1	2,500	0.46	14	Natural gas	Combined Cycle	CLP[C]
India	27	120 - 1148	0.51 - 0.89	1 - 18	Natural gas	Combined Cycle	CLP[C],CEA[D]
		114 - 912	0.36 – 0.63	11 – 39	Natural gas	Single Cycle	
Brazil	1	311	0.39	7	Natural gas	Combined Cycle	ENEL (2011)
Morocco	1	348[E]	0.41	5	Natural gas	Combined Cycle	ENEL (2011)
Singapore	1	1,470[F]	0.47	2	Natural gas	Combined Cycle	Kannan et al. (2005)
Mexico	4	2 - 23	0.49 - 0.61	2 - 23	Natural gas	Combined Cycle	CEC (2011)
Total	**335**	**241,799**					
Oil fired power plants							
USA	34	100 – 1590	0.85 - 1.74	13 - 58	Light or heavy fuel oil	Single Cycle	EIA-923 data 2012[G]
		116	0.74	15	Light fuel oil	Combined Cycle	
Australia	1	414	1.01	11	Light fuel oil	Single Cycle	AEMO[B]
India	1	165	0.64	15	Light fuel oil	Combined Cycle	CEA[D]
Mexico	13	113 - 1546	0.83 - 1.42	11 - 42	Light or heavy fuel oil	Single Cycle	CEC (2011)
Total	**49**	**24,347**					

[A] http://www.enipower.eni.it/it/pages/dove-operiamo/dove-operiamo.shtml;
[B] http://www.aemo.com.au/Consultations/National-Electricity-Market/Closed/~/media/Files/Other/planning/0410-0029%20zip.ashx; Combustion phase emissions were calculated from combustion efficiency and carbon content and fuel use was derived using heat content from Cuevas-Cubria et al. (2011)
[C] https://www.clpgroup.com/ourvalues/report/Pages/sustainabilityreport.aspx; Combustion phase emission were reported including scope 1 and 2 (purchased electricity and steam) emissions.
[D] http://www.cea.nic.in/reports/planning/cdm_co2/cdm_co2.htm
[E] Calculated from data for the ENEL-owned part of the plant (32%).
[F] Calculated from data for one cycle (367.5 MW).
[G] http://www.eia.gov/electricity/data/eia923/
[H] Age was defined as the year of reported emissions data minus the year of construction
MW = megawatts; kg CO_2-eq/kWh = kilograms carbon dioxide equivalents per kilowatt-hour.

MODEL FITTING

Before model fitting the reported emission factors and the predictors of plant age, capacity and capacity factor were log-transformed. Variance inflation factors (VIFs) were calculated to investigate multicollinearity among the predictors. Multicollinearity was considered acceptable when VIFs were below 5 (Zuur et al. 2009), and predictors exceeding this threshold would have to be excluded from the model building. However, VIFs were not higher than 2 for any predictor (see tables S2 and S3 in the supporting information on the Web). For visual inspection, we also included pair plots of the predictors in figure S1 in the supporting information on the Web.

The statistical program R was used to develop all models (R Team 2012). A linear mixed-effects model was fitted using the lme function from the package "nlme" (Pinheiro et al. 2015), where coefficients were fitted by means of REML (restricted maximum likelihood) estimation. A linear mixed-effects model is similar to a multiple linear regression model, but can deal with heteroscedasticity in the data by allowing the error distribution to vary between different groups (Zuur et al. 2009). In our study, the categorical predictors (fuel and technology type) were seen as separating groups. Additionally, the error in the intercept was estimated by allowing for different intercepts for five different world regions based on the data (India, United States, Mexico, Australia, and Rest of the World), which were assumed to be randomly distributed. The model was fitted based on 70% of the data (training data), randomly selected after making sure the percentages of each category (SC-oil, SC-gas, CC-oil, and CC-gas) were approximately equal in the training and validation sets. Predictor values for each plant in the training data and the validation set are shown in the Supporting Information (tables S4 and S5 in the supporting information on the Web, respectively).

The following regression was used to estimate LC GHG emissions per kWh produced:

$$E_{GHG} = \beta_0 + \beta_1 \cdot x_1 + \ldots + \beta_n \cdot x_n + \varepsilon_{t,f} \qquad \textbf{Equation 1}$$

where E_{GHG} is the logarithm of the LC-GHG emission factor (kg CO_2-eq/kWh), β_0 is the intercept of the model, β_1 to β_n are the model coefficients, and x1 to xn are the model predictors log capacity, log age, technology cycle type, and fuel type. The plant characteristics oil and single cycle type were modeled as binary variables in the model (either true (1) or false (0)). All oil power plants scored "true" for oil as a fuel, whereas all natural gas power plants scored "false" for oil fuel type. Plants that scored false on SC as predictor were CC power plants. The normally distributed error (ε), with a mean value of 0, has a different standard deviation for each combination of technology type t and fuel type f.

To determine the relative importance of each of the predictor variables, standardized regression coefficients for the non-categorical predictors were derived (Eriksson et al. 2003). To that end, log-transformed predictors were standardized to z-scores by mean centering and dividing by the standard deviation before model fitting.

MODEL EVALUATION

We evaluated model performance using the coefficient of determination (R^2). A value of 1 reflects a perfect model fit, whereas a model with an R^2 equal to or below 0 has no added value compared to using the average of the measured data (Legates and McCabe 1999). R^2 was calculated according to equation 2:

$$R^2 = 1 - \frac{\sum_i (y_i - y_{(pred,i)})^2}{\sum_i (y_i - mean(y))^2} \qquad \textbf{Equation 2}$$

where y_i is the actual GHG emission factor of plant i and $y_{pred,i}$ is the predicted GHG emission factor of the same plant. We report the R^2 for the model fitted on the training data set (70% of the data) as R^2_{train}. For the model applied to the remaining 30% of the reported data, we report R^2_{pred}, whereby the mean (y) in the denominator refers to the test set mean, rather than the training set mean, to avoid overly positive estimations of predictive power, following the recommendations by Schüürmann and colleagues (2008). The distinction is trivial in our case, however, because our training and test set means are very close (0.64 and 0.63 kg CO_2-eq/kWh, respectively). Additionally, we performed a cross-validation by splitting the training set in two sets containing 90% and 10% of the data, respectively. We repeated model fitting for all ten subsets, where the 90% was used for training and the 10% for testing. None of the ten test sets were overlapping with one another. For every test set, this resulted in a measured and a modeled value for each observation. We calculated an overall coefficient of determination based on all these pairs, termed R^2_{cv}.

Residual standard errors (RSE) were calculated based on the model developed with the 70% training set, whereby the RSEs were differentiated between the groups included in the model (SC, CC, oil, and natural gas). To identify whether the heteroscedasticity in the data set was adequately captured by this model configuration, we plotted normalized residuals for all plants against the individual predictors and against the fitted values (see figure S2 in the supporting information on the Web).

To estimate the uncertainty in the predictions for individual power plants, we calculated 95% prediction intervals. Predictions intervals were calculated by combining the RSEs and the uncertainty in the fit of the model's coefficients. The latter was calculated by the predictSE function in the package "AICcmodavg" (Mazerolle 2015).

MODEL APPLICATION

The WEPP database reports a total capacity of currently operational natural gas- and oil-fired power plants above 100 MW without cogeneration of around 1,300,000 MW. Of these, the 384 power plants included for model development have a total capacity of 266,236 MW (around 20% of the total) (see table 1 as well as table S1 in the supporting

information on the Web). For illustration, we applied our model to the 2,538 gas- and oil-fired power plants above 100 MW without cogeneration worldwide included in the WEPP database. Results were compared to emission factors taken from the ecoinvent database (Moreno Ruiz et al. 2013). ecoinvent reports country-specific emission factors, from which the minimum and maximum emission factors per region were selected. By excluding cogeneration plants, we neglected around 10% of total current gas- and oil-fired generation capacity by plants above 100 MW.

Results

MODEL PERFORMANCE

The model fitted to the 70% training data set resulted in the following coefficients for the predictors log age, log capacity, fuel, and technology type of power plants (equation (3)):

$$E_{GHG} = -0.25(\pm 0.026) - 0.03(\pm 0.008) \cdot logC + 0.04(\pm 0.008) \cdot logA + 0.14(\pm 0.006) \cdot OIL + 0.17(\pm 0.007) \cdot SC \qquad \textbf{Equation 3}$$

where log C is the logarithm of the capacity, log A is the logarithm of the age, OIL is oil as fuel, and SC is single cycle as technology type. The explained variance was 89% for the training set and the cross-validation (R^2_{train} and R^2_{cv} of 0.89; see table S6 in the supporting information on the Web for model coefficients) and 81% (R^2_{pred} of 0.81) for the predictions in the validation data set (see also figure S3 in the supporting information on the Web for predicted values and ranges of the plants in the validation set). Residual standard errors were 0.04 for SC gas-fired plants, 0.03 for CC gas-fired plants, and 0.08 for SC oil-fired plants. The standard error of the intercept was 0.025. For CC oil-fired plants, the RSE could not be estimated reliably because there was only one power plant of this category in the training data set.

According to the standardized coefficients, fuel type and technology type were more important as predictor than log capacity and log age (see table S7 in the supporting information on the Web). Figure 4.1 shows reported and estimated emissions factors and 95% prediction intervals for the 270 observations used for model development. Plant units are sorted according to increasing reported emission factors. Three clusters of power plant emission factors can be distinguished in figure 4.1. The plants with lowest emissions factors (up to plant numbered 177, shown in circles) are CC gas power plants. SC gas plants (triangles) have higher emission factors, whereas oil plants exhibit the highest emission factors. Absolute prediction intervals also increase from CC natural gas– to oil-fired power plants. Consistent with the ranges of reported emission factors shown in table 1, predicted emission factors of these different types of power plants do not overlap

significantly. GHG emission factors were underestimated particularly for the four oil plants with very high emission factors (>1.4 kg CO_2-eq/kWh).

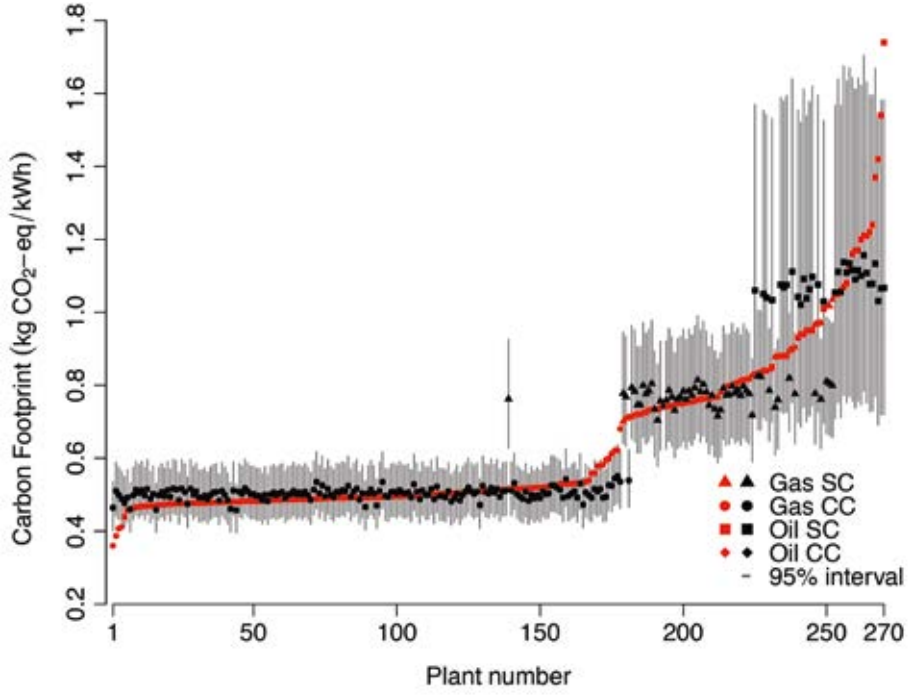

FIGURE 4.1 Reported (red) and estimated (black) GHG emission factors and 95% prediction intervals (gray lines) for single cycle gas plants (triangles), combined cycle gas plants (circles), single cycle oil plants (squares), and combined cycle oil plants (diamonds). Observations are sorted by increasing emission factors. GHG = greenhouse gas.

Additional Predictor: Capacity Factor

For the model with the capacity factor included, coefficients were fitted as (equation (4)):

$$E_{GHG} = -0.28(\pm 0.02) - 0.03(\pm 0.007) \cdot logC + 0.05(\pm 0.007) \cdot logA + 0.22(\pm 0.011) \cdot OIL + 0.14(\pm 0.007) \cdot SC - 0.04(\pm 0.007) \cdot logCF \quad \textbf{Equation 4}$$

where log C is the logarithm of the capacity, log A is the logarithm of the age, OIL is oil as fuel, SC is single cycle, and log CF the logarithm of the capacity factor.

The explained variance increased from 89% to 92% (R^2_{train}). The RSE decreased from 0.04 to 0.03 for SC gas plants and from 0.08 to 0.07 for SC oil plants. No change in RSE was observed for CC gas plants.

Figure 4.2 shows the observed and estimated emission factors and 95% prediction intervals for the model including capacity factor.

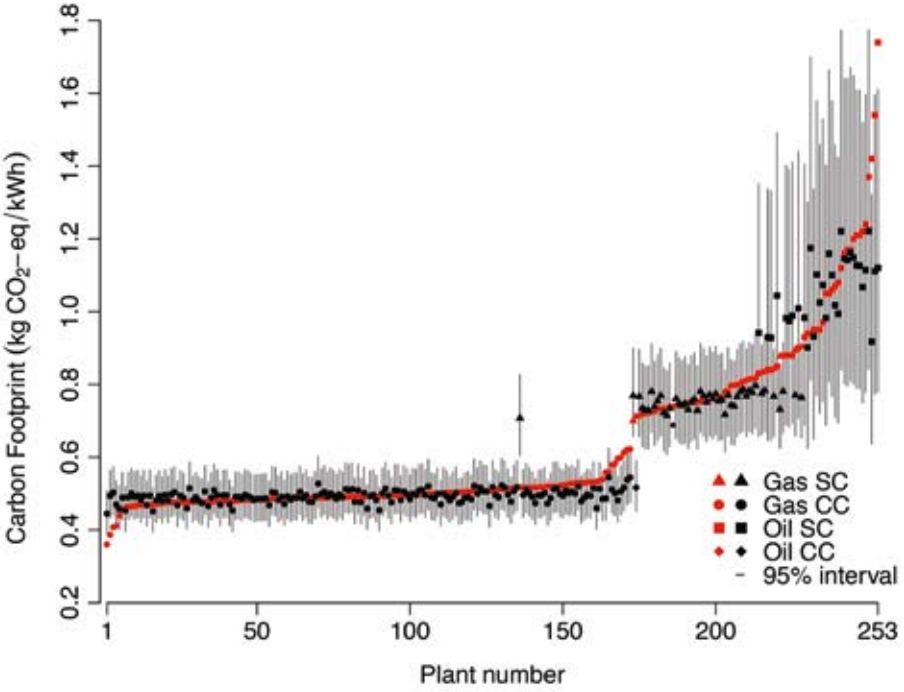

FIGURE 4.2 The effect of including the capacity factor as additional explanatory variable. Reported (red) and estimated (black) GHG emission factors and 95% prediction intervals (gray lines) for single cycle gas plants (triangles), combined cycle gas plants (circles), single cycle oil plants (squares), and combined cycle oil plants (diamonds). Power plant observations are sorted by increasing emission factors. GHG = greenhouse gas.

APPLICATION

Figure 4.3 shows the distribution of LC-GHG emission factors of noncogeneration natural gas- and oil-fired power plants that are 100 MW and above, reported in the WEPP database. For comparison, emission factors taken from the ecoinvent Database (Moreno Ruiz et al., 2013) are also shown. The three peaks in all the panels of figure 4.3 reflect the differences in emissions between CC natural gas–fired power plants, single cycle natural gas–fired power plants, and oil-fired power plants. For most regions, except Europe and the Middle East, ecoinvent emission factors for each group of natural gas power plants were lower than model estimates. For oil, the difference between high and low country emission factors were larger, and emission factors are generally larger in ecoinvent than in our model.

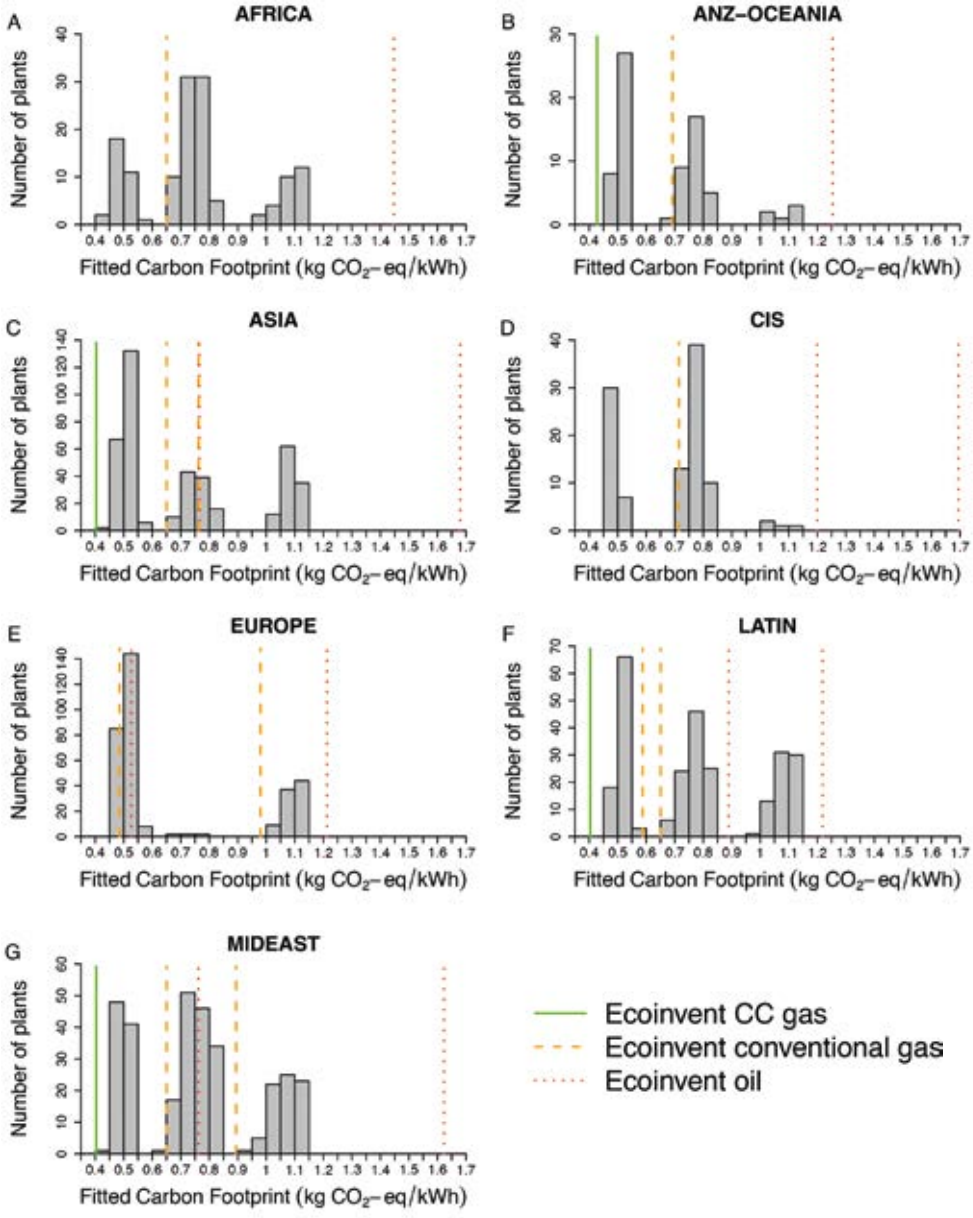

FIGURE 4.3 Histograms of emission factors predicted with our model per region of the world. Regions: (a) Africa; (b) ANZ-Oceania: Australia, New Zealand, and Oceania; (c) Asia; (d) CIS: Commonwealth of Independent States; (e) Europe; (f) LATIN: Latin America; and (g) MIDEAST: Middle East. Vertical lines indicate the lowest and highest regional GHG emission factors in the ecoinvent Database version 3.0. GHG = greenhouse gas.

Discussion

MODEL PERFORMANCE

The regression model developed was able to capture much of the variability in LC-GHG emissions per kWh produced by gas- and oil-fired power plants. This is in line with Hauck and colleagues (2014) who found that variability in LC-GHG emission factors of gas-fired power plants was primarily owing to technological differences. However, our model was not able to capture plants with very high emission factors (i.e., >1.4 kg CO_2-eq/kWh), as also found by Steinmann and colleagues (2014b) for combustion CO_2 emissions from coal-fired power plants. No systematic bias could be deduced from the residual plots (see figure S2 in the supporting information on the Web). Additionally, histograms of the residual deviation between predictions and observations were generally normally distributed based on visual inspection (see figure S4 in the supporting information on the Web).

MODEL REPRESENTATIVENESS

GHG emissions resulting from electricity generation can differ between countries, possibly because of differences in maintenance or cooling systems. Our model covers regional differences by assuming a random intercept that is allowed to vary across regions (India, United States, Mexico, Australia, and Rest of the World). Results show that the standard error of the intercept is 0.025. Because we use a log-transformed model, this means that approximately 95% of the predictions have an intercept within a factor of 1.12 from the fitted value of -0.25.

For most countries (except the United States, Singapore, and Italy) we employed generic upstream emission factors from ecoinvent. The total variation in upstream emission factors over all countries available in ecoinvent was a factor of 10, depending on whether gas is taken from sources close by or has to be transported as liquefied gas. Upstream emissions, however, generally do not contribute to more than 10% of total LC-GHG emissions (see also Hauck et al. 2014). For oil-fired power plants, few region-specific upstream emissions (Switzerland, Europe, and Rest of the World) were available and these were within a factor of 3 of one another.

Table 4.1, in combination with table S1 in the supporting information on the Web, indicates that our training set does not include the full range of the power plants available in the WEPP database. Predictions for very high-capacity plants (>2,000 to 3,000 MW) fall outside the training domain and should be interpreted with care. There are, in total, five gas-fired power plants with a capacity above 3,000 MW in Russia and Saudi Arabia. All other natural gas–fired power plants are well within the applicability domain of our

training set. For oil, eight power plants were outside the training domain, located mainly in Saudi Arabia and Ukraine.

MODEL INTERPRETATION

Estimated emission factors for CC plants were typically closer to reported emission factors than for SC plants and oil-fired power plants. SC and oil-fueled power plants are often used to intermittently provide electricity in periods of peak demand and thus do not make full and constant use of their capacity. These results indicate that for peak demand electricity generation, capacity and age are less strong predictors because they do not address how much of the capacity is actually used. Including capacity factor as an additional predictor reduced the residual standard error for SC natural gas– and oil-fired power plants, but not for CC power plants.

The difference in standardized coefficients for fuel and technology type versus other predictors in our model (around a factor 10; see table S7 in the supporting information on the Web) is much larger than differences between standardized coefficients (age, capacity, type of coal, and per capita gross domestic product [GDP]) found by Steinmann and colleagues (2014b) (around a factor of 2). These results highlight the importance of distinction in plant technology and fuel type for estimating LC-GHG emissions from natural gas– and oil-fired power plants. This finding indicates that relatively good estimates of LC-GHG emission factors can also be obtained by using a model with technology and fuel type as predictors without further specification of the age and capacity of the plant. This conclusion is further corroborated by the fact that differences within a certain technology or fuel type were small, whereas differences between groups were much larger (figure 4.1 and figure 4.2 as well as figure S3 in the supporting information on the Web).

Concluding Remarks

We developed a regression model to estimate LC-GHG emission factors per kWh of electricity generated by natural gas– and oil-fired power plants. The model captures the main differences in observed emissions data and was evaluated to be more robust than using the average of the reported data. We found that technology and fuel type were, by far, the most important predictors for LC-GHG emission factors. Our results can be useful for life cycle assessment and carbon footprinting in several ways. First, life cycle emission factors of individual plants can be directly utilized in system boundaries that include these specific plants. Second, the variation in regional or country-averaged electricity footprints can be estimated based on our model results and considered in more generic assessments. Additionally, for countries where no emission factors are available, these

can be calculated from the available technologies and fuels using our model. If the marginal producers are known, changes to the GHG emissions of the electricity mix can be assessed in detail. Consequences of policies for maintaining or phasing out certain technologies can be modeled. A similar modeling approach could be used for other combustion-related electricity generation, such as from biomass.

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CHAPTER 5

How Many Environmental Impact Indicators Are Needed in the Evaluation of Product Life Cycles?

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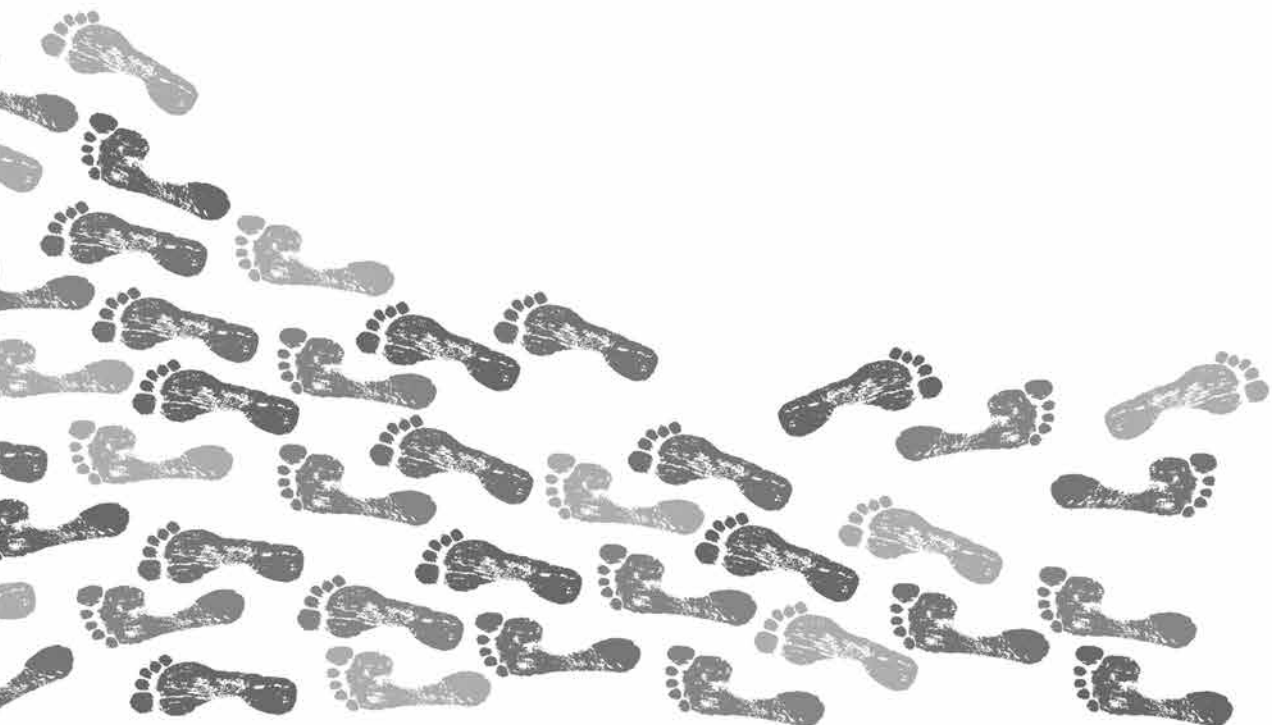
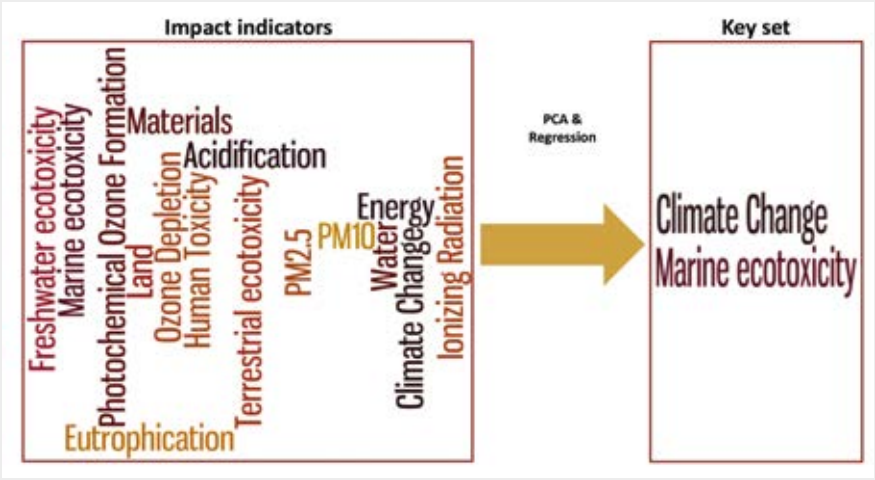


Abstract



Numerous indicators are currently available for environmental impact assessments, especially in the field of Life Cycle Impact Assessment (LCIA). Because decision-making on the basis of hundreds of indicators simultaneously is unfeasible, a nonredundant key set of indicators representative of the overall environmental impact is needed. We aimed to find such a nonredundant set of indicators based on their mutual correlations. We have used Principal Component Analysis (PCA) in combination with an optimization algorithm to find an optimal set of indicators out of 135 impact indicators calculated for 976 products from the ecoinvent database. The first four principal components covered 92% of the variance in product rankings, showing the potential for indicator reduction. The same amount of variance (92%) could be covered by a minimal set of six indicators, related to climate change, ozone depletion, the combined effects of acidification and eutrophication, terrestrial ecotoxicity, marine ecotoxicity, and land use. In comparison, four commonly used resource footprints (energy, water, land, materials) together accounted for 84% of the variance in product rankings. We conclude that the plethora of environmental indicators can be reduced to a small key set, representing the major part of the variation in environmental impacts between product life cycles.

Introduction

Over the course of the last two decades a wide variety of methods for quantifying environmental impacts have been introduced into the area of Life Cycle Impact Assessment (LCIA) (Hauschild et al., 2013). There are clear differences in coverage and complexity of the various LCIA methods available. Damage-based indicators, also called endpoint indicators, provide insight in the impact of emissions and resource use through the full cause-and-effect chain, which ultimately leads to ecosystem and/or human health damage (Goedkoop et al., 2013). Midpoint indicators provide a proxy for environmental damage by modeling only part of the cause-impact pathway. An example is the well-known global warming potential to quantify the contribution of various greenhouse gas emissions to climate change in terms of integrated radiative forcing (IPCC, 2013). Finally, resource footprints estimate the resources required in a life cycle without further impact or damage modeling. Cumulative energy demand is an example of such an indicator (Hirst, 1974; Arvidson et al., 2012; Arvesen & Hertwich, 2015; Frischknecht et al., 2015). Additional variation in indicators results from the fact that there are several competing methods available that quantify the same type of effect but with different models and data. For example, the TRACI method (Bare, 2011) and the EDIP method (Hauschild & Potting, 2005) both provide midpoint indicators for the impacts due to acidification.

A key question that this wide variety of available methods raises is whether the outcome of a Life Cycle Assessment (LCA) will change among different indicators and methods (Dreyer et al., 2003; Owsianiak et al., 2014; Bueno et al., 2016) Furthermore, it is unpractical to base decisions for environmental product optimization or environmental policy on dozens of indicators simultaneously. Endpoint damage models solve the problem of having too many indicators, but this goes at the expense of increased uncertainty, as uncertainties involved in damage modeling can be very large (Van Zelm et al., 2007, 2009; Rosenbaum et al. 2008).

Therefore, as an alternative to the endpoint damage models, there is a clear need to provide a limited set of indicators that is sufficiently small for efficient communication and decision-making but at the same time representative of the overall environmental impact. Several attempts have been made to find a representative subset of relevant indicators. In a study commissioned by the Joint Research Centre of the European Commission (JRC), various midpoint and endpoint indicators and methods were qualitatively compared in terms of scientific and stakeholder acceptance (Hauschild et al. 2013). However, with 14 different recommended midpoint indicators, the set is still quite large, and some of the methods have since then undergone quite significant changes. Moreover, the JRC study did not consider any redundancy among the recommended indicators caused by similarity in the underlying processes that cause the emissions and environmental impacts. Others have suggested using a "resource-based indicator family", consisting of a set of resource footprints covering the cumulative demand of land, water, carbon (or fossil energy), and,

potentially, materials (Galli et al, 2012). However, while these resource footprints are easy to use and communicate (European Resource Efficiency Platform, 2014), they may not account for the full range of impacts employed in the damage-based methodologies. Finding a set of indicators that is optimal in both its size and coverage requires a more systematic and quantitative way of reducing the number of indicators. A few studies have attempted to achieve this via Principal Component Analysis (PCA) (Pozo et al., 2012; Brunet et al., 2012; Sabio et al., 2012; Li et al., 2012; de Saxcé et al., 2014). If correlations between indicators are high, substantial dimensionality reduction can be achieved by PCA. For example, only two out of 11 indicators were needed to cover more than 95% of the total variance of the environmental impacts within a set of nine household electronic products (Gutiérrez et al., 2010). A more recent study, covering 17 impact indicators for two product categories (electricity and oil), employed a slightly different and novel technique to demonstrate that the number of impact indicators can be greatly reduced (Pascal-González et al., 2015). However, while these studies provided valuable insights for one or a few method(s) and/or product group(s), their coverage has been too small to answer questions about which set of indicators is optimal in a more general sense. The search for an optimal set of indicators using PCA has, to the best of our knowledge, not yet been applied over a large range of products and impact assessment methods.

Here, we aim to find an optimal set of environmental indicators to cover the variance in the rankings of a large number of products. We selected 976 products and 135 environmental indicators from the ecoinvent 3.1 database (Moreno Ruiz et al., 2013) as input for our analysis. We combined PCA with multiple regression to arrive at the minimum set of indicators explaining the major part of the variance in the product rankings. Apart from this minimum set, we also evaluated the extent to which four commonly used resource footprints (fossil energy, water, land, and materials) were representative of the variation in product rankings.

Materials and Methods

PRODUCTS

All products and corresponding environmental impacts were taken from the ecoinvent database (version 3.1). Environmental impacts of all products are expressed per kilogram of product. To avoid overlap among the products, we applied the following selection criteria:

– Aggregated product categories (e.g., “inorganic chemicals”) were removed from the data set.

– In case of identical products, we preferred the global or "rest-of-the-world" market mix over specific subtypes based on particular production methods or regions. For example, we selected global market rye grain and excluded organic rye grain and Swiss rye grain.
– In the case of products with almost identical production chains (e.g., butanol and iso-butanol), we selected the products with the largest overall amount of emissions or resource extractions.

After applying the first two criteria, there were 1002 products remaining. To apply the third criterion, we then searched for products with (nearly) identical product chains. This was done by dividing every emission/resource extraction of a product by the same emissions/resource extractions of all other products. This yielded 1001 sets of 1869 ratios for each product. If these ratios were (almost) equal for all emissions and resources considered (coefficient of variation <0.01), two products were considered identical. Identical products found this way are usually products for which the impacts are allocated at the very last point of the product chain (such as butanol and iso-butanol). Only the one with the highest overall impact (i.e., average ratio >1) was retained. Our final selection contained 976 products (Table S1), which we grouped into seven categories: Chemicals (435), Plastics (64), Ores, minerals and fuels (91), Building materials (72), Processed biobased products (80), Agricultural and forestry products (106), Metal products and electronics (128).

INDICATORS

Ecoinvent (Moreno Ruiz et al., 2013) reports a total of 692 impact indicators. Our method and the algorithm that we employed to find the optimal set of indicators is not suitable for use on sets of data with (almost) perfectly correlated data (i.e., a correlation coefficient of approximately 1), because two perfectly correlated indicators are indistinguishable (Orestes Cedeira et al., 2015). Therefore, we excluded impact indicators that met at least one of the following criteria:

– Newer versions of the same impact indicator were assumed to fully replace the older ones. Therefore, we only used the most recent version of each indicator. For example, the endpoint indicator calculated with the Ecoscarcity 2013 (Frischknecht et al., 2013) method was retained, while the same endpoint indicators from Ecoscarcity 2006 and 1997 were excluded.
– For most environmental impact indicators multiple versions are provided, either including or excluding long-term emissions. These long-term emissions can stem from landfill sites, long after the product is disposed. For most indicators there is no difference between the versions including and excluding the long-term emissions. For toxicity indicators, however, excluding the emissions on a long-term leads to an underestimation of the damage. Therefore, only the indicator versions including the long-term emissions were retained for our analysis.

– After these first two steps, the remaining set of 161 indicators included several indicators that are identical for different impact assessment methods. For example, the Ozone Depletion Potential (ODP) for an infinite time horizon is calculated in the same way in the CML2001 (Guinée et al., 2002), EDIP2003 (Hauschild & Potting, 2005) and Impact2002 (Jolliet et al., 2003) methods. Similarly, there are several indicators for global warming that are identical for different methods. In order to check whether there was complete correlation between the indicators we used the "trim. matrix" function on the rank correlation matrix of the 976 products in the R package "subselect" (Orestes Cedeira et al., 2015). If two or more indicators were found to be indistinguishable, only one indicator was retained by the algorithm. This resulted in the removal of 26 indicators that all showed a correlation of 1 to one or more of the other indicators.

After this procedure we retained a set of 135 environmental indicators for 976 products. The 135 environmental indicators belong to 13 different methods (Table 5.1).

TABLE 5.1 Impact assessment methods, numbers of indicators and corresponding main categories as included in the analysis.

Impact assessment method	Number of indicators	Category
CML2001 [r]	49	Midpoint indicators
EDIP 2003 [r]	21	
Impact 2002 [r]	14	
ReCiPe [r]	31	
TRACI [r]	9	
EcoIndicator99 [r]	3	Endpoint indicators
Ecological scarcity2013 [r]	1	
EPS2000 [r]	1	
Impact 2002 [r]	3	
ReCiPe [r]	3	
Fossil energy footprint *	1	Resource footprints
Water footprint *	1	
Material footprint *	1	
Land footprint *	1	

r references per method: CML (Guinée et al., 2012), EDIP (Hauschild & Potting, 2002), Impact (Jolliet et al., 2003), ReCiPe (Goedkoop et al., 2013), TRACI (Bare, 2011), Ecoindicator (Goedkoop & Spriensma, 2001), Ecological Scarcity (Frischknecht et al., 2013), EPS (Steen 1999, 1999b).

* Calculated from the inventory outcomes of the ecoinvent database

DATA ANALYSIS

We employed PCA combined with regression analysis to find the minimum set of indicators necessary to adequately describe the variance in product rankings among the full set of impact indicators. In PCA the total variation in a data set is rewritten as a set of noncorrelated linear combinations of the original variables (in our case, the indicators), which are called principal components. The first principal component describes the maximum amount of variance and subsequent principal components explain decreasing amounts of variance. If there is a large correlation between variables, the first couple of principal components will cover the majority of the variance in the data set, and these components can be used as a highly parsimonious summary of the total data set (Cadima & Jolliffe, 2001).

First, we performed a PCA on the rank correlation matrix, i.e. the correlation matrix of the data set after ranking the products on each of the 135 indicators from 1 to 976 (see Table S2). This transformation to rank scores was done to give equal weight to each product in the data set and to each impact indicator (i.e., each indicator now has the same mean and standard deviation). It is desirable to give equal weight to each product because the analysis of impact per kilogram of product is an arbitrary choice that does not reflect differences in production volumes or value to society. Without this transformation the correlation structure would be dominated by a few products that have very high impacts per kilogram (for example the precious metals gold and platina).

Second, we determined the number of nontrivial components with the Avg-Pa (Average parallel analysis) stopping rule as described by Peres-Neto et al. (2005). This stopping rule is a criterion which tells whether a component describes more or less variance than one would expect if it was based on purely randomized data. Because we work with product rankings rather than impact scores, we adjusted the procedure to work with randomized product rankings rather than normally distributed random data. All integers from 1 to 976 were randomly sampled to create a data set with the same number of rows (976) and columns (135) as the original data. This was repeated 1000 times. A PCA was then performed on each of the 1,000 randomized data sets, and the average variance explained by each component was calculated. If a component explained more variance in the original data than in the randomized data, the component was considered nontrivial.

Third, to interpret the nontrivial components, the loading of each indicator as well as the principal component scores per product (and product group) were plotted. Biplots of the loadings show the association between the indicators and the principal components: the more extreme (high or low) the loading, the more representative the indicator is of that component. The principal component scores show the associations between the observations and the principal components, thus revealing the similarity of the indicators and products.

Fourth, to find a subset of the original indicators most closely associated with the nontrivial principal components, we calculated the amount of variance in principal components scores that could be explained by subsets of the original indicators. Subsets of any number of indicators can be tested, whereby a set comprising all indicators would cover 100% of the variance and smaller subsets would cover less. The best set, in terms of explained variance, for each number of indicators was found by using the "improve" algorithm from the package "subselect" (Orestes Cedeira et al., 2015) in the statistical program R (R Core team, 2015). The improve algorithm uses multiple linear correlation to determine the amount of explained variance.

Fifth, we defined the optimal size of the indicator set by using the explained variance of the so-called nontrivial principal components as a benchmark. The indicator set with the lowest number of indicators and an explained variance equal to or higher than the explained variance of the nontrivial components was considered to be the preferred set of indicators.

Finally, we tested the extent to which a set of four resource footprints (fossil energy, land, water and material use) covered variance in our data set by using the multiple linear correlation analysis on all principal component scores, as mentioned above. Note that these four resource footprints were not part of the set of 135 indicators.

Results

PRINCIPAL COMPONENTS AND INDICATORS

The number of nontrivial components was four, which together covered 92.0% of the total variance in the data set. The majority of the variance (83.3%) was covered by the first component, with 3.9%, 3.1%, and 1.9% covered by the three consecutive components (Figure 5.1). Since all correlations in the database were positive, the first component can be seen as an overall indicator of environmental impact. Indicators that are most similar to other indicators (i.e., have the highest mutual correlations) have the highest absolute loadings on this component. For the first component these were the indicators related to freshwater and marine ecotoxicity. However, most other indicators showed very similar loadings (Figure S1, see SI1 for a more extensive analysis of the principal components). Indicators with the lowest absolute loadings on the first component were related to land use, which means that indicators related to land use are least correlated to all other indicators. On the second principal component, high loadings were found for indicators related to land use and terrestrial ecotoxicity while indicators related to fossil energy use and global warming had low loadings. This means that after taking into account the fact that impact-intensive products are generally impact-intensive according to all impact

indicators; products that use relatively large amounts of land are likely to use a relatively limited amount of fossil energy and vice versa. Indicators related to ionizing radiation (i.e., from the use of nuclear energy) and indicators of ozone depletion were further distinguished from the rest by components 3 and 4. See Figures S1 and S2 for the loadings of all indicators on the first four components.

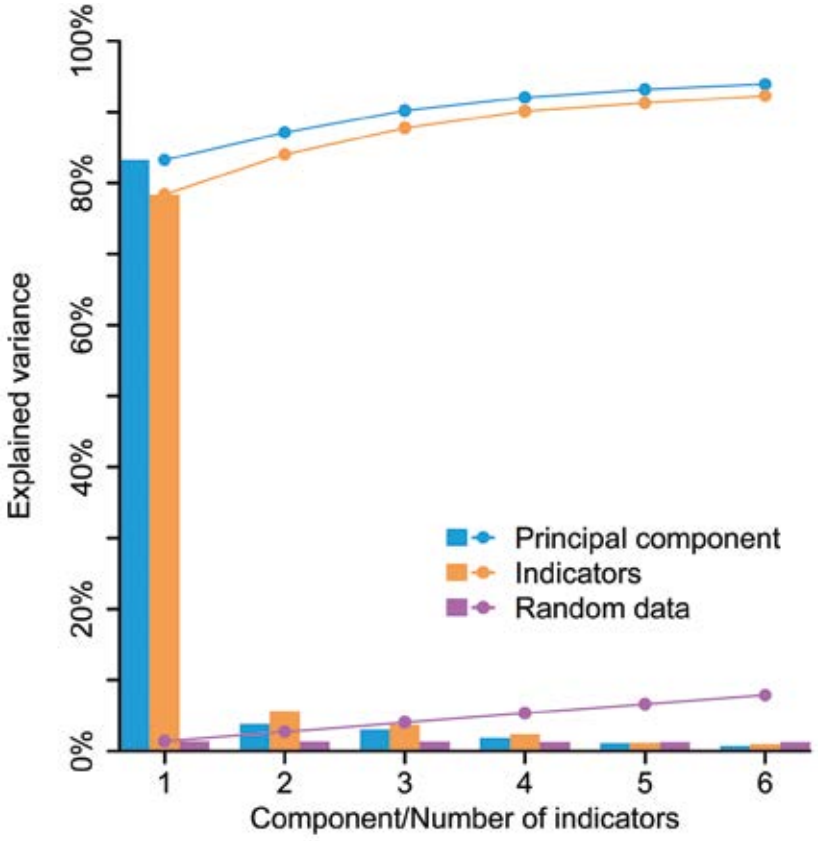


FIGURE 5.1 Variance explained per principal component based on our data set (blue), per principal component based on random data (purple), and by the best set of indicators (orange). Solid lines with dots indicate the cumulative variance explained.

PRODUCTS

The scores per principal component (Figure 5.2) indicate how the products are related to each of the components. Products with the highest and lowest overall ranks showed the most extreme scores on the first principal component. On a per kg basis, we found the highest impacts (lowest scores on the first principal component) for metal products and electronics (which include very high-priced and energy-intensive products such

as gold) and the lowest impacts for ores, minerals, fuels and building materials. On the second component a clear distinction could be seen between the products on a biological base (agricultural and forestry products and processed biobased products) and the rest of the products. This coincided with the high loadings for (agricultural) land use on the second principal component. A number of plastics showed the lowest scores on the third component. These plastics have relatively small emissions of ozone depleting substances as a result of their production process compared to the other emissions. The highest scores are found among the inorganic chemicals.

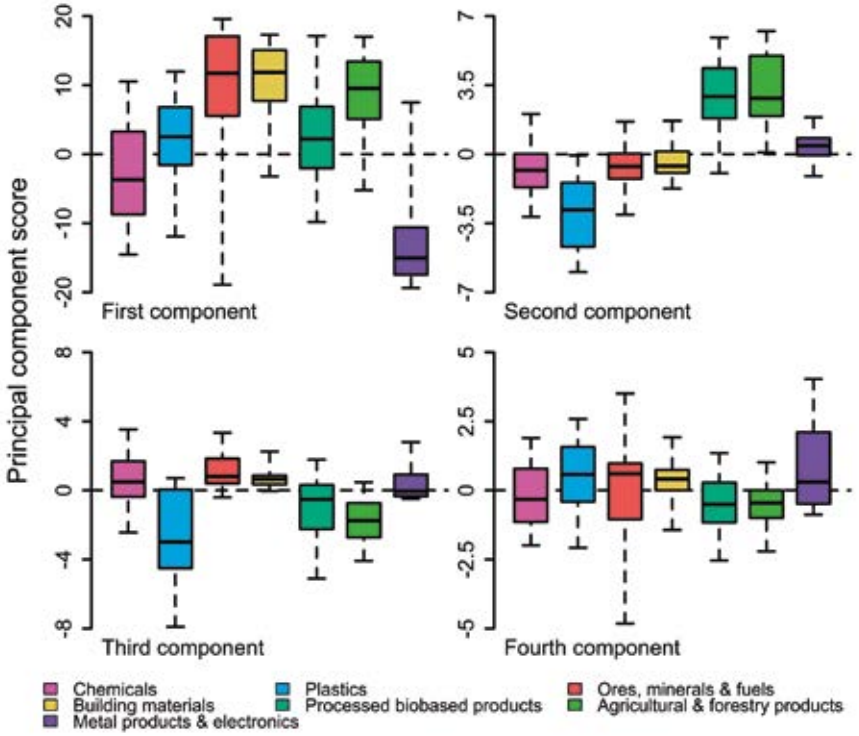


FIGURE 5.2 Boxplots of principal component scores per product and product group: colored boxes cover the interquartile distance, black bars inside the boxes denote the medians, whiskers extend to the 5th and 95th quantiles.

BEST SET OF INDICATORS

A set of six indicators was needed to cover slightly more variance than the first four principal components (i.e., 92.3% and 92.0% respectively; Figure 5.1). The best set of six indicators contained indicators of climate change, ozone depletion, terrestrial ecotoxicity, the combined ecosystem effects of acidification and eutrophication, marine ecotoxicity, and land use (Table 5.2).

The four resource footprints together accounted for an explained variance of 84.3% (Table 2). The results suggest that the fossil energy indicator, with an explained variance of 62.8%, is a reasonable indicator of overall impact. The explained variance can be raised to 76.5% by adding land use and then to 83.8% by adding material use. The water footprint explained only 0.5% of additional variance; this is due to the fact that water consumption is related to both the energy-intensive process of electricity generation and the land-intensive process of crop production.

TABLE 5.2 Best sets of impact indicators and the variance explained by sets up to six indicators, and the variance explained by the resource footprints.

#	Impact indicator	Method: Full name of indicator	Explained variance
1	Marine ecotoxicity	ReCiPe: METP100a (I)	78.4%
2	Climate change	CML2001: upper limit of net GWP100a*	84.0%
	Marine ecotoxicity	ReCiPe: METPinf (H)	
3	Land use	Impact2002: land occupation	87.8%
	Human toxicity	ReCiPe: HTPinf (E)	
	Climate change	ReCiPe: GWP100a (H)	
4	Climate change	CML2001: upper limit of net GWP100a	90.1%
	Ozone depletion	CML2001: ODP40a	
	Land use	Impact2002: land occupation	
	Marine ecotoxicity	ReCiPe: METPinf (E)	
5	Climate change	CML2001: GWP20a	91.3%
	Ozone depletion	CML2001: ODP40a	
	Terrestrial ecotoxicity	CML2001: TAETP20a	
	Acidification & eutrophication	Impact2002: terrestrial acidification & eutrofication	
	Marine ecotoxicity	ReCiPe: METPinf (E)	
6	Climate change	CML2001: GWP20a	92.3%
	Land use	CML2001: Land use: competition**	
	Ozone depletion	CML2001: ODP40a	
	Acidification & eutrophication	Impact2002	
	Marine ecotoxicity	ReCiPe Midpoint E: METPinf	
	Terrestrial ecotoxicity	ReCiPe Midpoint I: TETP100a	

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* Upper limit of GWP100a: a method where the upper values of several uncertain GHGs are used rather than the most likely value

** Like the land footprint this consists of an unweighted summation of different land uses, however not all types are included

Resource-based sets		
1	Fossil energy	62.8%
	Land	37.9%
	Water	58.1%
	Material	54.3%
2	Fossil Energy, Material	76.5%
3	Fossil Energy, Land, Material	83.8%
4	Fossil Energy, Land, Material and Water	84.3%

Abbreviations:
METP: Marine EcoToxicity Potential
GWP: Global Warming Potential
HTP: Human Toxicity Potential
ODP: Ozone Depletion Potential
T(A)ETP: TerrestriAl EcoToxicity Potential
inf/100a/40a/20a: Time Horizons of infinite duration and 100, 200 and 40 years respectively
(I): Individualist perspective, (E): Egalitarian perspective, (H): Hierarchist perspective

Discussion

Our analysis revealed a large amount of redundancy in a set of 135 impact indicators, since a single indicator already covered 78.4% of the variance in the ranking of 976 products. This result is in line with earlier research in which large correlations between a single indicator (energy demand) and different impact indicators were found (Huijbregts et al. 2006, 2010). However, even though one indicator might be able to cover a large proportion of the damage over a wide range of products, within certain product groups it may be less useful to distinguish products from each other (Laurent et al., 2012). As the scores of the individual products demonstrate, several indicators are needed to distinguish products within specific groups. For example, biobased products are mostly separated by the amount of land use, while some plastics have relatively high emissions of ozone depleting substances; therefore, an indicator that takes this into account is necessary to distinguish products within this group. The requirement of a limited set of indicators is in line with the findings from Gutierrez et al. (2010) who used a PCA-based approach for data reduction. These authors found that three indicators (respiratory inorganics, ozone depleting substances, and minerals) were needed to cover the majority of the variance in environmental impacts of a small set of household electronics. Pascual-Gonzalez et al. (2015) applied a combination of multiple regression and an approach called MILP (Mixed-Integer-Linear-Programming) to reduce the number of impact indicators for a large number of oil and electricity products. Fossil energy demand, respiratory inorganics, and ozone depletion constituted the best set for oil, while for electricity the different types of primary energy carriers (water, wind, nuclear, and fossil) and an indicator of climate change were needed. Our study, adds to these insights, by providing an application of a data reduction technique on a data set that is both larger and more diverse than used up to now.

According to our results, the best indicator set includes indicators of global warming (which is strongly correlated to all other indicators), land use, and ozone depletion, supplemented by indicators for the combined effect of acidification and eutrophication (these two impacts are combined into one indicator in the IMPACT 2002 methodology), and terrestrial and marine ecotoxicity. While this set maximizes the amount of explained variance, these six indicators are not necessarily the most preferable according to additional criteria, such as the RACER (Relevant, Accepted, Credible, Easy, and Robust) criteria (Lutter & Giljum, 2008). For example, the problem of ozone depletion is becoming less relevant due to successful emission reduction policies (WMO, 2011) and the indicators of toxicity (including the statistically best indicator for marine ecotoxicity) are not always robust, due to the large uncertainties involved in their calculations (Van Zelm et al., 2007, 2009; Rosenbaum et al. 2008). As the loadings of the indicators (Figure S1) on the first component (which covers 83.3% of the total variance) show, there are several indicators with approximately the same explanatory power. This means that alternative sets of indicators can be defined which are only marginally worse in terms of explained variance compared to the set of six indicators derived from our analysis. The resource footprints are relatively easy and robust to calculate. Being indicators of resource use rather than indicators of environmental impact, it was not known whether they can be used as a proxy for environmental impacts. Our results indicate that they cover the variance in impact indicators quite well (84% explained variance with four indicators), which suggests that these indicators are relevant for use in the area of LCIA. Using simple resource footprints would reduce the need for the complicated mid- and endpoint damage models.

In this study we have used product rankings calculated on a 1 kg basis, to give insight in the variation between very diverse products. It can be argued that other bases of comparison, for instance, based on products with the same functional unit, are more in line with one of the main applications of LCA: product optimization. Comparing products with the same functional unit was done by Sabio et al. (2012) who found four relevant environmental indicators for hydrogen supply chains, thereby also demonstrating that a small set of indicators was a sufficient base for the comparison of similar product alternatives. The products used in our study are mostly quite simple commodities, with only the electronics category covering more complex consumer products, such as LCD screens. Furthermore, the analysis was based on cradle-to-gate data, whereby the product's use and disposal are not taken into account. The use phase of products can be energy-intensive, meaning that, if included, products with long use times would generally rank higher on indicators related to energy use, such as indicators of climate change. It is difficult to predict how the correlation structure, and therefore the indicator selection, would change when more complex products or use phase data are taken into account. The correlation between indicators could either increase or decrease, resulting in more or less explained variance for indicator sets of each size. However, in the case of taking into account the use phase, it is likely that there will be more explained variance with the same number of indicators, since all indicators related to energy use will increase simultaneously for products with long use times.

Additionally, the coverage of the ecoinvent database may not be complete in terms of the inventory flows included (i.e., the extent to which relevant emissions and resource extractions are included for all products) and in terms of (novel) impact pathways covered. Limiting the inventory flows to a limited number of well-studied pollutants may result in an overestimation of the correlations between the impact indicators that are eventually calculated from these flows, for example not all of the toxic chemicals covered by the USEtox model (Rosenbaum et al., 2008) are available in the ecoinvent database. Similarly, leaving out potentially relevant damage pathways (for example ecosystem damage caused by tropospheric ozone formation) may also cause an overestimation of the amount of variance that can be covered with a limited number of indicators. Despite these limitations, it should be noted that the ecoinvent database is one of the largest databases available for life cycle assessment, with clear guidelines on how to ensure completeness and consistency of the data as much as possible (Weidema et al., 2013).

Finally, spatially explicit impact assessment methods, as recently developed for several impact categories, including water (Verones et al., 2013), land (de Baan et al., 2013), acidification (Roy et al., 2014) and eutrophication (Azevedo et al., 2013) were not included in the assessment. This is due to the fact that coupling of spatially explicit inventory and impact information is still not common practice in LCA databases, including ecoinvent 3.1. Spatially explicit methods use a different amount of impact for the same environmental intervention, which can reorder the ranking of the impact indicator, depending on the location where the intervention takes place. Whether this results in more or less correlation between the different impact indicators cannot be known *a priori*. Regionalization may increase the amount of variance to be explained by a small set of indicators and therefore limit the coverage of our recommended set; however, regionalization can potentially also increase the correlations between indicators. This would be the case if regionalization results in several impact indicators that are consistently higher than average in one country. Products that rely heavily on that country as a sourcing region will then have a higher rank for all these indicators of impact, resulting in a higher correlation between the indicators than one would observe without regionalization of the impacts. It is recommended to redo the PCA-regression procedure after the introduction of spatially explicit impact assessment methods in common LCA practice.

Summarizing, we introduced a procedure for systematically selecting a set of impact indicators that is optimal in covering the maximum amount of variance with a minimal number of indicators. With this method we have demonstrated that reducing the number of indicators in our data set from 135 to six indicators is feasible without losing more than 8% of the total variance. Although it is unlikely that any practitioner would have used 135 indicators simultaneously, there was no reason to discard any of the indicators *a priori* other than for reasons of convenience. Our results can be seen as comforting for LCA practitioners, since we showed a clear overlap between and within methods. For the first time, we have demonstrated a large dimensionality reduction to be feasible over a wide range of indicators and products. This suggests that the plethora of indicators available for

product assessments is largely superfluous and that a small set of key impact indicators is sufficient for product optimization and environmental policy. Alternatively, a set of 4 resource footprints covering 84% of the total variance may be used.

Acknowledgment

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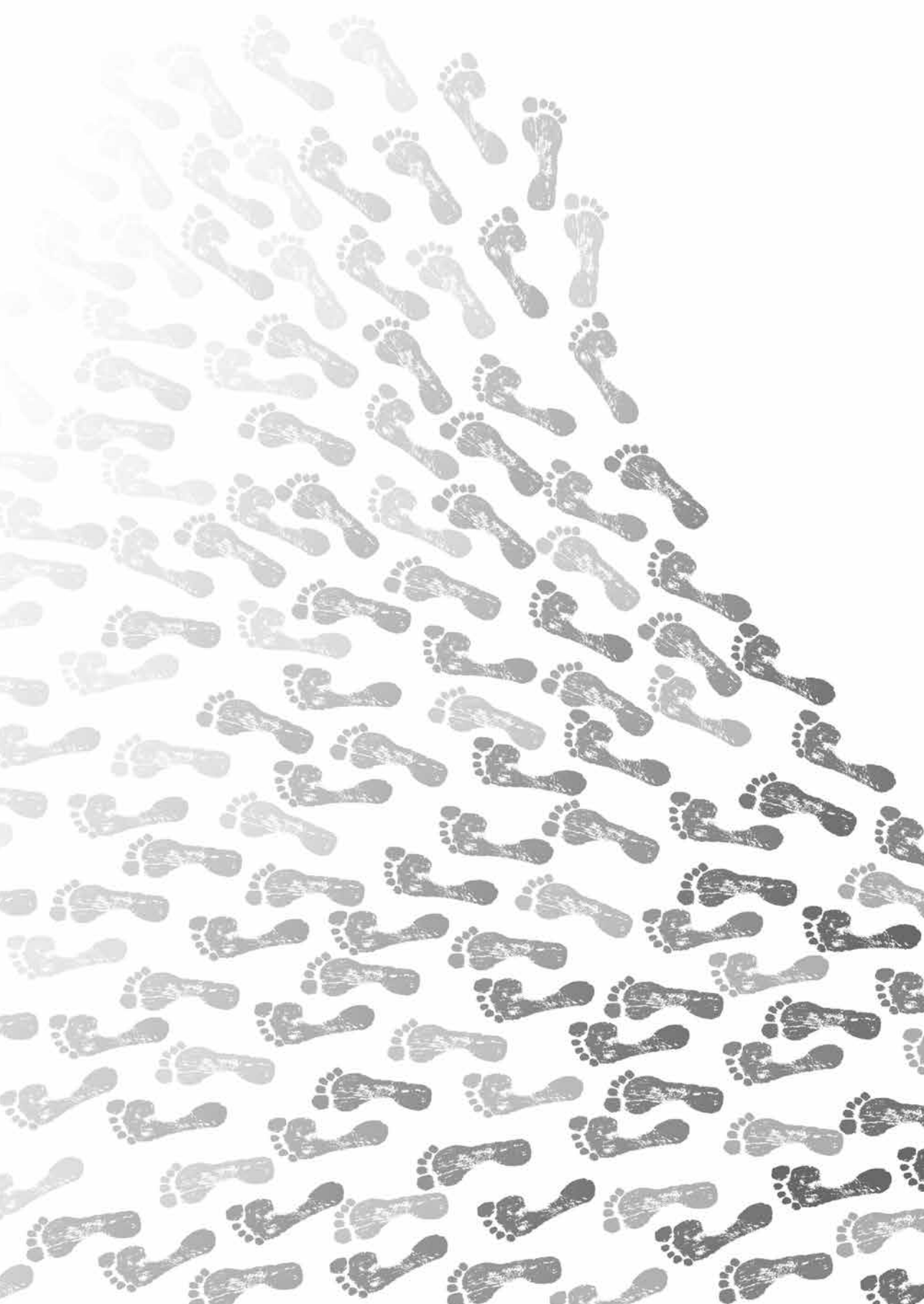

CHAPTER 6

Headline environmental indicators revisited with the global multi-regional input-output database EXIOBASE

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Abstract

Environmentally Extended Multi-Region Input Output (EEMRIO) databases are used to quantify numerous environmental pressures and impacts from a consumption perspective. However, for targeted communication with decision makers, large sets of impact indicators are unfavorable. Small sets of headline indicators have been proposed to guide environmental policy, but these may not cover all relevant aspects of environmental impact. The aim of our study was to evaluate the extent to which a set of four headline indicators (material, land, water and carbon) is representative of the total environmental impact embedded in an EEMRIO database. We also used principal component analysis (PCA) combined with linear regression to investigate which environmental indicators are good candidates to supplement this headline indicator set, using 119 environmental indicators linked to the EEMRIO database EXIOBASE. We found that the four headline indicators covered 59.9% of the variance in product-region rankings among environmental indicators, with carbon and land already explaining 57.4%. Five additional environmental indicators (marine ecotoxicity, terrestrial ecotoxicity, photochemical oxidation, terrestrial acidification, and eutrophication) were needed to cover 95% of the variance. In comparison, a statistically optimal set of seven indicators explained 95% of the variance as well. Our findings imply that there is (i) a significant statistical redundancy in the four headline indicators and (ii) a considerable share of the variance is caused by other environmental impacts not covered by the headline indicators. The results of our study can be used to further optimize the set of headline indicators for environmental policy.

Introduction

Environmentally Extended Multi-Regional Input-Output (EEMRIO) analysis is a method to quantify the environmental impacts from a consumption perspective on a global scale (Wiedmann et al. 2007; Wiedmann 2009; Tukker and Dietzenbacher, 2013; Wood et al. 2015). Examples of environmental impact indicators in input-output databases include land use, water consumption, greenhouse gas emissions, material use, particulate matter emissions and nitrogen emissions (Yu et al. 2013; Hoekstra and Mekonnen 2012; Steen-Olsen et al. 2013; Davis and Caldeira, 2010; Peters and Hertwich, 2008; Wiedmann et al., 2015; Tukker et al. 2016, Ghertner and Fripp, 2007; Oita et al., 2016).

While using a set of multiple complementary indicators is helpful to cover all relevant aspects of environmental impact, it is considered unfeasible and also unnecessary to base policy decisions on dozens of indicators simultaneously. In response to the potential overload of environmental indicators, small sets of (resource) indicators, called headline or dashboard indicators, have been proposed to serve as a basis for environmental policy (e.g. Galli et al. 2012, European Resource Efficiency Platform, 2014). However, the smaller the proposed headline set of indicators, the higher the chance that the set is not representative of all relevant impact pathways. Various authors evaluated the usefulness of the cumulative energy demand (CED) or the carbon footprint as proxy indicator for environmental damage (e.g. Huijbregts et al. 2010; Röös et al. 2013; Kalbar et al. 2017, Simas et al. 2017). While relatively high correlations are found for most metrics of environmental damage, there are also impact categories (such as freshwater ecotoxicity) for which neither cumulative energy demand nor carbon footprint are good proxies. Focusing on just one indicator of impact clearly does not cover all relevant aspects of environmental impact. Systematic searches for an optimal set of indicators based on correlations between indicators were performed by Berger and Finkbeiner (2011) for indicators of resource scarcity and by Lasvaux et al. (2016) for a large number of indicators used to quantify environmental impacts of the building sector. Lasvaux et al. (2016) showed that five dimensions of environmental impact related to the building sector should be covered, namely fossil energy consumption, ecotoxicity, ionizing radiation and ozone depletion, land use and mineral depletion.

Eurostat (2017) proposes to use a headline set consisting of the material, land, water and carbon footprint. Recently, Steinmann et al. (2016) applied an indicator reduction procedure and showed that a headline set of four resource footprint indicators (energy, water, land and material) together accounted for 84% of the variance in product impact rankings on 161 indicators of impact for a set of nearly 1000 different commodities. It is crucial that a proposed small set of headline indicators to be used for policy making does covers all relevant types of environmental impact. This is also acknowledged by the European Commission, stating that the headline set of indicators can be supplemented with more specific thematic indicators if necessary (Eurostat, 2017). Since the number of

potential thematic indicators is high, it is important to find an optimal balance between simplicity and exhaustiveness.

The goal of this study was to reveal the extent to which a set of four headline indicators (material, land, water and carbon footprints) is representative of the total environmental impact embedded in the EXIOBASE database. We also investigated with a statistical analysis which environmental indicators are good candidates to supplement this headline indicator set. Finally, we applied our methodology on the full set of indicators to find an optimal set of indicators from a purely numerical point of view.

Materials and methods

EXIOBASE

While a number of EEMRIO models are available (see Tukker & Dietzenbacher, 2013), we used the EEMRIO EXIOBASE (base year 2011; version 3.2.4) in this study because of the relatively large coverage of emission and resource types (Wood et al. 2015). EXIOBASE includes 200 products with a relatively large amount of detail (Table 1). For example, agricultural production is broken down into 15 product groups based on different livestock species and different crop types which have dissimilar environmental impact. These 15 product groups are followed down the supply chain into 12 more groups which include manufactured products related to food. Energy commodities are likewise detailed in EXIOBASE, with 69 types of energy carriers distinguished, based on IEA energy balances (IEA 2012), and including the disaggregation of the electricity generation sector into 12 types of electricity producers. Further detail is included in the mining sector (11 types of ores and quarrying) and the manufacturing sector, which includes 42 types of manufacturing products in addition to the manufactured energy and food products previously identified. Not all countries produce all products.

In terms of environmental pressures, EXIOBASE records emissions to air and water, as well as land use, material extraction and water use. Water accounts are provided for both blue water and green water and in terms of water consumption and withdrawal. Material accounts are provided in terms of energy content and mass of both used and unused extraction. Unused extractions form the part of the extraction that does not enter the economic system (for example excavated soil with no further economic use during building activities). Land accounts are broken down by activity (e.g. forestry vs pasture). Air emissions accounts are provided for 27 substances, broken down by source (combustion, non-combustion, agricultural, waste). All greenhouse gas emission categories are covered except emissions from land use, land use change and forestry. In addition, agricultural emissions of nitrogen and phosphorous to water are included (See Stadler et al., 2017 for a more extensive description of EXIOBASE 3).

TABLE 6.1 Summary of EXIOBASE version 3

	EXIOBASE 3
Baseyear(s)	1995 – 2011
Products	200
Industries	163
Countries	44 (28 EU member plus 16 major economies)
Rest of the world regions	5 (Europe, Asia, Africa, America, Middle East)
Water accounts	194 (Water blue and green per source, including final demand)
Material accounts	69 (Energy products, including final demand) 222 (Used extractions) 222 (Unused extractions)
Land accounts	14 (Including build up land for final demand)
Emissions	27 (from combustion including final demand) 27 (non-combustion) 3 (HFC, PFC, SF6) 5 N/P/SOx (from waste) 7 N/P (from agriculture)

Calculation of the environmental multipliers by products follow the standard demand model of Leontief (1966), where environmental pressures per million euro Q are calculated via:

$$Q=S*(I-A)^{-1}$$

Where the vector S denotes the environmental stressors (e.g. land, water, material accounts) per unit output of each product-region combination; the matrix A denotes the direct coefficients representing the global economic structure (I is an identity matrix of appropriate size). A full description of the variables and derivation of the Leontief calculation is available in various references (e.g. Miller and Blair, 2009). Q is known as the multiplier matrix in input-output economics, and in this study it denotes the effect in terms of environmental pressure that is generated for each unit of final demand. It corresponds to the "system process" in life-cycle assessment.

ENVIRONMENTAL IMPACT INDICATORS

To allow for a meaningful comparison across studies we use the same set of indicators as Steinmann et al. (2016). This set includes indicators from all major Life Cycle Impact Assessment (LCIA) methods (CML 2001, Ecoindicator 99, Ecological Scarcity 2013, EDIP 2003, EPS 2000, Impact 2002, ReCiPe 2008 and TRACI) as well as the resource-based indicators (land, water, material and energy). Only the latest version of each impact assessment method was included. The impact assessment methods include so-called

midpoint and endpoint indicators. Midpoint indicators are used to quantify the impact for a single impact category, such as acidification or global warming, whereas endpoint indicators are more comprehensive indicators of damage which include multiple impact categories to come to an impact in terms of overall ecosystem damage, overall human health damage or even a combined score of human health and ecosystem impacts. Per assessment method we included all midpoint indicators as well as endpoint indicators related to damage to ecosystems or human health. We excluded indicators reflecting resource scarcity because of a lack of adequate input data. For example, total amounts of extracted and used ore are available, but the amount of metal present in that ore cannot be (directly) calculated from those amounts. This means that the impact on metal scarcity cannot be meaningfully calculated. We used characterization factors to quantify the environmental impact indicators, thereby summarizing the amount of damage per unit of each environmental extension. To calculate the headline indicators we summed all used extractions, including the metal ores, (in kilotons) for the material footprint. The land footprint was calculated by summing all types of land use, the water footprint was calculated by summing all types of blue water consumption, while the carbon footprint was calculated by using the characterization factors from the midpoint ReCiPe 2008, Hierarchist method.

For the analysis we selected the consumptive environmental impacts of the 6,982 product-region combinations with a final demand of at least 1 million euro. We used the characterization factors as implemented in Ecoinvent version 3.1 (See Table S1 for a complete overview of all characterization factors per environmental extension). However, since the number of environmental extensions in EXIOBASE is limited, not all 161 initial indicators could be included. Indicators were excluded if no environmental extensions related to an impact indicator were present in EXIOBASE, which was the case for indicators of ionizing radiation and ozone depletion. In the end 119 different indicators (including the four headline indicators) were retained, from eight different LCIA methods.

To reveal the intrinsic relationships among all indicators, both within and across LCA methods, we calculated Pearson's correlation coefficients between the indicators based on their underlying characterization factors. To that end, extensions which did not contribute to an indicator, i.e. did not have a characterization factor, were given a value of 0 for that indicator. The correlation matrix is provided as supplementary table (Table S2). We then calculated the rank scores of the product-region combinations (ranging from 1 for the product-region combination with the lowest impact to 6,982 for the product-region combination with the highest impact for the concerned impact indicator) for each indicator and found that 21 impact indicators showed a perfect correlation (Spearman's rho = 1) with at least one other indicator in the dataset. Note that perfectly correlated rank scores can occur even if the characterization factors from the underlying methods are not perfectly correlated. Since our indicator optimization approach (see next section) is not able to deal with perfectly correlated indicators, we removed 14 indicators *a priori*. While many of the remaining indicators also showed very high correlations (up to 0.99),

these are automatically grouped together in the optimization procedure. It was therefore not necessary to further reduce the number of indicators a priori. See table S3 for a full list of the environmental impact indicators included and removed. The 105 remaining indicators are summarized per category and impact type in table 6.2.

TABLE 6.2 Included number of indicators per methodology and impact category

LCIA method	Acidification & malodorous air	Climate change	Eutrophication	Ozone formation & PM	Toxicity	Footprint based	Endpoint	Total
Midpoint methods								
CML 1999	2	5	2	5	24	-	-	38
EDIP 2003	1	3	4	2	5	-	-	15
Impact 2002+	2	1	1	2	3	1	-	10
ReCiPe 2008	3	3	1	2	11	-	-	20
TRACI	1	1	1	2	3	-	-	8
Endpoint methods								
Ecoindicator 99	-	-	-	-	-	-	3	3
Ecological scarcity 2013	-	-	-	-	-	-	1	1
EPS 2000	-	-	-	-	-	-	1	1
Impact 2002+	-	-	-	-	-	-	2	2
ReCiPe2008	-	-	-	-	-	-	3	3
Resource methods								
Footprints	-	-	-	-	-	4	-	4
Total	**8**	**13**	**9**	**13**	**46**	**6**	**10**	**105**

EVALUATION OF HEADLINE INDICATORS

To evaluate the extent to which the set of four headline indicators is representative of the total environmental impact embedded in EXIOBASE, we followed the two-step procedure as proposed by Steinmann et al. (2016). According to this procedure, first the dimensionality in the full set of indicator values is determined based on a principal component analysis (PCA). Next, a linear regression analysis is used to relate the resulting principal components to a selection of indicators (in this case the four headline indicators, if needed supplemented with one or more thematic indicators) and evaluate the amount of variation explained. Principal component analysis was performed on the correlation matrix of the rank scores for the 105 indicators. We compared the explained variance of each component to the average explained variance of the same component based on a PCA on random data with the same number of indicators (105) and observations (6,982). Because we use rank scores, each random dataset (1,000 in total) was a reordering of the numbers 1 to 6,982. A component was considered non-trivial if the explained variance of a component in our dataset was larger than the average explained variance based on the

random datasets. This procedure is an adaptation of the approach described by Peres-Neto et al. (2005).

In a second step, we combined the set of four headline indicators with the midpoint environmental impact indicators used in the first step and used these as predictors of the principal component scores in a linear regression analysis. We excluded the endpoint indicators (n=10) as possible predictors because these are composite indicators that require multiple underlying indicators as input. To define the optimal size of the indicator set, we used the explained variance of the non-trivial principal components as a benchmark. We started with headline set of indicators (material, land, water and carbon footprints) to evaluate the amount of variation explained by this key set. Next, we supplemented this set with one additional thematic indicator at a time, selecting from the 91 midpoint indicators included in the PCA, in such a way that the resulting set covered the maximum amount of variance. This procedure was repeated until the amount of explained variance was equal or higher than that of the set of non-trivial components. We also employed this methodology without starting with the headline set of indicators. In that approach we started with one indicator that covered most of the variance and supplemented this with additional indicators until the required amount of variance was covered. This yields best set of indicators from a purely numerical perspective, i.e. without including the headline set *a priori*.

INTERPRETATION

To interpret the meaning of the non-trivial components, a twofold approach was used. Firstly, the indicators with the highest and lowest loadings were compared for the first four principal components. Loadings are the weights given to each indicator for each principal component. Indicators contrast each other on a component (meaning they would lead to different rankings), if one indicator has a negative loading and another has a positive loading. Principal component scores can be calculated by taking the sum-product of the loadings for a principal component and the standardized original rank scores that principal component. Secondly, the scores of the individual products were assessed for the first four principal components to see which types of products score are particularly associated to that component. This analysis contributes to the interpretation of the components and provides insight into which type of indicator is most appropriate to differentiate between products of a certain product type. Products with the most extreme scores are said to be separated from each other by a component. We divided the products into eight different categories for this purpose (agricultural & food products, electricity, fossil fuels, metals & electronics, minerals chemicals & plastics, non-food bio-based products, services, waste & recycling). Results from this analysis can be found in the Supporting Information (section SI 2). A list with the names of each product and its corresponding category is provided in as supplementary Table S4. All analyses were performed in the R environment (R Core team 2016).

Results

Six non-trivial components were found, which explained 95.3% of the variance in the dataset (Figure 6.1). The majority of the variance in the dataset was explained by the first component (58.9%). Consecutive non-trivial components explained 22.5%, 7.4%, 3.2%, 2.1% and 1.2% of the variance (see SI 1 and table S3 for an interpretation of the principal components). Because the six non-trivial components covered 95% of the variance, we searched for the smallest subsets of indicators that explains this amount of variance. With all correlations between the impact indicators being positive the first component can be seen as representative of overall impact. As a single indicator the carbon footprint represents this impact fairly well (41.6% explained variance). Adding the land footprint as second indicator raises the explained variance to 57.4%, while the four headline indicators together explained 59.9% of the variance (Table 6.3, Figure 6.1). This means that a substantial part of the variance in product rankings is not explained by the headline set of indicators, and that additional thematic indicators are necessary to cover the missing impacts. Adding an indicator of marine ecotoxicity boosted the explained variance to 85.3%. In total five additional thematic indicators were necessary to cover >95% of the variance (Figure 6.1). This set contained the headline indicators (carbon, land, water and material footprints) as well as indicators of marine ecotoxicity, terrestrial ecotoxicity, photochemical ozone formation, terrestrial acidification, and eutrophication.

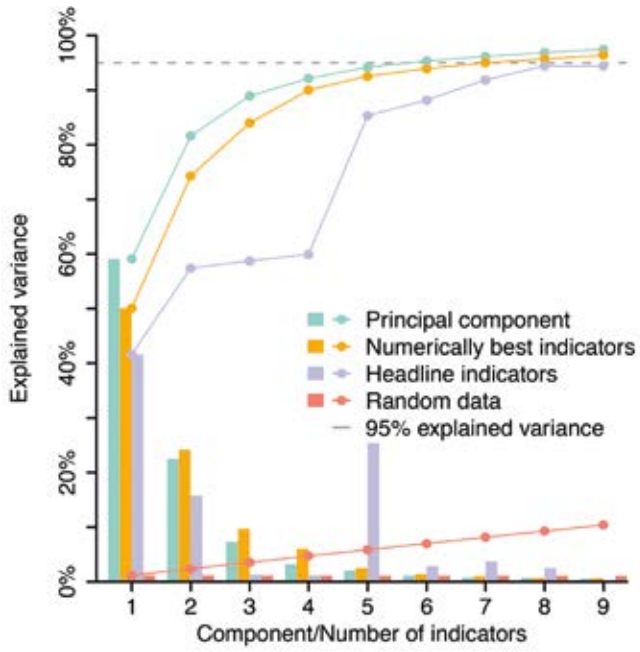

FIGURE 6.1 Explained variance per principal component (green bars), numerically best indicator set (orange bars), the headline indicator set plus additional thematic indicators (purple bars) and random data (pink bars) and the corresponding cumulative explained variance (dotted lines with the same colors).

From a purely numerical point of view, the headline set of indicators is not optimal because there is overlap between the different headline indicators. For example, the water footprint correlates well with the land footprint (Spearman's rho = 0.84), meaning that these two footprints lead to a similar ranking between product-region combinations and there is little added value in using both in EXIOBASE. Results of the numerical analysis show that 50.1% of the variation in ranks scores could be covered by a single indicator of particulate matter formation (Figure 6.1, Table S5). Adding an indicator of freshwater toxicity increased the explained variance to 74.3% and further adding an indicator of marine ecotoxicity raised the explained variance to 84.0%. In order to explain 95% of the variance in product-region ranks, a set of seven indicators was needed. This set contained indicators of particulate matter formation, freshwater aquatic ecotoxicity, marine ecotoxicity, climate change, terrestrial ecotoxicity, photochemical oxidation and land occupation (Table 6.3).

TABLE 6.3 Explained variance of sets of headline indicators supplemented by additional thematic indicators (sizes 1 to 9) and the numerically best set of impact indicators

#	Indicator name	Method	Explained variance
Headline indicators			
1	Carbon		41.6%
2	Carbon & Land		57.4%
3	Carbon, Land & Material		58.7%
4	All headline indicators (Carbon, Land, Material, & Water)		59.9%
5	Headline indicators		85.3%
	+ Marine ecotoxicity (20 year time horizon)	CML 2001	
6	Headline indicators		88.2%
	+ Marine ecotoxicity (20 year time horizon)	CML 2001	
	+ Terrestrial ecotoxicity (infinite time horizon)	ReCiPe 2008	
7	Headline indicators		91.8%
	+ Marine ecotoxicity (20 year time horizon)	CML 2001	
	+ Terrestrial ecotoxicity (infinite time horizon)	ReCiPe 2008	
	+ Photochemical oxidant formation	ReCiPe 2008	
8	Headline indicators		93.6%
	+ Marine ecotoxicity (20 year time horizon)	CML 2001	
	+ Terrestrial ecotoxicity (infinite time horizon)	ReCiPe 2008	
	+ Photochemical oxidant formation	ReCiPe 2008	
	+ Terrestrial acidification	TRACI	
9	Headline indicators		95.2%
	+ Marine ecotoxicity (20 year time horizon)	CML 2001	
	+ Terrestrial ecotoxicity (infinite time horizon)	ReCiPe 2008	
	+ Photochemical oxidant formation	ReCiPe 2008	
	+ Terrestrial acidification	TRACI	
	+ Eutrophication	CML 2001	

>>

Numerically best indicator set			
7	Particulate matter formation (Hierarchist) [1]	ReCiPe 2008	95.0%
	Freshwater aquatic ecotoxicity (infinite time horizon)	CML 2001	
	Marine ecotoxicity (infinite time horizon)	ReCiPe 2008	
	Global warming (100 year time horizon)	EDIP 2003	
	Terrestrial ecotoxicity (100 year time horizon, Individualist)	ReCiPe 2008	
	Photochemical oxidation (Maximum Increment Reactivity)	CML 2001	
	Land occupation damage to ecosystem quality	Impact 2002+	

[1] The ReCiPe methodology uses three archetypical viewpoints to deal with value choices in modeling consistently. Perspectives include Individualist (short-term perspective, nature is resilient), Hierarchist (average perspective, nature has limited resilience) and Egalitarian (long-term perspective, nature is vulnerable)
TRACI = Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts.

Discussion

Our analysis showed that a set of four headline indicators, consisting of the material, land, water and carbon footprints, covers around 60% of the variance in product-region rankings based on a set of 119 impact indicators applied to the EXIOBASE EEMRIO database. In order to explain more than 95% of the variance present in the EXIOBASE dataset, this headline set needs to be supplemented by five more indicators. Alternatively one could employ a numerically optimal set of seven indicators. It is interesting to note that the resulting number of nine indicators (or seven for the numerically optimal set) is smaller than the number of impact categories that was originally present in the dataset. These findings are in line with other studies on the potential for data reduction in terms of environmental indicators (Pozo et al. 2012, Brunet et al. 2012, de Saxcé et al. 2014, Sabio et al. 2012, Li et al. 2012 and Gutierrez et al. 2010, Pascual-González et al. 2016). Compared to the original impact categories that were included, no indicators of human toxicity, particulate matter formation and freshwater ecotoxicity are among the supplemented headline set of indicators. This means that the emissions underlying these impact categories are correlated to other environmental extensions in the database, which may be caused by processes (i.e. the burning of coal) that generate multiple emissions simultaneously (for example carbon dioxide, particulate matter and lead). Because of these correlated emissions, part of the impacts resulting from these can be covered by proxies from other impact categories.

One of the reasons such high correlations between indicators were found is that several impact indicators are based on the same limited number of extensions. For example, there are 46 different indicators of toxicity (out of 119 indicators in total) which are all calculated based on the emissions of 11 different toxic substances. It might be argued that part of this correlation is caused by the fact that not all relevant toxicants were included in EXIOBASE. LCA databases, such as ecoinvent (Moreno Ruiz et al., 2015), may include up to a few hundred different emissions of toxicants and toxicity information for even

more substances is available through toxicity models such as USEtox (Rosenbaum et al. 2008). With a limited amount of underlying emissions, consisting mostly of heavy metals (which are relatively well covered in EXIOBASE), the toxicity indicators can be considered as overrepresented in the LCIA methods used here. Note, however, that there are also intrinsic differences between the included toxicity indicators for different ecosystems. While the ecotoxic effects are often calculated through extrapolation from one ecosystem to another (freshwater, marine and terrestrial), the characterization factors between the different types of toxicity indicators are not strongly correlated. This is because the fate part of the characterization factor is specific to the receiving compartments (marine vs freshwater vs terrestrial environment), which results in characterization factors for chemical impacts in different ecosystems that are intrinsically different.

Another limitation of our study is that various impact categories, such as metal scarcity, ozone depletion and ionizing radiation, had to be excluded because corresponding extensions are not available in EXIOBASE. This might give an overestimation of the amount of variance that can be explained with a limited number of indicators. Regardless of the cause of the correlations however, our results do show that not all impact indicators are required for efficient communication of the results of an EEMRIO database.

The reduction in number of indicators in this study, based on the consumption of 1 million euros of products from EXIOBASE, was approximately equal to the reduction for the ecoinvent dataset, which was based on 1 kilogram of each product (Steinmann et al. 2016). In that study, 92.3% of the variance could be explained by six indicators, compared to 95.0% for the numerically optimal set of seven indicators in the current study. Given that the earlier study was based on the ecoinvent dataset, which includes a much larger number of different emissions than EXIOBASE and therefore also has more variation in impact indicators, we expected that it would have a lower reduction potential. However, the differences between products and therefore the correlations between indicators are larger when they are compared on a 1 kilogram basis. The ranked impacts of 1 kilogram of gold are much larger than those of 1 kilogram of corn, for example. On a 1 million euro basis, this effect is weakened because of the price differences between the products. In other words, 1 million euro represents a lot more kilograms of grain than gold, making the impact per million euro more similar. Despite this effect, we still found that the consumption of services had the lowest impacts while the consumption of metal products and electronics category still showed the highest impacts per million euros spent (See SI 2). While allowing for an equal base of comparison between indicators, the use of rank scores partly neglects the fact that some impacts might be very similar across product-regions whereas other indicators may show much more variation. By transforming each indicator to rank scores (as opposed to simply standardizing the impacts per indicator) the potential to distinguish between highly variable and non-discriminating indicators is lost. We feel that the use of rank scores is justified, however, because without transforming the scores to ranks the product-region combinations with the highest impacts would have dominated the correlation structure.

While there are numerous differences between a bottom-up approach like ecoinvent version versus a more top-down EEMRIO model, results show a remarkable similarity as well. In the study from Steinmann et al. (2016), the best set of six indicators included indicators of climate change, land use, acidification & eutrophication, ozone depletion, marine ecotoxicity and terrestrial ecotoxicity. The numerically optimal set of seven indicators in this study included four indicators of the same impact categories (climate change, land use, marine ecotoxicity and terrestrial ecotoxicity). Emissions of ozone depleting substances (as defined by the WMO, 2011) are not included in the EXIOBASE extensions, hence no indicators for this impact category could be included in this study.

We have demonstrated that the set of four headline indicators as proposed by Eurostat (2017) was not able to fully represent the environmental impacts embedded in EXIOBASE. This means that supplementing this set with additional thematic indicators is recommended. A limitation of using the indicators identified in this study is that they are optimal in terms of explained variance only. For policy making, however, additional criteria, such as the societal acceptance and relevancy of the indicators are of vital importance as well. These criteria have been formalized under the acronym RACER (Relevant, Accepted, Credible, Easy and Robust) (Lutter and Giljum, 2008) and represent additional considerations when assessing the usefulness of an indicator. It is questionable whether the toxicity indicators we identified are regarded robust enough by policy makers, giving their relatively large uncertainties (Rosenbaum et al. 2008). Nonetheless, they do cover an aspect of environmental impact that cannot be approximated by simple footprints of resource use. Overall our results are promising for policy makers, who aim to design environmental policies for product manufacturers for example. Instead of focusing on a large number of conflicting indicators, we argue that a relatively small subset of indicators can be used to guide environmental policy.

CHAPTER 7

Resource Footprints are Good Proxies of Environmental Damage

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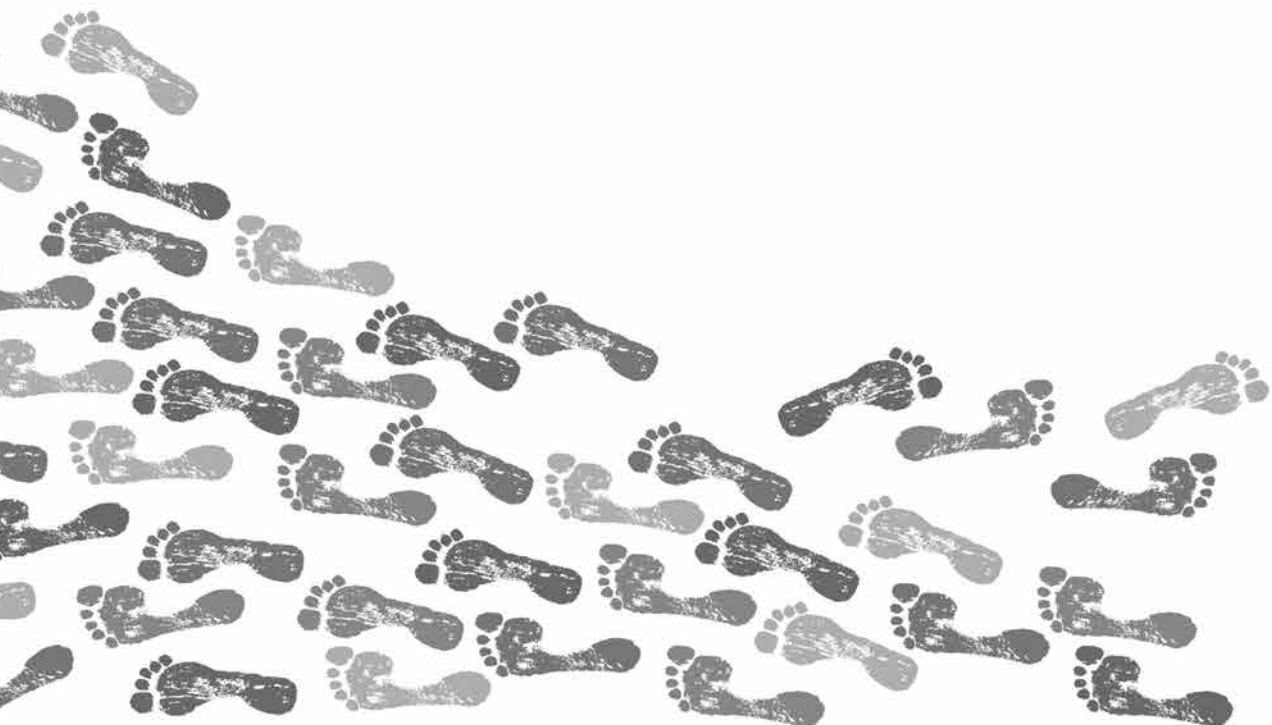
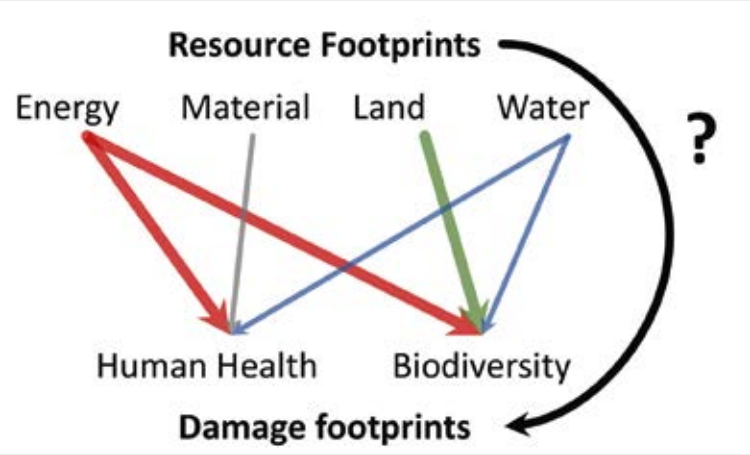


Abstract



Environmental footprints are increasingly used to quantify and compare environmental impacts of for example products, technologies, households, or nations. This has resulted in a multitude of footprint indicators, ranging from relatively simple measures of resource use (water, energy, materials) to integrated measures of eventual damage (for example, extinction of species). Yet, the possible redundancies among these different footprints have not yet been quantified. This paper analyzes the relationships between two comprehensive damage footprints and four resource footprints associated with 976 products. The resource footprints accounted for >90% of the variation in the damage footprints. Human health damage was primarily associated with the energy footprint, via emissions resulting from fossil fuel combustion. Biodiversity damage was mainly related to the energy and land footprints, the latter being mainly determined by agriculture and forestry. Our results indicate that relatively simple resource footprints are highly representative of damage to human health and biodiversity.

Introduction

Apart from welfare and increased longevity, our modern industrialized society has brought unintended environmental and social impacts, for example on biodiversity and human health. As illustrated by the so-called DPSIR framework (Driver, Pressure, State, Impact, and Response) (Smeets & Wetering, 1999), human needs (e.g., need for food) result in environmental pressures (e.g., use of fertilizer) which change the state of the environment (e.g., polluted surface water). This in turn results in impacts (e.g., biodiversity decline) and eventually a societal response to these impacts (e.g., reduced fertilizer use) (Figure 7.1). In line with this framework, biodiversity impacts are assessed by integrated assessment studies, such as the Millennium Ecosystem Assessment (Millennium Ecosystem Assessment, 2005) and the Global Biodiversity Outlooks (Secretariat of the Convention on Biological Diversity, 2014) which quantify the influence of human drivers on species decline. Similarly, in the Global Burden of Disease studies the damage to human health of a number of (environmental) factors, such as fine particulate dust concentrations, is assessed in terms of Disability Adjusted Life Years (GBD risk factors collaborators, 2015).

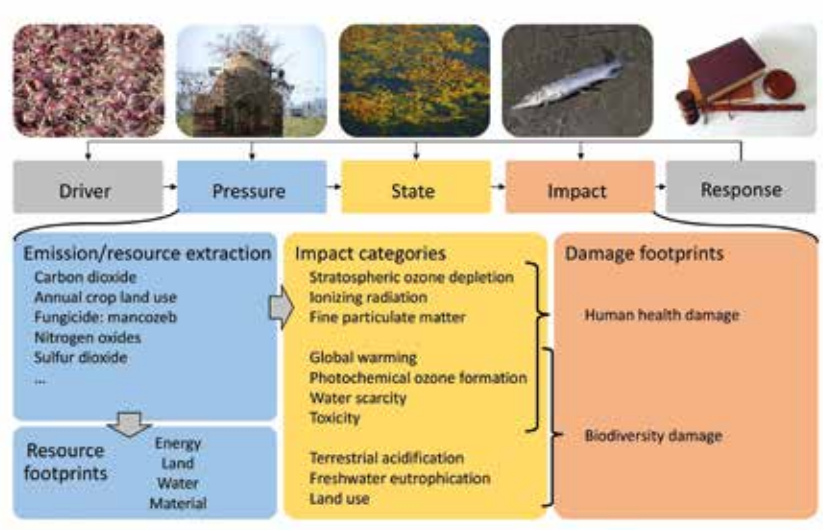


FIGURE 7.1 Schematic overview of the DPSIR chain and calculation of resource and damage footprints. The DPSIR chain shows how a primary human need (Driver), such as the need for food (onions), may lead to a resource extraction or substance emission, in this case fertilizer application (Pressure), resulting in a change in the abiotic environment, like eutrophication (State), a corresponding ecological response, like fish death (Impact), and eventually a societal reaction, such as environmental legislation on fertilizer application (Response). Resource and damage footprints are calculated based on all emission and resource extractions (located in the Pressure part of the DPSIR chain) that are associated with the production of, in this case, 1 kg of onions. Emissions, extractions, and resource footprints are retrieved from the ecoinvent database. The five emissions/resource extractions that ultimately contribute most to biodiversity damage induced by onion production are displayed. The state of the environment is calculated via different routes in several impact categories, which can ultimately result in damage to human health, biodiversity damage, or both. The ReCiPe methodology provides the factors necessary to convert the amount of emissions/resource extractions into environmental damage.

For purposes of environmental accountability and efficient damage remediation, impacts on biodiversity or human health can be allocated to specific products, technologies, cities, or nations, resulting in so-called footprints. Different types of footprints have been developed. Damage footprints approximate the anthropogenic impact on human health and ecosystems by encompassing as many relevant resource extractions, substance emissions, and cause-effect pathways as possible (Hauschild, 2005; Hellweg & Milà i Canals, 2014; Bjørn et al., 2014; Nordborg et al., 2017). The comprehensiveness of the damage footprints comes, however, at a cost. Not only do damage footprint calculations require large amounts of input data but also their outcomes are associated with large uncertainties because of the assumptions and simplifications made when quantifying intricate environmental cause-effect chains (Hellweg & Milà i Canals, 2014). As an alternative approach, the pressure part of the DPSIR chain can be used to quantify so-called resource footprints (Giljum et al., 2011; Tukker et al., 2016). Examples of resource footprint indicators (Hoekstra & Wiedmann, 2014) include land use (Weinzettel et al., 2013; Yu et al., 2013), water consumption (Feng et al., 2011; Hoekstra & Mekonnen, 2012), raw material extraction (Bruckner et al., 2012; Giljum et al., 2015; Wiedmann et al., 2015) and life cycle energy use (Arvidsson & Svanström, 2016). Because they are situated early on in the DPSIR chain, such resource footprint indicators are relatively straightforward to calculate and communicate, yet they are unlikely to represent the total environmental impact of a particular anthropogenic entity (Galli et al., 2012; Fiala, 2008). For example, environmental impacts primarily due to emissions of toxic substances are poorly represented by resource footprints (Huijbregts et al., 2010; Laurent et al., 2012) Moreover, certain footprints are considered overly simplistic for use in environmental assessments. For example, material footprints that merely sum the amounts of all raw materials needed fail to consider that the environmental impacts associated with their extraction and processing can be highly material-specific (van der Voet et al., 2005).

In short, the different footprint approaches involve clear trade-offs between comprehensiveness and representativeness, on the one hand, and data requirements, computational efforts, and reliability, on the other. A vital question in this context, therefore, is how damage footprints are connected to the more straightforward resource footprints (Huijbregts et al., 2010; Hoekstra & Wiedmann, 2014; Fang et al., 2014). Various studies investigated mutual correlations among footprint indicators (Berger & Finkbeiner, 2011; Röös et al., 2013; Lasvaux et al., 2016; Steinmann et al., 2016). These studies focused on quantifying redundancies among different types of indicators and generally found that 4 to 6 indicators are enough to cover virtually all variance among different footprint indicators. Other studies looked specifically at resource-damage relationships (Huijbregts et al., 2010; Kalbar et al., 2017) but considered bivariate relationships only, demonstrating that the cumulative energy demand was a useful proxy for environmental damage for most product categories, except for biobased products. Up to now, the relationship between multiple resource and damage footprints has never been systematically quantified. Knowledge of the relationships between both sets of indicators will clarify the extent to which resource footprints may serve as proxies for damage to humans and biodiversity.

In this study, we analyzed the relationships between two state-of-the-art damage footprints and four resource footprints associated with the manufacturing of 976 products (Supporting Information data file S1). Damage footprints pertain to human health and biodiversity, which are expressed in years of disabled life or shortened lifespans and in local species losses, respectively. Resource footprints reflect the use of fossil energy, raw materials, land, and water. To quantify the damage and resource footprints associated with each product, we used resource use and emission data from the ecoinvent database (v3.1) (Moreno Ruiz et al., 2013). To quantify damage to human health and biodiversity, we multiplied the products' resource uses and emissions with so-called characterization factors that aggregate relevant environmental cause-effect pathways (Figure 7.1), thus yielding an estimate of the total amount of damage per unit of resource use or emission for each product (Goedkoop et al., 2009; Huijbregts et al., 2016). We then applied multiple log–linear regression to link each of the two damage footprints to the four resource footprints. To elucidate the primary cause-effect pathways underlying the relationships between the damage and resource footprints, we calculated the contribution of each emission and resource use to the two damage footprints of each of the 976 products.

Methods

PRODUCT SELECTION AND LIFE CYCLE SCOPE

We based our analysis on the ecoinvent database (version 3.1). This database contains "cradle-to-gate" life-cycle data on 1,597 types of emissions representing numerous substances emitted to various environmental compartments (air, water, and soil) and 272 entries regarding the use of resources, including groundwater and surface water, fossil fuels, minerals, and various types of land cover. For our analysis we selected all products with emissions and resource extractions expressed per kg of product. The "cradle-to-gate" life cycle perspective of the database implies that we covered the production part of the products' life cycles, thus including resource use and damage from extraction of the raw materials up to the delivery to the market. Following the product selection procedure by Steinmann and co-workers, (2016) we applied the following selection criteria to minimize overlap between products:

- Individual products (e.g., concrete block) were preferred over aggregated categories (e.g., "construction materials").
- For identical products, for which different production regions or production methods were available, we selected the global or "rest-of-the-world" market mix instead of specific subtypes based on particular production methods or regions.
- Some products share (almost) identical production chains (such as isobutanol and butanol). In these cases we selected the products with the largest overall amount of interventions.

Similarity among the product chains was checked by dividing all interventions related to the production of 1 kg of a product by all the interventions of all other products. In case of an identical production chain, the ratios for all interventions are the same. Two products were considered to come from the same production chain if the coefficient of variation of these ratios was <0.01. Like in the paper by Steinmann and co-workers (2016) the final set contained 976 products, from seven categories: Agricultural & forestry products (106), Building materials (72), Chemicals (435), Metal products & electronics (128), Ores, minerals & fuels (91), Plastics (64), and Processed biobased products (80) (see data file S1 for the names of all products).

RESOURCE FOOTPRINTS

We quantified four resource footprints for each product: nonrenewable energy demand, raw material use, land use, and freshwater consumption. Energy demand (MJ) was quantified as the total amount of fossil energy required, including energy from oil, coal, gas, and peat. Raw material use (kg) was calculated as the total amount of all raw materials extracted from the earth, excluding fossil fuels because these were already covered by the energy demand calculations. Biotic resources were not included in the material footprint. Metal extractions as reported in ecoinvent were converted to ore extractions by dividing by the metal-specific ore grades, as reported in ecoinvent (Moreno Ruiz et al., 2013). In case of multiple metals derived from the same ore (e.g., silver and gold), we used the maximum ore extraction needed to obtain the required amount of any of the metals, in order to avoid double counting of ore produced. The land footprint ($m^2 \cdot yr$) was quantified as the total area of land used over time, irrespective of the type of land use, and not including land transformation. The employed blue water footprint covers the life cycle consumptive use of water. Freshwater consumption (m^3) was defined as the amount of evaporated water plus the amount of water that is incorporated in the products. This consumption was calculated as the difference between freshwater extracted from nature and the amount of water returned. In 245 out 976 cases the water evaporation (calculated by summing all emissions of water to the air) exceeded the amount of extracted water minus the amount of returned water. In these cases the evaporation was used as approximation of the total water consumption.

DAMAGE FOOTPRINTS

We calculated the human health and biodiversity damage footprints of each product by summing the resource uses and emissions multiplied with the corresponding characterization factors (CFs), i.e. factors representing the amount of damage per unit of resource use or emission, as

$$DF_{x,p} = \sum_i I_{i,p} \cdot CF_{i,x}$$

where $DF_{x,p}$ is the damage footprint for category x (human health or biodiversity) and product p, $I_{i,p}$ is the amount of resource use or emission i associated with product p, and $CF_{i,x}$ is the characterization factor for resource use or emission i and damage category x (damage to human health or biodiversity) (Hauschild & Huijbregts, 2015). We calculated human health damage as disability-adjusted life years (DALYs; yr) induced by climate change, stratospheric ozone depletion, toxicant exposure, photochemical ozone formation, particulate matter formation, water stress, and ionizing radiation (Huijbregts et al., 2016). Biodiversity loss was calculated as the time-integrated local species loss (species • yr) due to climate change, terrestrial acidification, photochemical ozone formation, freshwater eutrophication, terrestrial ecotoxicity, freshwater ecotoxicity, marine ecotoxicity, water stress, agricultural land occupation, and urban land occupation (Huijbregts et al., 2016). See Supporting Information Table S1 for a more detailed description of the impact pathways considered in these impact categories and the sources of the underlying data.

To account for spatial variability in damage we used country-specific CFs for acidification, freshwater eutrophication, and water consumption and region-specific CFs for fine particulate matter formation and photochemical ozone formation. There were 156 countries for which acidification, freshwater eutrophication, and water consumption CFs were provided by the ReCiPe methodology (Huijbregts et al., 2016). Each of these countries was assigned to one of the 58 regions for fine particulate matter formation and photochemical ozone formation (Supporting Information data file S2).

To avoid artificial environmental benefits for human health and biodiversity, net negative emissions of metals to agricultural soils due to metal uptake in crops, as reported in ecoinvent v3.1, were not considered in our cradle-to-gate analysis. Furthermore, we neglected potential human health impacts of pesticide uptake by crops, as we did not have information whether the crops were used for food, feed, or biofuels. Finally, only the off-target biodiversity impacts of chemical emissions to agricultural soil were considered. This was done to avoid double counting with the biodiversity impact caused by agricultural land occupation.

REGRESSION MODELING

We used multiple linear regression (least-squares fitting) to relate the damage footprints to the resource footprints. To account for spatial variability in impacts, we performed the regression analysis for each of the 156 countries separately, thereby implicitly assuming that all emissions and resource extractions required for each of the 976 products occur in that specific country. Because the footprints varied up to 10 orders of magnitude (based on all products), all footprints were log-transformed prior to model fitting. In regression models, high correlations among explanatory variables (in our case, the resource footprints) lead to unstable regression coefficients. If this is the case, it becomes impossible to determine which of the predictors is responsible for which share of the

variance (Field, 2009; Zuur et al., 2009). Therefore, we fitted all possible combinations of predictors and removed the regression models for which any of the predictors had a Variance Inflation Factor (VIF) larger than 5 (Field, 2009). We then ranked the remaining models according to Akaike's Information Criterion (AIC) (Akaike, 1974) which enabled us to select the most parsimonious model per country, damage footprint, and product group (Supporting Information Table S2). We calculated Cook's distances for the full model set to assess the influence of individual products on the regression coefficients (Cook & Weisberg, 1982). Cook's distances were below the threshold of 1 in all cases; therefore, all individual products were retained in the analysis. All analyses were performed in the statistical program R (R Core team, 2012). Plotting of all figures except Figure 7.1 was performed with the package "Cairo" (Urbanek et al., 2012) and VIFs were calculated with the package "HH" (Heiberger, 2013). Plots of the model residuals were created to analyze the accuracy of the predictions as well as check for potential violations of regression assumptions (Supporting Information Figures S7 and S8). The plots revealed that the errors in the prediction did not systematically deviate from the expected normal distribution.

CAUSE-EFFECT PATHWAYS

To elucidate the relationships between the damage and resource footprints, we first calculated the contribution of each individual resource extraction or emission to the damage to human health or biodiversity of each product, as

$$FF_{x,i,p} = \frac{I_{i,p} \cdot CF_{i,x}}{\sum_i I_{i,p} \cdot CF_{i,x}}$$

where $FF_{x,i,p}$ is the fraction of the damage footprint of product p for category x (human health or biodiversity) caused by resource extraction or emission i, $I_{i,p}$ is the amount of resource extraction or emission i associated with product p, and $CF_{i,x}$ is the characterization factor for resource extraction or emission i and damage category x. Per damage footprint, we ranked the median contributions $FF_{x,i,p}$ over all products and per product group. This analysis was performed only for the default ReCiPe characterization factors, i.e. country-specific differences due to spatial variability were not included.

DAMAGE SCENARIOS

Damage footprint calculations require particular assumptions and choices, for example with respect to the time horizon considered, the cause-effect pathways to be included, and the expected ability of humans and ecosystems to mitigate or adjust to future damage. In the ReCiPe methodology, these assumptions and choices are aggregated in three scenarios that reflect differences in value choices based on Cultural theory considerations (Thomson et al., 1990; Hofstetter et al., 2000; De Schryver et al., 2011). Each of these scenarios is represented by a coherent set of characterization factors. To assess the

influence of these different scenarios on our results, we performed the damage footprint calculations and subsequent regression analyses based not only on the characterizations of the default scenario but also according to the two other scenarios. The "high resilience" scenario assumes that ongoing technological and economic developments enable mankind to mitigate future damage, therefore giving more weight to present-day effects than future damage and accounting only for well-established cause-effect relationships. The "low resilience" scenario reflects the view that nature is fragile, that all possible cause-effect paths need to be accounted for (precautionary principle), and that a long time horizon is most adequate.

Results

HUMAN HEALTH DAMAGE

Overall, the four resource footprints accounted for more than 90% of the variation in human health damage. Human health damage was primarily associated with fossil energy use, followed by the use of raw materials, water, and land (Figure 7.2, Supporting Information Figures S1 and S2). The strong association between human health damage and fossil energy use reflects adverse health effects due to the emissions of carbon dioxide (CO_2), fine particulate matter, and sulfur dioxide (SO_2) associated with the combustion of fossil fuels (Figure 7.2 and Supporting Information Figure S3). Emissions of CO_2 and other greenhouse gases lead to climate change, which in turn lead to increased malnutrition due to crop failures and increased transmission of infectious diseases (Watts, 2015). Fine particulate matter, including sulfur aerosols produced by SO_2 emissions, has adverse effects particularly on people suffering from lung or heart diseases (Lelieveld et al. 2015; Brauer, 2016). As the small error bars indicate (Figure 7.2), the associations between damage and resource footprints were not sensitive to spatial variation in impacts between the 156 countries included in our analysis.

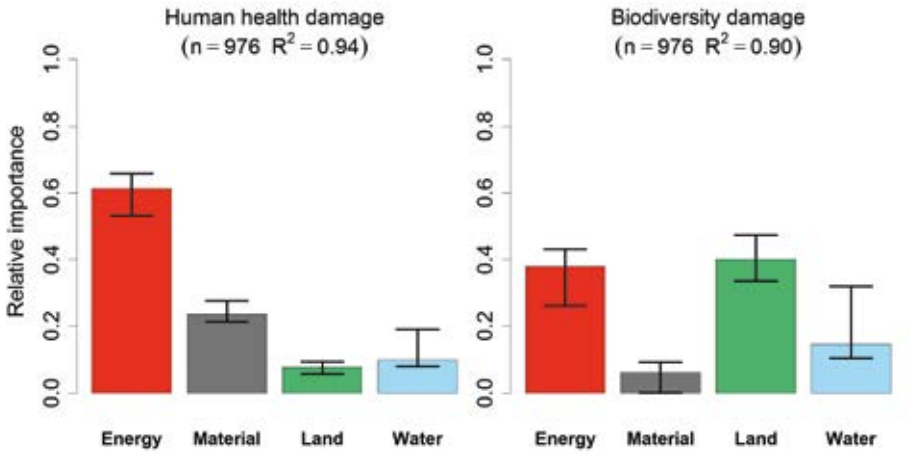


FIGURE 7.2 Associations between human health damage (left) and biodiversity damage (right) and four resource footprints (Energy, Material, Land, Water). The relative importance is expressed as standardized coefficients of log–linear regression models based on 976 products. Error bars display the 90% confidence interval in predictor importance, resulting from spatial variability in damage. R^2 was calculated as the mean value obtained from the 156 country-specific regression models.

BIODIVERSITY DAMAGE

The four resource footprints also accounted for at least 90% of the damage to biodiversity (Figure 7.2, Supporting Information Figures S4 and S5). Overall, damage to biodiversity could be approximated in particular by the combination of the land and energy footprints. Land use is generally acknowledged as an important driver of biodiversity loss because it leads to the destruction or modification of natural habitats (Alkemade et al., 2009; Newbold, 2015). The importance of fossil energy demand is primarily attributed to CO_2 emissions associated with fossil-fuel combustion (Figure 7.3 and Supporting Information Figure S6). Climate change induced by these emissions may result in biodiversity loss through shifts or reductions in the ranges of species (Alkemade et al., 2009, Urban, 2015). Acidification as a result of SO_2 emissions also had a relatively large contribution to the overall biodiversity damage (Figure 7.3). The relative impacts of the resource footprints showed more variation among the 156 countries than for human health impacts (Figure 7.2). This is due to biodiversity damage by water stress being highly location-specific, with higher impacts in countries with greater water scarcity.

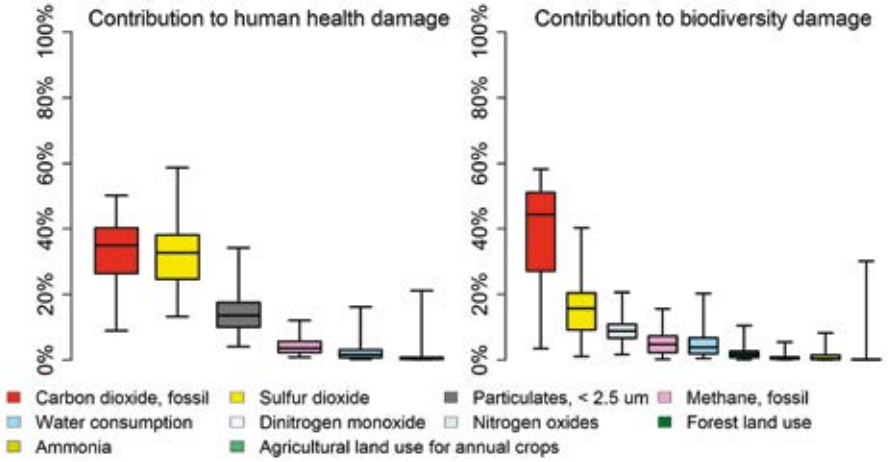


FIGURE 7.3 Contributions of major resource extractions or substance emissions to human health damage (left) and biodiversity damage (right). Boxplots represent quartiles and 90% intervals encompassing the 976 products.

Discussion

Over the past 20 years, a variety of footprint assessment methods have been developed, ranging from relatively simple resource- or emission-based indicators to more comprehensive damage-based indicators. Recently, an explicit call has been made for the various methods to be harmonized and for the representativeness of the resource-based footprints to be evaluated (Hoekstra & Wiedmann, 2014). Using a comprehensive damage assessment methodology and state-of-the-art life-cycle data associated with a large number of products, we found that four relatively straightforward resource footprints accounted for the majority of the variation in damage to human health and biodiversity.

The ecoinvent 3 database, as used in our study, is comprehensive in terms of included environmental flows and also has a clear set of data quality guidelines. Similarly, the ReCiPe 2016 method is a state-of-the-art method to quantify damage on an end point level. Other impact assessment methods might use different characterization factors and therefore come to different estimations of the environmental damage. However, studies aimed at comparing different impact assessment methods generally find very strong correlations between impact categories from different methods (Berger & Finkbeiner, 2011; Röös et al., 2013; Lasvaux et al., 2016; Steinmann et al., 2016). These findings make it likely that the choice of impact assessment method is not very influential. Our findings are also consistent with independent studies that acknowledge the importance of energy and land use as primary drivers of human health and biodiversity impacts (Millennium

Ecosystem Assessment, 2005; Secretariat of the Convention on Biological Diversity, 2014; GBD risk factors collaborators, 2015). Our study is, however, not without limitations. One limitation is that not all emissions related to the products' life cycles are reported in the ecoinvent database. For example, emissions of nanoparticles are not included, and therefore any potential damage that these may cause to biodiversity or human health cannot be included either. A second limitation is that in the ReCiPe method not all impacts are included, such as ocean acidification, which would also lead to an underestimation of the biodiversity damage footprint. Both of these limitations may result in weaker correlations between resource and damage footprints, if the missing emissions or damage pathways are unrelated to overall resource use. A third limitation is that we focused on the "cradle-to-gate" phase of the products' life cycles. We do expect, however, that the resource footprints are also representative of the environmental damage caused during the use and waste phases ("gate-to-grave"). For example, for buildings and household appliances, damages from the use and waste phases are dominated by energy and/or water use (Blengini and Di Carlo, 2010; EPA, 2013).

The relationships observed between resource and most of the analyzed damage footprints were consistent across product groups (Supporting Information Figures S1 and S4), countries, and assumptions used in the damage calculations. The latter can be observed from the similarity among the results of the default damage, high-resilience, and low resilience scenarios, which represent three coherent sets of assumptions commonly used in environmental impact assessments (Supporting Information Figures S2 and S5). There were only three main exceptions to these general findings, resulting in lower explanatory power of the resource footprints or shifts in their relative importance. First, particularly if the damage of a particular entity is primarily caused by process-specific emissions of toxic substances, the resource footprints are less representative of the damage. For human health damage, this was the case for plastics and building materials ($R^2 \approx 70$-80%, Supporting Information Figure S1). The manufacturing of some of these products is associated with substantial process-specific emissions of certain substances. During the manufacture of some plastics for example, long-lived hydrochlorofluorocarbons are emitted which lead to ozone depletion and global warming, resulting in human health damage not closely related to overall amounts of resource use. For biodiversity damage, the explanatory power of the four resource footprints was slightly lower for plastics ($R^2 = 71\%$) and processed biobased products ($R^2 = 84\%$) (Supporting Information Figure S4), because the global warming effect of certain process-specific emissions is not well-captured by the resource footprints. Second, the associations between biodiversity damage and resource footprints tended to vary across products. For example, the damage from agricultural, forestry, and biobased products was primarily due to land use, whereas the impacts of the other product groups were primarily related to fossil energy use (Supporting Information Figures S4 and S6). Third, the relative contributions of land and energy use also varied depending on whether the damage calculations followed a default or high-resilience as opposed to a low-resilience scenario (Supporting Information Figure S5). In the low-resilience scenario, which assumes a limited capability of humans and

ecosystems to adjust to change, the damage is calculated over a time horizon longer than the default of 100 years. This results in a substantial increase in the contribution of the energy footprint at the expense of the contribution of the land footprint.

Critics of resource footprints argue that environmental impacts cannot be adequately captured by simple, one-dimensional indicators, whereas their advocates stress that the simplifications involved are necessary to ensure that the indicators speak to policy makers and the general public (Giljum et al. 2011, Hoekstra & Wiedmann, 2014; Lifset, 2014). By relating two comprehensive damage indicators to four straightforward resource footprints, we have demonstrated that resource footprints are representative screening indicators of damage to human health and biodiversity. Our analysis further revealed that human health damage is primarily induced by fossil energy use, whereas biodiversity damage is primarily related to both land and fossil energy use. Thus, we conclude that energy and land footprints provide valuable proxies for the overall environmental damage produced by a particular entity.

Acknowledgment

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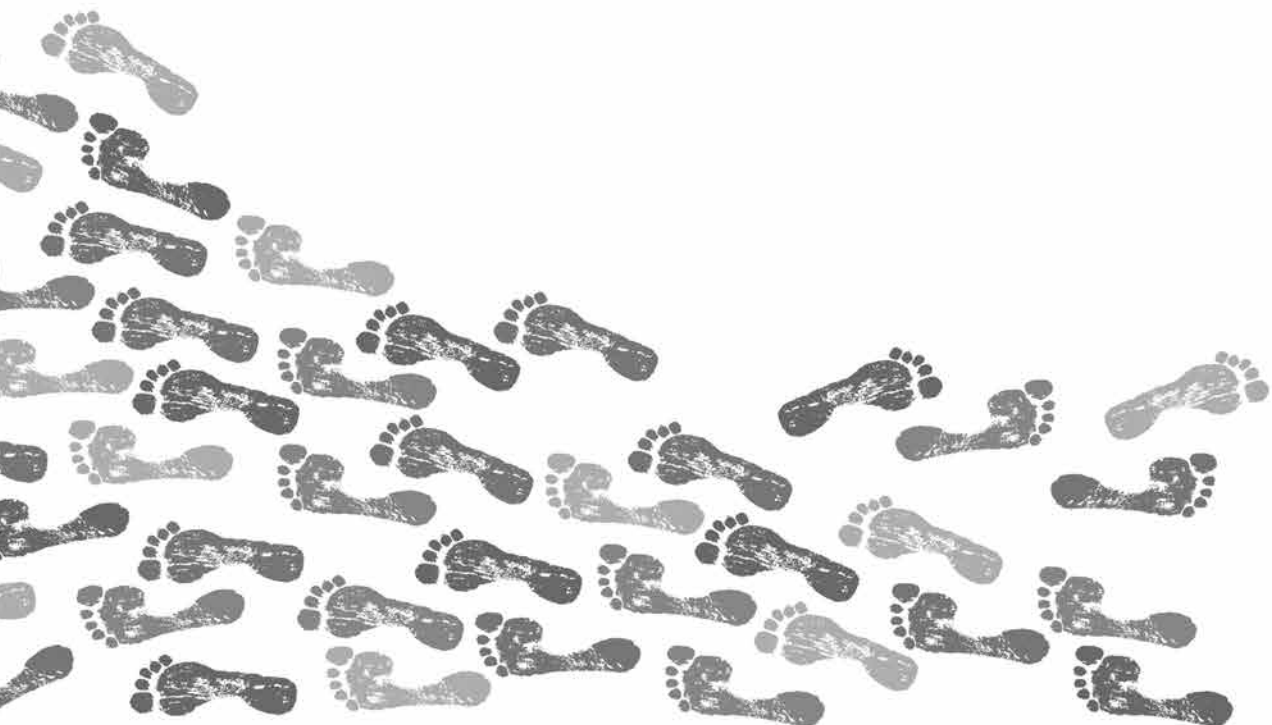
CHAPTER 8

Synthesis



In this thesis the potential for reduction of uncertainty and redundancy in environmental footprinting was explored. More specifically the following two research questions were addressed:

1 To what extent can uncertainty in environmental footprints be quantified and reduced, with a focus on the carbon footprint of fossil-fired power plants?
2 What is the optimal representative set of impact indicators to be used for environmental footprinting?

The first research question was dealt with in Chapters 2-4. Separating uncertainty from variability in the supply chains of individual power plants demonstrated that the majority of the spread in carbon footprints was caused by variability, the remaining uncertainty was small (Chapter 2). Plant-specific differences in efficiency were the main determinants of variability between power plants. Where plant efficiency data was lacking, regression techniques were employed to estimate missing combustion phase greenhouse gas emissions on an individual power plant level, thereby also quantifying the uncertainty caused by the regression models (Chapter 3 & 4). The results of these Chapters are discussed in section 8.1. The second research question was answered in Chapters 5-7. Optimal sets of impact indicators were identified with a combination of Principal Component Analysis (PCA) and multiple linear regression (Chapters 5 & 6). The potential of using resource-based footprints as proxies of environmental damage was also explored (Chapter 7). The results of these approaches are discussed in section 8.2. The overall conclusions and recommendations and the overarching lessons that can be learnt from these studies are presented in section 8.3.

Reducing uncertainty

UNCERTAINTY AND VARIABILITY

In Chapter 2, parametric uncertainty was separated from spatial and technological variability in the carbon footprints of coal-fueled power plants in the United States. This was done by calculating power plant-specific carbon footprints with corresponding uncertainty ranges. The results showed that little uncertainty remains (95% intervals were generally within +/- 2%) if one accounts for the variability between supply chains and especially variability in efficiencies of power plants. A similar study for natural gas power plants in the United States was performed by Hauck et al. (2014), likewise the variability in efficiency between power plants was found to be more important than the uncertainty in the upstream stages. Separating uncertainty and variability is a time-consuming and data-intensive process and despite the best efforts to gather spatially and technologically explicit data, there are still limitations to this study. Temporal variability

was covered in a rudimentary way by assessing the differences in efficiency between consecutive years. The results from this analysis showed that the least efficient power plants in the base year (2009) were also the ones with the highest temporal variability in efficiency. Possibly, these plants have been used continuously during one year, but only briefly or highly intermittently in another year, yielding relatively low power output per unit of fuel input during the years in which they are used less. Power plants that are designed to run as baseload plants require modifications to deal with varying loads. Without these modifications the plant efficiency decreases strongly in case of frequent shut-downs and start-ups (Henderson, 2014). Chapter 3 and 4 also demonstrated that power plants that are operated close to their maximum capacity during the year (i.e. have high capacity factors) have lower carbon footprints. The regression model employed in Chapter 4 showed a larger error for single cycle power plants compared to the combined cycle plants which likely reflects the fact that the former are often used to meet peak demands (i.e. more variable production over time) while the latter primarily provide baseload power. This results in prediction uncertainties for single cycle gas plants that are approximately twice as large as those for combined cycle gas plants and even up to four times as high for oil plants, meaning that the models could differentiate between the types of plants but not between the best and worst plants within a specific type. More plant specific data on the (expected) variability in electricity production is necessary to provide a more certain prediction of the carbon footprint.

With the increasing role of renewable electricity generation, fossil-fueled power plants will be used primarily to balance variable loads in the near future (Schill, 2014, Schill et al. 2017). A decrease in the efficiency of fossil fueled power plants can be expected due to this shift of function from baseload plants to peaker plants. The magnitude of this decrease will depend on which measures are taken to facilitate operating of power plants with variable power output. A further complicating factor is that the costs ($ investment costs/kg CO_2 captured) of retrofitting power plants with CCS-technology (carbon capture and storage) are lower for baseload power plants than for plants that operate with variable power outputs (Middleton & Eccles, 2013). To determine which configuration of fossil power plants (with or without CCS technology) and renewables leads to the lowest environmental impact, all these aspects need to be taken into account.

REGRESSION MODELS

In order to estimate the fossil carbon footprints of electricity production in power plants located in other countries than the United States, regression models were applied in Chapters 3 and 4. Applying these regression models introduces additional uncertainty in the carbon footprints compared to empirical estimates, with relatively low uncertainty for combined cycle gas plants, intermediate uncertainty for coal-fueled power plants and high uncertainty for single cycle gas and oil plants.

Local-linear regression approaches proved to be slightly better than the standard multiple linear regression, in Chapter 3 the former explained 61% of the variance while the latter only explained 49%. Local-linear models have the disadvantage that the most influential predictors cannot be identified in the same way as for the global linear models, making the interpretation of the local-linear models less straightforward. The lack of a relationship between predictors and response that is equal across the applied whole range of values also means that the original dataset needs to be provided in order to make predictions with local linear regression for other power plants, which may be an issue if the training dataset contains proprietary information. In contrast, with the global models only the fitted coefficients are necessary to make predictions. One issue that was encountered in Chapter 3, was the presence of very high carbon footprints for some of the coal-fired power plants in the dataset for India. The global linear models employed could not adequately predict these numbers, suggesting that the relationships with some covariates/predictors or variables not included in the model may be non-linear. This can explain the better performance of local regression models, which weigh similar data points more strongly than others, compared to global regression models that give equal weight to each data point. In Chapter 4, the models' errors were incorporated in a more sophisticated way compared to Chapter 3. A mixed-effect model, in which the error of prediction was allowed to vary across different types of electricity plants, was used for the prediction of oil- and gas-fueled power plants. The mixed-effect model structure allows to attribute the uncertainty in an appropriate way. If used on the dataset for coal plants in Chapter 3, more uncertainty would have been attributed to the Indian power plants than to power plants from other countries, reflecting the large spread in carbon footprints found for India. The carbon footprints of fossil power plants were, in general, linearly related to the selected predictors. For other products or impacts a linear relationship between predictors and environmental footprints may not hold. Wernet and co-workers (2008) and Song and co-workers (2017) employed Artificial Neural Networks (ANN) to predict the environmental impacts of a number of different chemicals based on their chemical properties. With an explained variance in rank scores of up to 74%, the ANN approach clearly out-performed the linear regression models (maximal explained variance 29%) in the study by Wernet et al. (2008).

OPPORTUNITIES

Despite the above-mentioned limitations, using regression models to predict carbon footprints of power plants can reduce uncertainties, covering approximately half of the variation in carbon footprints for coal plants and 80% for gas and oil plants. The application of regression models is not limited to the power sector. In principal one can apply regression models to any data-scarce product category in LCA, provided that the data is available to build the models on. The CO_2 emissions of power plants were predicted in Chapters 3 & 4 by employing readily available technological power plant characteristics. In Chapter 7, emissions of carbon dioxide and sulfur dioxide, and land occupation were demonstrated to be important contributors to environmental damage. The importance of

land as contributor to environmental impact indicates that future studies aimed towards reducing uncertainty could focus on predicting land requirements particularly related to the agricultural and forestry sector. Recent studies assessing the variability in the footprints of agricultural systems in Iran demonstrate that variability in yields (amount of produce per unit of area) is highly correlated with variability in environmental impacts per unit of production of wheat (Heidari et al., 2016, 2017). Regression-based models have the potential to predict spatial differences in yields by using topographic and/or climatic conditions as predictors. Another interesting area to apply regression models, is the category of household domestic appliances where individual behavior during the use phase of the product/service may be a main driver of variability in environmental impact (Di Sorrentino et al., 2016). Regression models to estimate for example the shower or laundry behavior of individuals based on a few characteristics can help to greatly reduce the uncertainty in their environmental impacts.

Reducing redundancy

INDICATOR SELECTION

In Chapters 5 and 6, the redundancy among midpoint indicators was quantified via Principal Component Analysis (PCA) combined with linear regression modeling. Both Chapters showed large correlations among different indicators as well as among different impact assessment methodologies. Chapter 5 demonstrates that 92.3% of the variance in rankings for a large set of products can be explained with just six different midpoint indicators (i.e. climate change, land use, ozone depletion, acidification & eutrophication, marine ecotoxicity and terrestrial ecotoxicity). However, another aspect to consider when suggesting any reduced set of environmental indicators is the extent to which they meet the RACER (Relevant, Accepted, Credible, Easy and Robust) criteria. Given the high uncertainty in toxicity indicators (Rosenbaum et al. 2008) and the diminishing relevancy of ozone depleting emissions as environmental problem (WMO, 2011), the representativeness of resource-based footprints was also explored. The resource-based footprints perform well on most of the RACER criteria, as they are relatively easy to calculate, statistically robust and therefore credible. They are, however, not always accepted in the field of life cycle impact assessment because their relevancy for environmental damage is disputed (e.g. van der Voet, 2005; Fiala, 2008). Together, the fossil energy, land and material footprints covered 83.8% of the variance in product rankings. Adding the water footprint had little effect since the land and water footprints were strongly correlated.

The land, water, material and carbon footprints were less representative of the impacts embedded in the EEMRIO model EXIOBASE. Only about 60% of the variance in product rankings could be explained by those four headline indicators (Chapter 6). The carbon footprint is strongly correlated to the fossil energy footprint (Spearman rank correlation, r = 0.92 for the set of products in Chapter 5), making these indicators grossly interchangeable. An indicator of marine ecotoxicity was necessary to increase the explained variance to more than 85% in EXIOBASE, demonstrating that the toxic impacts were not strongly related to the resource footprints. One of the limitations of using an EEMRIO model like EXIOBASE is, however, that only a small number of emissions is typically taken into account, challenging the generality of this finding. For instance, most emissions that are included consist of metals, potentially resulting in an overrepresentation of these metals as drivers of toxic impacts. Other, not-included toxic emissions, may be more strongly correlated to the resource footprints than the metals are.

While Chapters 5 and 6 focused on the redundancies between midpoint indicators, Chapter 7 showed more specifically how well the more complicated endpoint damage footprints can be approximated by the simpler resource based methods. For a set of 976 products, a combination of the energy and land footprint explained about 90% of the variance in damage to human health and ecosystems. These two footprints can be considered as good proxies of damage because a large part of the environmental damage is caused by a small number of fossil energy-related emissions, such as greenhouse gas and sulfur dioxide emissions, or land use types (mainly agricultural land use). The publication of Chapter 7 in the journal Environmental Science and Technology led to the submission of a comment debating the issue of what a good proxy is. The usefulness of using the resource footprints as a proxy was discussed because they might lead to a different ranking among products than the original damage footprints. In our reply we demonstrated that in 92% of all product-by-product comparisons the ranking between products remained unchanged. The reply to this comment is added to this thesis as Appendix 8.

Based on the analyses in Chapters 5 and 6, it appears that three environmental footprints related to land and (fossil) energy (or GHG emissions) and toxicity embrace a large share of resource, midpoint and endpoint footprints in an LCA and EEMRIO setting. These three footprints can be used as the basis for environmental product assessments. Chapter 7 shows that the contribution of the toxicity indicators to ecosystem and human health damage is negligible and suggests that the use of two resource footprints could even be enough to provide a sufficiently detailed environmental footprint of products and services. This raises an interesting question: can we now indeed be confident that looking solely at land and fossil energy in environmental product assessments is sufficient? To answer this question it is worthwhile to look back at the assessments of biodiversity (MEA, 2005) and human health (Murray et al. 2012; GBD Collaborators, 2015) introduced in Chapters 1 and 7 to see if at least all major drivers of impact are covered by the proposed proxy indicators. While climate change (which is for a large part caused by fossil energy use) and habitat

loss are among the top drivers of biodiversity loss, they are not the only ones. The impact caused by habitat fragmentation and introduction of invasive exotic species is currently not covered in any of the environmental damage footprints used in LCA or EEMRIO. In principle it is possible to link both (part of) the introduced invasive species and habitat fragmentation to life cycle transport requirements and land use. Approaches to include habitat fragmentation due to land occupation are still under development. The meta-population capacity of a landscape can be used to derive a so called Species Fragmented Area Relationship (SFAR), which relates both the area and degree of fragmentation to the number of present species (Hanski & Ovaskainen, 2000; Hanski et al., 2013). This SFAR could be a starting point to derive spatially explicit characterization factors to be used for impact assessment. This approach has not yet been implemented however. A different approach was used by Chaplin-Kramer et al. (2017) who included habitat fragmentation in their assessment of the effects of indirect land use change. Their approach is based on a simplified relationship between patch-size and mean species abundance (MSA) of natural areas derived from the GLOBIO model (Schipper et al., 2013). Incorporation of this approach in existing LCIA methods is difficult because exact knowledge of the spatial configuration of the used land is necessary to calculate this metric. Characterization factors for invasive species introduced via the transport of goods via the Rhine-Main-Danube canal have been derived by Hanafiah et al. (2013). Their results show that in the river Rhine more than 70% of the total freshwater ecosystem impact may be caused by the introduction of invasive species, demonstrating the potential relevance of including this indicator. Unfortunately by covering only a small part of Europa, the spatial coverage is too limited to be used in the life cycle impact assessment methods. With the current level of technology, transportation requires fossil fuels and causes both fragmentation and the introduction of invasive species via the construction of roads and canals. In addition to the direct effects of habitat loss (which are already included in the impact assessment methods) land use has an additional indirect effect through habitat fragmentation. It is therefore hypothesized that the importance of fossil energy demand and land use as proxies for biodiversity damage, as found in Chapter 7, would remain the same or even increase if these two additional damage pathways were to be included. Note that in the future, with the transition towards a transportation sector that is fueled by renewable electricity, the correlation between transportation and fossil fuel use is likely to become a lot weaker while the required transport infrastructure will still lead to introduction of exotic species and habitat fragmentation. This would limit the relative importance of fossil energy demand as proxy for ecosystem damage. The final major driver of biodiversity loss that is not included in environmental damage footprints of products is overexploitation of natural resources (for example through fisheries). Two studies on fisheries have quantified the impacts of overexploitation on a fish stock or midpoint level (Emanuelsson et al., 2014; Langlois et al., 2014), but these studies cannot be used directly to link overexploitation due to fish catch to an overall endpoint effect on biodiversity. If overexploitation were to be included, it seems likely that the direct exploitation effect will be responsible for a large proportion of the environmental damage for products directly causing overexploitation, such as canned tuna or wild game meat. Including this impact

pathway would therefore result in a lower predictive power of the resource footprints for these products. Among the top 20 causes of human health loss in DALY (Murray et al., 2012) are depressive disorders, AIDS/HIV, road traffic accidents, lower back pain and self-harm, none of which are covered in the environmental human health impact calculations. However, not all these impacts need to be covered, only those that can be linked to environmental cause-and-effect pathways should be included. Of all of these causes it seems feasible and reasonable to attribute (a part of the) road traffic accidents to transportation. Fries & Hellweg (2014) have demonstrated that if road accidents were to be included, they would be responsible for 26% of the total human health impacts for Switzerland. Values for other countries are not presented in that study, making inclusion in LCIA methods not yet possible. Including road accidents is likely to have a similar effect on the relationship between resource and damage footprints as including habitat fragmentation and invasive exotic species has for ecosystems.

OPPORTUNITIES

The latest developments in life cycle impact assessment methodologies acknowledge that there is a large spatial variability in impact. Regionalized characterization factors are now provided for a number of impact categories in the ReCiPe and LC-Impact methods (Huijbregts et al. 2016, Verones et al. 2016). No spatially explicit factors were used in Chapters 5 and 6, while in Chapter 7 only a first simple test of the effects of regionalized characterization factors was performed. This was done by assuming that all emissions, water and land use occur in one country and fitting the regression model based on the characterization factors for that country. This procedure was repeated for 158 different countries. Such an approach can be seen as a sensitivity analysis rather than an assessment of the true spatial variability among impacts. Spatial variability had a larger influence on the predictive power of the resource footprints for biodiversity impacts than for human health. For human health the fossil energy footprint remained the most important predictor while for biodiversity impacts, spatial variability often reversed the roles of the fossil energy footprint and the land footprint as the most important predictor. Whether the representativeness of the small indicator sets also holds if the spatial variability in impacts is fully taken into account remains to be tested. The limited coverage of toxicity indicators in EEMRIO models can potentially be improved as well. Right now the toxicity indicators calculated with EXIOBASE only represent metal toxicity, including non-metal toxicants may help to present a more complete picture of the toxic impacts caused by our economy. Another way to improve the impact assessment models is to include those major drivers of biodiversity and human health damage that are attributable to one (or more) of the life cycle interventions.

Conclusions and recommendations

Overseeing the work in all Chapters, the main conclusions of this thesis are:

- Technological variability in the carbon footprint of fossil-fired power plants is larger than uncertainty.
- Regression analysis can be used to predict the carbon footprints of fossil-fired power plants with low uncertainty for combined cycle gas plants, intermediate uncertainty for coal fueled power plants and relatively high uncertainties for single cycle gas and oil plants.
- The search for an optimal set of indicators for a large range of products yields a statistically best set consisting of a limited set of six environmental indicators (climate change, land use, ozone depletion, acidification & eutrophication, marine ecotoxicity and terrestrial ecotoxicity).
- Sets of key performance indicators based on the resource footprint for energy, material, land and water perform well for a set of products from a life cycle database Ecoinvent, for the EEMRIO model EXIOBASE ecotoxicity was also part of the key indicators
- Land and fossil energy are useful proxies of endpoint environmental damage.
- Overall, environmental footprints related to fossil energy (or GHG emissions), land and toxicity embrace a large share of resource, midpoint and endpoint footprints derived via the Ecoinvent and EXIOBASE datasets.

Recommendations for future work based on the findings of these thesis are:

- Development of regression models for other product groups in LCA, especially in those cases where variability is expected to play an important role (e.g., agricultural products, consumer behavior) and can be related to few characteristics of the product/system.
- Investigation of the influence of temporal variability on life cycle greenhouse gas emissions from both renewable and fossil electricity generation.
- Evaluation of the robustness of the optimal set of environmental indicators with spatially-differentiated impact assessment methods.
- Improvement of the impact assessment methods by including those major drivers of biodiversity and human health damage that are attributable to specific life cycle interventions, such as the introduction invasive species, habitat fragmentation and road accidents.

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Appendices

APPENDIX 1: SUPPLEMENTAL MATERIAL FOR:

CHAPTER 2: A METHODOLOGY FOR SEPARATING UNCERTAINTY AND VARIABILITY IN THE LIFE CYCLE GREENHOUSE GAS EMISSIONS OF COAL FUELED POWER GENERATION IN THE UNITED STATES

TABLE S1 Parameter values and uncertainty ranges for all uncertain foreground parameters

Parameter	Unit	Type of distribution	Geometric mean (lognormal) Most likely value (beta-pert)	Geometric standard deviation (lognormal) Range (uniform, beta-pert)	Source
Mining phase					
CH_4 release fraction post-mining	(m^3 CH_4/kg coal) / (m^3 CH_4/kg coal)	Beta-Pert	0.325	[0.25-0.40]	(EPA 2011)
CH_4 release factor surface mining	(m^3 CH_4/kg coal) / (m^3 CH_4/kg coal)	Lognormal	1 + 1	1.4	(EPA 2011)
CH_4 release underground mining through ventilation	kg CH_4/ kg coal	Lognormal	$5.3 \cdot 10^{-3}$ [a]	1.17	(EPA 2011), (IPCC 2006)
CH_4 release underground mining through degasification	kg CH_4/ kg coal	Lognormal	$2.4 \cdot 10^{-3}$ [b]	1.03	(EPA 2011), (IPCC 2006)
Coal use for surface mining	kg coal used/ kg coal produced	Lognormal	$1.5 \cdot 10^{-6}$	1.58	(Censusbureau), (Dones et al. 2007b)
Distillate use for surface mining	l/kg coal	Lognormal	$1.4 \cdot 10^{-3}$	1.58	(Censusbureau), (Dones et al. 2007b)
Residual use for surface mining and supporting activities	l/kg coal	Lognormal	$2.0 \cdot 10^{-4}$	1.58	(Censusbureau), (Dones et al. 2007b)
Gasoline use for surface mining	l/kg coal	Lognormal	$5.6 \cdot 10^{-5}$	1.58	(Censusbureau), (Dones et al. 2007b)
Coal use for underground mining	l/kg coal	Lognormal	$5.0 \cdot 10^{-4}$	1.58	(Censusbureau), (Dones et al. 2007b)
Residual use for underground mining and supporting activities	l fuel / kg coal	Lognormal	$7.3 \cdot 10^{-6}$	1.58	(Censusbureau), (Dones et al. 2007b) See also S 2.1
Gasoline use for underground mining	l fuel / kg coal	Lognormal	$1.4 \cdot 10^{-5}$	1.58	(Censusbureau), (Dones et al. 2007b)

Electricity use for surface mining	kWh/kg coal	Lognormal	$6.3 \cdot 10^{-3}$	1.41	(Jaramillo et al. 2007), (Dones et al. 2007b)
Electricity use for underground mining	kWh/kg coal	Lognormal	$1.7 \cdot 10^{-2}$	1.41	(Jaramillo et al. 2007), (Dones et al. 2007b)
Transport phase					
Heavy fuel use oceanic transport	kg/tkm	Lognormal	$2.5 \cdot 10^{-3}$	1.41	(Spielmann et al. 2007)
Diesel use barge	kg/tkm	Lognormal	$9.4 \cdot 10^{-3}$	1.14	(Spielmann et al. 2007)
Diesel use truck					
	kg/tkm	Lognormal	$2.7 \cdot 10^{-2}$	1.03	(Spielmann et al. 2007)
Diesel use train	kg/tkm	Lognormal	$2.5 \cdot 10^{-3}$	1.35	(Spielmann et al. 2007)
Air speed over train	km/h	Lognormal	$4.9 \cdot 10^{-1}$	1.58	(QueenslandRail-Limited 2008) see also "Use Phase"
Mine location	None	Uniform		[-1 – 1]	This report
Plant location	None	Uniform		[-1 – 1]	This report
Use phase					
CO_2 emission from complete combustion of coal	kg CO_2/GJ	Lognormal	State average	[1.01]	(Hong and Slatick 1994; Roy et al. 2009) See Table S2 for state averages
Background processes See "Use Phase" and Table S4					
GWP[c]					
AGWP20 CH_4	Wm^{-2} yr(kg CO_2)-1	Lognormal	1.8 • 10-12	1.25	(IPCC 2007)
AGWP20 CO_2	Wm^{-2} yr(kg CO_2)$^{-1}$	Lognormal	2.5 • 10-14	1.1	(IPCC 2007)
AGWP100 CH_4	Wm^{-2} yr(kg CO_2)$^{-1}$	Lognormal	2.2 • 10-12	1.25	(IPCC 2007)
AGWP100 CO_2	Wm^{-2} yr(kg CO_2)$^{-1}$	Lognormal	8.7 • 10-14	1.1	(IPCC 2007)
AGWP500 CH_4	Wm^{-2} yr(kg CO_2)$^{-1}$	Lognormal	2.2 • 10-12	1.25	(IPCC 2007)
AGWP500 CO_2	Wm^{-2} yr(kg CO_2)$^{-1}$	Lognormal	2.9 • 10-13	1.1	(IPCC 2007)

a Release factor is calculated as a lognormal distribution + 1, because the minimum value is 1. According to EPA, 1993 if emissions are low, only the in situ content in the coal that is actually mined is released (release factor 1), however, in other cases, methane from surrounding strata is also be released (factor >1).

b The larger uncertainty range of ranges estimates provided by IPCC (IPCC 2006) was taken, because uncertainty estimates depend on measurement frequencies and determination method that could not be determined for all plants; total CH_4 releases from underground mining are calculated to come 69% from ventilation and 31% from degasification.

c In order to calculate the GWP of a GHG for a certain time horizon, the Absolute Global Warming Potential (AGWP) of that GHG is divided by the AGWP of the reference gas (CO_2) for that time horizon. Therefore parameter uncertainty in the GWP of CH_4 is caused by both uncertainty in the AGWP of CH_4 itself and the AGWP of CO2

MINING PHASE

Census bureau information on fuel use in mines

Fuel uses in underground and surface mines are derived from the economic census 2002 of the US census bureau (Censusbureau). These numbers are divided by the production in 2002 as reported by the EIA (EIA 2006) to arrive at consumption numbers per fuel and mine type as shown in Table S1. Fuel use for supporting activities is also reported by the census bureau. From the fuel use emission factors are derived in the same way as for the combustion phase (based on heat content, carbon content, CO_2/C ratio).

For surface mines, CH_4 emissions were calculated based on the in situ content of CH_4 per coal basin and the release factors for surface mining. Post-mining emissions for both surface and underground mines were based on the CH_4 content and the post-mining release factor. Median/most likely values and uncertainty ranges for release factors were taken from EPA (EPA 2011). For underground mines the CH_4 emissions were based on the US total emission from underground mining. This number was divided by total production from underground mines to arrive at an emission factor per kg coal produced. This information was also provided by the EPA (EPA 2011). Corresponding uncertainty estimates for emissions from ventilation and degasification were provided by the IPCC (IPCC 2006). Ventilation uncertainty factors were applied to 69% of the underground emissions and degasification uncertainty factors were applied to 31% of underground emissions (derived from EPA (EPA 2011)). Residual fuel use for supporting activities was reported as a total number (for surface and underground mining) by the census bureau and was distributed over surface and underground mining according to their contribution to total coal production. The residual fuel use for supporting activities was added to the overall residual fuel use, table S1 displays the total residual fuel use.

CO_2 emissions from mining were derived from fuel and electricity use at the mines. Uncertainty factors for fuel use and electricity use are taken from Ecoinvent (Dones et al. 2007b) and are shown in table S3.

TABLE S2 Coal basin-state attribution, adopted from EPA(EPA 2010), Table A-114

State	State Abbrevation	Coal basin	Methane content surface (m^3/kg) and Geometric standard deviation, between parentheses	Methane content underground (m^3/kg) and Geometric standard deviation, between parentheses	Carbon dioxide emission (kg CO_2/GJ coal for complete combustion)
Kentucky	KY	Central Appalachia (E KY), Illinois	$7.8 \cdot 10^{-4}$ [1.8], $1.1 \cdot 10^{-3}$ [1.8]	$4.7 \cdot 10^{-3}$ [1.8], $2.0 \cdot 10^{-3}$ [1.8]	88.0 [1.01], 87.4 (Kentucky West) (BIT) [1.01]
Tennessee	TN	Central Appalachia	$7.8 \cdot 10^{-4}$ [1.8]	$4.7 \cdot 10^{-3}$ [1.8]	88.0 (BIT) [1.01]
Virginia	VA	Central Appalachia (VA)	$7.8 \cdot 10^{-4}$ [1.8]	$4.7 \cdot 10^{-3}$ [1.8]	88.7 (BIT) [1.01]
Illinois	IL	Illinois	$1.1 \cdot 10^{-3}$ [1.8]	$2.0 \cdot 10^{-3}$ [1.8]	87.5 (BIT) [1.01]
Indiana	IN	Illinois	$1.1 \cdot 10^{-3}$ [1.8]	$2.0 \cdot 10^{-3}$ [1.8]	87.5 (BIT) [1.01]
Montana	MT	N. Great Plains (WY, MT)	$6.2 \cdot 10^{-4}$ [1.8]	4.9 • 10-4 [1.8]	90.1 (BIT), 91.7 (SUB), 94.8 (LIG) All: [1.01]
North Dakota	ND	N. Great Plains (ND)	$1.7 \cdot 10^{-4}$ [1.8]	$4.9 \cdot 10^{-4}$ [1.8]	94.1 (LIG) [1.01]
Wyoming	WY	N. Great Plains (WY, MT)	$6.2 \cdot 10^{-4}$ [1.8]	$4.9 \cdot 10^{-4}$ [1.8]	88.8 (BIT) [1.01], 91.4 (SUB) [1.01]
West Virginia	WV	Central Appalachia (WV), Northern Appalachia	$7.8 \cdot 10^{-4}$ [1.8] $1.9 \cdot 10^{-3}$ [1.8]	$4.7 \cdot 10^{-3}$ [1.8] $4.3 \cdot 10^{-3}$ [1.8]	89.0 (BIT) [1.01]
Maryland	MD	Northern Appalachia	$1.9 \cdot 10^{-3}$ [1.8]	$4.3 \cdot 10^{-3}$ [1.8]	90.4 (BIT) [1.01]
Ohio	OH	Northern Appalachia	$1.9 \cdot 10^{-3}$ [1.8]	$4.3 \cdot 10^{-3}$ [1.8]	87.2 (BIT) [1.01]
Pennsylvania	PA	Northern Appalachia	$1.9 \cdot 10^{-3}$ [1.8]	$4.3 \cdot 10^{-3}$ [1.8]	88.4 (BIT) [1.01]
Arizona	AZ	Rockies	$6.6 \cdot 10^{-4}$ [1.8]	$4.5 \cdot 10^{-3}$ [1.8]	90.2 (BIT) [1.01]
Colorado	CO	Rockies	$6.6 \cdot 10^{-4}$ [1.8]	$4.5 \cdot 10^{-3}$ [1.8]	88.7 (BIT) [1.01], 91.4 (SUB) [1.01]
New Mexico	NM	Rockies	$6.6 \cdot 10^{-4}$ [1.8]	$4.5 \cdot 10^{-3}$ [1.8]	88.4 (BIT) [1.01], 89.8 (SUB) [1.01]
Utah	UT	Rockies	$6.6 \cdot 10^{-4}$ [1.8]	$4.5 \cdot 10^{-3}$ [1.8]	87.7 (BIT) [1.01], 89.0 (SUB) [1.01]
Alabama	AL	Warrior	$9.6 \cdot 10^{-4}$ [1.8]	$8.3 \cdot 10^{-3}$ [1.8]	88.3 (BIT) [1.01]
Mississippi	MS	Warrior	$9.6 \cdot 10^{-4}$ [1.8]	$8.3 \cdot 10^{-3}$ [1.8]	(LIG) Geomean of all other states
Kansas	KS	West Interior	$9.5 \cdot 10^{-4}$ [1.8]	$4.4 \cdot 10^{-3}$ [1.8]	87.2 (BIT) [1.01]
Louisiana	LA	West Interior	$9.5 \cdot 10^{-4}$ [1.8]	$4.4 \cdot 10^{-3}$ [1.8]	91.8 (LIG) [1.01]

Missouri	MO	West Interior	$9.5 \cdot 10^{-4}$ [1.8]	$4.4 \cdot 10^{-3}$ [1.8]	86.5 (BIT) [1.01]
Oklahoma	OK	West Interior	$9.5 \cdot 10^{-4}$ [1.8]	$4.4 \cdot 10^{-3}$ [1.8]	88.5 (BIT) [1.01]
Texas	TX	West Interior	$9.5 \cdot 10^{-4}$ [1.8]	$4.4 \cdot 10^{-3}$ [1.8]	87.9 (BIT) [1.01], 91.8 (LIG) [1.01]

Notes: States in bold are attributed to more than one coal basin. Emission factors are provided by EPA (EPA 2010) in Table A-116. For the Rockies and West Interior and basins these are on different level of detail then table S1. For mines that could not be attributed to one of these sub-basins Monte Carlo simulations were used, the geometric average for the basin is reported here, the range was assumed to be the 95% confidence interval of a lognormal distribution. The same applies for Tennessee in Central Appalachia. Here the average of emissions factors for Central Appalachia (VA) and (WV), because those were the only ones available. Carbon dioxide emissions are listed per coal type, abbreviations stand for Bituminous coal (BIT), Subbituminous coal (SUB) or Lignite (LIG). Information for lignite coal from Missippi (MS) was lacking, therefore the geomean from other Lignite producing states was used. Uncertainty ranges for the methane content and carbon dioxide emissions are given between parentheses, sources are (Diamond et al. 1986) and (Roy et al. 2009) respectively (see also section 3).

Transport phase

Most coal is transported by rail, on direct lines from mine to power plant (McCollum 2007). The locations of the mine's county and the plant's ZIP area were used to calculate the distance between plant and mine in Google maps. Thereby it is assumed that highway distances are a reasonable approximation of rail road distances. For coal that is transported via waterways the same method of calculating the distance is used, even though the canals/rivers may not run exactly parallel to roads. For each plant-mine combination the primary mode of transport was acquired from the EIA, ignoring any secondary modes of transport. The primary mode of transport reported by the EIA was assumed to the correct one, regardless of the travel distance. An exception was made for imported coal. About 2% of the total coal mass delivered to plants is imported from mines in Colombia, Venezuela, and Indonesia. Transport distance was estimated by calculating the distance from the centroid of the foreign country to the centroid of the receiving plant's county. For imported coal all transport was assumed to be by transoceanic freight ship. Therefore any transports sheets that reported a different type of transport than transoceanic freight ship for imported coal were corrected.

Incomplete mine or transport information

Not all power plants that are listed in the EIA 923 file, have corresponding usable mine and transport information. Plant-mine transports with a lack of mine information amount to ca. 1% of total mass of coal delivered. The overall average mining emissions (kg GHG/kg coal) were assigned to these plant-mine pairs for all greenhouse gases.

All rail transport was assumed to be by a diesel powered trains. Fuel use of trains, trucks and ships per ton-km is uncertain. Uncertainty in the fuel use per ton-km for diesel fuelled trains was derived from ICF International (ICFInternational 2009). Uncertainty in fuel use for interoceanic freight ships, barges and trucks were all taken from the ecoinvent database (Spielmann et al. 2007). Transport emissions for transport by conveyor belt neglected, because this type of transport is only used when coal mine and power plant are directly adjacent (transport distance was assumed to be negligible).

For some mines the exact county location was not known. In these cases the great-circle distance between the mine's state centroid and the power plant location was calculated. Great-circle distances are, by definition, the shortest route from point a to b, however roads rarely follow the shortest route exactly. To determine the relation between the great-circle distances and the road distances, a regression analysis of all plant-mine combinations with known road distances and the corresponding great circle distances was performed. The regression result was then used to convert the great-circle distances for the mines with unknown locations into road distance approximations. The regression procedure was implemented for 11.3% of all plant-mine combinations (367 out of 3241 plant-mine combinations).

Coal loss during rail transport

According to Ecoinvent (Dones et al. 2007a), estimations of coal losses during transport vary from 0.05-1% during rail transport, with an additional loss during storage between 0.05-0.1%. However because loss prevention techniques are available and because not all coal types have the same tendency to form dust, Ecoinvent uses a total loss (transport and storage) of 0.1% for European coal and 0.2% for coal from other sources than Europe.

Experimental research on coal dust losses during transport has led to varying results (Lazo and McClain 1996; Ferreira et al. 2003). Based on the work of Ferreira (Ferreira et al. 2003) and their own on site measurements, the Queensland Rail company (QueenslandRailLimited 2008) applies Equation S1 to calculate the coal losses, taking into account the wind speed above the wagons.

$$M = k_1 \cdot \upsilon^2 + k_2 \cdot \upsilon + k_3 \qquad \textbf{Equation S1}$$

Where:
M = Mass emissions rate of coal dust (g/km/ton coal)
$k_1 = 0.378 \cdot 10^{-4}$ ($h^2 \cdot$ g/ton/km^3)
$k_2 = -0.126 \cdot 10^{-3}$ ($h \cdot$ g/ton/km^2)
$k_3 = 0.63 \cdot 10^{-4}$ (g/km/ton)
υ = air velocity over surface of the train (km/h)

The air velocity over the surface of the train is dependent on both the wind speed and the travelling speed of the train. In this study the air speed over the surface of the train was defined as an uncertain parameter. By using equation S1 the coal loss for different air velocities could be calculated. In conditions with no wind and a relatively low speed (40 km/h) this leads to a loss of 0.055 g/km/ton. A train travelling at high speed (90 km/h) in strong winds, could experience an air velocity of up to 120 km/h, which would result in a 0.53 g/km/ton. By multiplying this loss by the transport distance the total coal loss (in gram/ton) during transport was determined.

Uncertainty in distances

Uncertainty in these distances may be estimated as follows: First, we assume that latitudes and longitudes of mines and plants are uniformly distributed with means μ and widths σ. We then assume that the centroids of the regions (e.g. ZIP codes) reported by the U.S. Census Bureau are estimators of the mean latitudes and longitudes, and the square roots of the land areas of these regions are estimators of σ. Assuming these distributions are both uniform, the distance between a mine i and plant j will also be uniform, i.e.

$$d_{ij} \sim U(g(\mu_i,\mu_j)-\Sigma_{ij}, g(\mu_i,\mu_j)+\Sigma_{ij}) \qquad \textbf{Equation S2}$$

where $g(\mu_i, \mu_j)$ is the average Google road distance between the centroids of the regions in which the mine and plant reside, and $\Sigma_{ij} = A_i^{1/2} + A_j^{1/2}$ is the half-width of the distribution. Multiplication of d_{ij} by the corresponding mass of coal transported yields the total transportation from mine to plant. This, in turn, is multiplied by an emission factor that models the impacts associated with the round trip fuel usage of the train. In the U.S., coal is transported via unit trains, which are the most fuel efficient type of rail transport. In the absence of data for an emission factor (e.g. kg CO_2eq/tonne/km coal transport), we recommend the use of the Ecoinvent model of freight rail transport. An Ecoinvent-based model for the emissions associated with transport may be expressed as a random number using Crystal Ball.

Use phase

In order to calculate the emissions during the use phase, the fuel efficiency of the power plants and carbon content of the coal are needed. The carbon content depends on the state in which the coal is mined and the type of coal. This carbon content is also uncertain a standard coefficient of variation (CV) of 1% was assumed, based on coal analyses by Roy et al (Roy et al. 2009). The same CV was applied to coal from all states.

Background processes

Background processes relate to:

- Mine construction and decommissioning
- Provision, maintenance and disposal of locomotives, wagons, barges and ships, railway tracks and port infrastructure
- Provision of the diesel for transport to a local storage facility
- Building and decommissioning of power plants

The CO_2 and CH_4 emissions that took place during these background processes were eventually related to the functional unit. Several uncertain background parameters can be grouped to generate (i.e.) one uncertain CO_2 emission factor for all background processes related to mining or different modes of transport. Equations S3-S8 show the calculations that were used to derive these parameters. By using Monte Carlo simulation (1000 simulation runs) the distributions of the calculated parameters were derived. The resulting means and their distributions are displayed in Table S3.

$$EF_{(g,i)} = (GHG_{construction(g,i)} + GHG_{decommissioning(g,i)}) \cdot Mine_i$$ **Equation S3**

EF = Emission factor (kg GHG/kg coal)
g = Type of greenhouse gas (CO_2 or CH_4)
i = Type of mine (surface or underground)
$GHG_{construction}$ = GHG emissions during construction of mine (kg GHG/mine)
$GHG_{decommissioning}$ = GHG emissions during decommissioning of mine (kg GHG/mine)
Mine = Amount of mine that is needed to produce 1 kg of coal (mine/kg coal)

$$EF_{train(g)} = \sum GHG_{process(i,g)} \cdot Process_{(i)}$$ **Equation S4**

EF_{train} = Emission factor (kg GHG/tkm)
g = Type of greenhouse gas (CO_2 or CH_4)
$GHG_{process}$ = Greenhouse gas emissions during process (kg GHG/process)
i = Type of process (Construction locomotive, Construction goods wagon, Maintenance locomotive, Maintenance goods wagon, Disposal locomotive, Construction railway track, Operation and maintenance railway track, Disposal railway track, Diesel at regional storage)
Process = Amount of process needed that is needed for 1 tkm (process/tkm)

$$EF_{truck(g)} = \sum GHG_{process(i,g)} \cdot Process_{(i)}$$ **Equation S5**

EF_{truck} = Emission factor (kg GHG/tkm)
g = Type of greenhouse gas (CO_2 or CH_4)
$GHG_{process}$ = Greenhouse gas emissions during process (kg GHG/process)
i = Type of process (Construction lorry, Operation lorry, Maintenance lorry, Disposal lorry, Construction of road, Operation and maintenance of the road, Disposal road, Diesel at regional storage)
Process = Amount of process needed that is needed for 1 tkm (process/tkm)

$$EF_{barge(g)} = \sum GHG_{process(i,g)} \cdot Process_{(i)}$$ **Equation S6**

EF_{barge} = Emission factor (kg GHG/tkm)
g = Type of greenhouse gas (CO_2 or CH_4)
$GHG_{process}$ = Greenhouse gas emissions during process (kg GHG/process)
i = Type of process (Construction barge, Maintenance barge, Construction ports, Operation and maintenance ports, Construction of canals, Operation and maintenance of canals, Diesel at regional storage)
Process = Amount of process needed that is needed for 1 tkm (process/tkm)

$$EF_{freight\ ship(g)} = \sum GHG_{process(i,g)} \cdot Process_{(i)}$$ **Equation S7**

$EF_{freight\ ship}$ = Emission factor (kg GHG/tkm)
g = Type of greenhouse gas (CO_2 or CH_4)
$GHG_{process}$ = Greenhouse gas emissions during process (kg GHG/process)
i = Type of process (Construction freight ship, Maintenance freight ship, Construction ports, Operation and maintenance ports, Diesel at regional storage)
Process = Amount of process needed that is needed for 1 tkm (process/tkm)

$$EF_{liquid\ fuel(i)} = Carboncontent_{(i)} \cdot Density_{(i)} \cdot 44/12$$ **Equation S8**

$EF_{liquid\ fuel}$ = Emission factor (kg CO_2/l fuel)
i = Type of fuel (Diesel, Gasoline or Residual)
Carboncontent = Carbon content of the fuel (kg C/kg fuel)
Density = Density of the fuel (kg fuel/l)
44/12 = Conversion factor from kg C to kg CO_2

TABLE S3 Parameters and distributions for background processes

Parameter	Unit	Type of distribution	Geometric mean and geometric SD	Calculated from source
CO_2 emissions for construction and decommissioning of a surface mine	kg CO_2/kg coal	Lognormal	$1.6 \cdot 10^{-2}$ [1.03]	(Dones et al. 2007b)
CO_2 emissions for construction and decommissioning of an underground mine	kg CO_2/kg coal	Lognormal	$3.8 \cdot 10^{-3}$ [1.04]	(Dones et al. 2007b)
CH_4 emissions for construction and decommissioning of a surface mine	kg CH_4/kg coal	Lognormal	$5.2 \cdot 10^{-6}$ [1.23]	(Dones et al. 2007b)
CH_4 emissions for construction and decommissioning of an underground mine	kg CH_4/kg coal	Lognormal	$5.7 \cdot 10^{-6}$ [1.22]	(Dones et al. 2007b)
Background CO_2 emissions for transport by train	kg CO_2/tkm	Lognormal	$1.1 \cdot 10^{-2}$ [1.07]	(Spielmann et al. 2007)
Background CO_2 emissions for transport by truck	kg CO_2/tkm	Lognormal	$1.5 \cdot 10^{-1}$ [1.23]	(Spielmann et al. 2007)
Background CO_2 emissions for transport by barge	kg CO_2/tkm	Lognormal	$1.5 \cdot 10^{-2}$ [1.18]	(Spielmann et al. 2007)
Background CO_2 emissions for transport by transoceanic freight ship	kg CO_2/tkm	Lognormal	$2.8 \cdot 10^{-3}$ [1.18]	(Spielmann et al. 2007)
Background CH_4 emissions for transport by train	kg CH_4/tkm	Lognormal	$2.4 \cdot 10^{-5}$ [1.14]	(Spielmann et al. 2007)
Background CH_4 emissions for transport by truck	kg CH_4/tkm	Lognormal	$5.6 \cdot 10^{-4}$ [1.21]	(Spielmann et al. 2007)
Background CH_4 emissions for transport by barge	kg CH_4/tkm	Lognormal	$3.5 \cdot 10^{-5}$ [1.19]	(Spielmann et al. 2007)

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Background CH_4 emissions for transport by transoceanic freight ship	kg CH_4/tkm	Lognormal	$7.8 \cdot 10^{-6}$ [1.31]	(Spielmann et al. 2007)
CO_2 emission for complete combustion of gasoline	kg CO_2/l	Lognormal	2.4 [1.03]	(EIA 1994)
CO_2 emission for complete combustion of diesel	kg CO_2/l	Lognormal	2.65 [1.02]	(EIA 1994)
CO_2 emission for complete combustion of residual fuel	kg CO_2/l	Lognormal	3.1 [1.04]	(EIA 1994)
CO_2 Emissions from electricity use	kg CO_2/ kWh	Lognormal	$4.6 \cdot 10^{-1}$ [1.38]	(Jaramillo et al. 2007)

Additional analyses

In addition to the analyses presented in the main manuscript we have also performed some additional analyses, for which the results are presented in this section. These analyses include the relative contribution of upstream processes for 3 time horizons, the variability and uncertainty per NERC region, an analysis of the temporal variability in plant efficiencies and an additional plant-mine pair analysis treating the unique mine-plant pairs (rather than the different power plants) as the unit of comparison.

Relative contribution of upstream processes

Figure S1 shows the relative contribution of upstream processes to the total life cycle greenhouse gas emissions for each individual power plant for 20, 100 and 500 year time horizons. Median percentages vary from 2.3% (minimum, 500 year time horizon) to 48.3% (maximum, 20 year time horizon). It should be noted however that the value of 48.3% is exceptionally large, the second highest upstream contribution was 27.0%. The reason for the relatively high upstream emissions for this particular plant is that all of its coal was transported by truck over a distance of approximately 1800 km, which results in very high transport emissions.

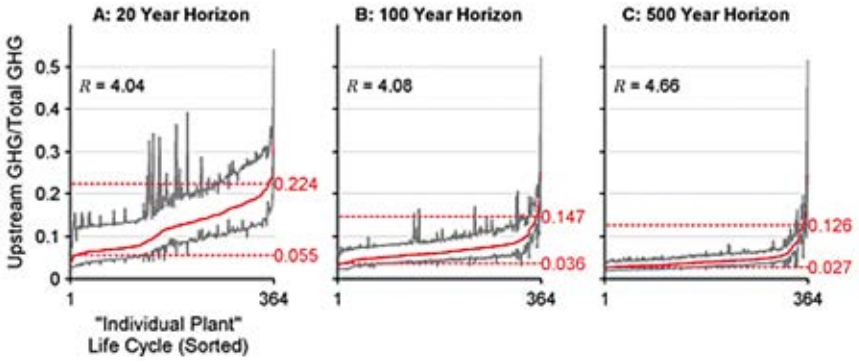

FIGURE S1 Upstream greenhouse gas emissions expressed as a fraction of total life cycle greenhouse gas emissions. Red solid lines illustrate average fractions; gray lines illustrate the 95% intervals. R is a quotient of the 97.5th and 2.5th percentiles (also displayed by the red dashed lines) of the median fractions of the upstream emissions – analogous to r for life cycle emissions.

Uncertainty and variability by NERC region

In Figure S2 we present weighted average life cycle GHG emissions for each North American Electric Reliability Corporation (NERC) region. Weighted average life cycle GHG emissions varied by about 7% among the NERC regions. Our estimates are generally lower, albeit slightly, than those reported by Ecoinvent(Dones et al. 2007b), with the exception of the FRCC region. The Ecoinvent database however is based on 2004 eGRID data instead of the 2009 EIA data we have used, which results in different net efficiencies reported by Ecoinvent. The ranking among different NERC regions, however, is the same. The MRO and FRCC regions have the highest and lowest life cycle GHG emissions respectively. Regional differences in life cycle GHG emissions result primarily from plant efficiencies in those regions.

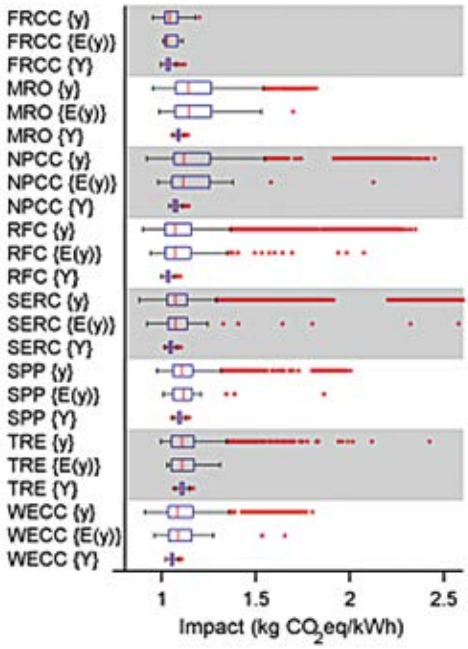

FIGURE S2 Effects of variability and uncertainty in U.S. NERC Regions. Sets of MC-generated GHG emissions resulting from MC simulations of all life cycles terminating in a NERC Region are denoted by {y}. Sets of the average GHG emissions resulting from all life cycles terminating in a NERC Region are denoted by {E(y)}. Sets of MC generated GHG emissions associated with the generation-weighted footprints of each region are denoted by {Y}. The sets {Y} illustrate the effect of uncertainty, whereas the sets {E(Y)} illustrate the effect of variability. The near equality of the interquartile distances among {E(y)} and {y} in each region demonstrates that variability is the primary cause of the range of life cycle emissions for coal power in each NERC Region. Plants per region: FRCC: 9; MRO: 47; NPCC: 15; RFC: 123; SERC: 114; SPP: 29; TRE: 13; WECC: 44.

Temporal variability in power plant efficiencies

In Figure S3 we demonstrate that the distribution of power plant efficiencies has remained fairly stable over a three year time period (2009-2011). Since power plant efficiency was the major contributor to the variability in emissions we expect the overall variability in the US carbon footprint to be fairly stable over time, thereby justifying our choice not to include this type of variability more explicitly in our analysis.

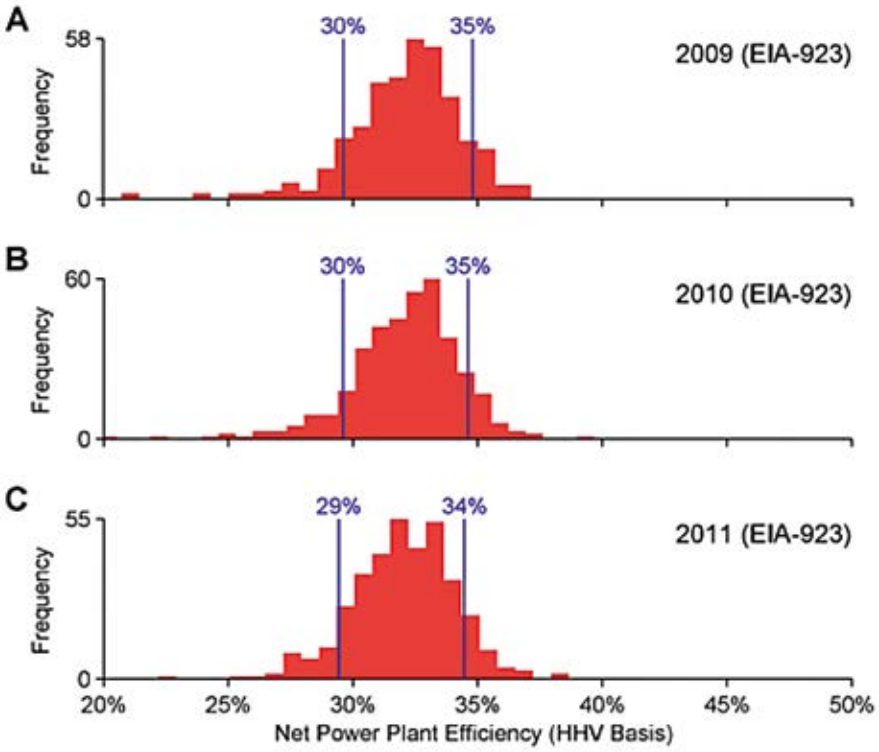

FIGURE S3 Efficiencies of U.S. coal fired power plants calculated from the EIA 923 Electricity Data File. Blue lines represent the 10th and 90th percentiles. The distributions of the efficiencies of the plants are essentially invariant with time.

PLANT-MINE PAIR ANALYSIS

In addition to the simulations described in the main text, Monte Carlo simulations were performed for each mine-plant combination, i.e. LCAs defined by system boundaries containing only one mine and one plant. 2295 plant-mine-pairs were analyzed, with the same selection criteria for plants specified in the main text. Results are illustrated in Figure S3A-C for the three main coal types used in the U.S., with rm defining the variability ratio for each "single mine to single plant" life cycle boundary.

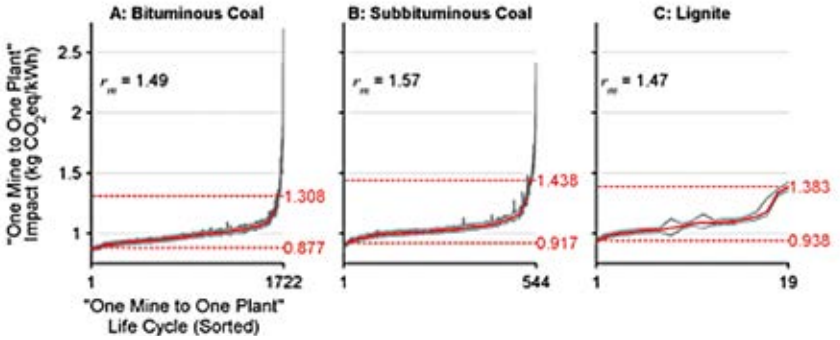

FIGURE S4 Life cycle greenhouse gas emissions for plant-mine pairs, for a) bituminous coal (1,722 plant-mine pairs), b) lignite (19 plant-mine pairs) and c) subbituminous coal (544 plant-mine pairs).

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APPENDIX 2: SUPPORTING INFORMATION FOR:

CHAPTER 3: HOW TO ADDRESS DATA GAPS IN LIFE CYCLE INVENTORIES: A CASE STUDY ON ESTIMATING CO_2 EMISSIONS FROM COAL-FIRED ELECTRICITY PLANTS ON A GLOBAL SCALE

SI 1 Calculation of CO_2 emissions factors from reported data

Estimates of plant level CO_2 emissions were made in a number of different ways, depending on the nature of available data. Firstly, the reported data had to meet at least one of the following criteria in order to be used:

- Emissions factors in kg CO_2/kWh were directly reported.
- Plant-level CO_2 emissions (kg) and net electricity generation (kWh) were reported
- Carbon content of the coal consumed (kg CO_2/MJ) and the net generation efficiency were reported

For European plants CO_2 emissions factors were reported directly [1]. For the US, CO_2 emissions factors were calculated based on the coal use and net electricity generation in a previous study by Steinmann et al. [2] US CO_2 emissions factors were adopted directly from that study. For the majority of the remaining data sources (plants from India, South Africa, China, Hong Kong and Bulgaria) [3-6], total emissions and net generation were available, which were used to estimate emissions factor. The Australian Energy Market Operator (AEMO) reports net generation efficiency (HHV) and the carbon content of the coal for Australian plants [7].

SI 2 Exploratory Data Analysis

The inverse of the emissions factors of all plants and the individual predictors were plotted against each other (Figure S1) to explore the relationships between the predictor variables and the response variable. Since the distribution of the predictors is skewed, a log transformation was tried out for all variables (except the fuel type). All possible combinations of the log-transformed and non-transformed predictors were fitted to determine the optimal combination of predictors (see main manuscript for details). The model with only log-transformed variables (apart from fuel type) was the best model. Subsequently the variance inflation factors (VIFs) for this combination of predictors were checked (Table S1), note the VIFs of the model with capacity factor as additional predictors are also reported in Table S1. All VIFs were below 2, indicating only limited multi-collinearity in the data.

SI 3 Analysis of the relative errors in the model fit

Figure S2 shows the relative error in the cross-validated training set (311 plants) and in the test set (133 plants) for both the multiple linear and the local linear regression models.

If both training and test sets are considered simultaneously for the multiple regression model, there are 19 plants for which the relative error is larger than 20% (5 over-, 14 underestimation). Without any other knowledge about a plant's characteristics this means that there is approximately 4.3% (19/444) chance of over or underestimating the emissions by 20%. Looking at the individual predictors, we can see that if the plant is older than 30 years this risk is 5.1% (13/274), when the capacity is smaller than 1000 MW this chance is raised to 7% (16 out of 243 plants), while a steam pressure below 125 Bar will likely result in a higher chance of over or underestimation, 11.6% or 15 out of 129 plants. Of the plants that have all three conditions combined, 92 in total, there are 12 plants (13.0%) with a relative error larger than 20%.

SI 4 Temporal variability of annual average emissions factors (US plants)

The annual average emissions factors for the 310 US coal plants (Figure S6) show an average difference of 3.5% (as a percentage of the mean) between the highest and the lowest reported values over a time period of 3 years. The largest ranges in emissions factors are observed for plants with the highest average emission factors over this time period. The four plants with an average emissions factor > 1.5 kg CO_2/kWh show an average difference of 33% between the extreme values, while the remaining 306 plants have an average difference of 3.1%.

SI 5 Including the capacity factor as additional predictor

The effect of adding the power plant's capacity factor as sixth predictor was analyzed. Model fitting and validation was done via the same methodology as for the models with five predictors. Although generally not available for all coal plants, the capacity factor was found to be one of the most important factors that determine the net operating efficiency of a power plant[8]. The capacity factor could be calculated for 420 plants in the full set. The predictive power of both regression models improved after introducing the capacity factor as additional predictor, R2 values, based on the test set, increased from 0.49 to 0.56 for the global regression and from 0.61 to 0.64 for the local linear regression. Both models with capacity factors (Figure S6) underestimate the emissions factors for power plants with a reported emission factor above 1.5 kg CO_2/kWh, this underestimation is stronger for the parametric multiple regression than for the local linear regression. From Figure S3 (panels K and L), it is evident that lower relative errors are associated with plants having capacity factors higher than 50%.

SI 6 Alternate regression models implemented

A number of alternate non-parametric regression models were implemented to compare against the local linear regression model used in this study. A simple nearest neighbors approach was tested[9]. Kernel regression using a Nadaraya-Watson average with a Gaussian kernel was also implemented[9]. Additionally, local linear regression on log-transformed values was tested. Local quadratic regression[10] was also tested, but this method yielded singularities during the computation of the optimal Gaussian weight function coefficient, and hence this method was not used. Local polynomial regression

(with polynomial order >2) was not tested because the number of variables being used in the regression is not small, which would result in a large number of total variables (including interaction terms) being required for polynomial regression. This would also likely increase the risk of overfitting. Of all the non-parametric regression models tested, the local linear regression using non transformed predictors showed the best performance with the lowest mean square error and R^2 for the training data set. The training and test set R^2 values for the alternate models are presented in Table S6.In addition, partial least squares regression was also tested[9], as an example of a data reduction regression method. However, this method did not yield results that were significantly different from the ordinary least squares approach. The training and test set R^2 values for this approach is also presented in Table S6.

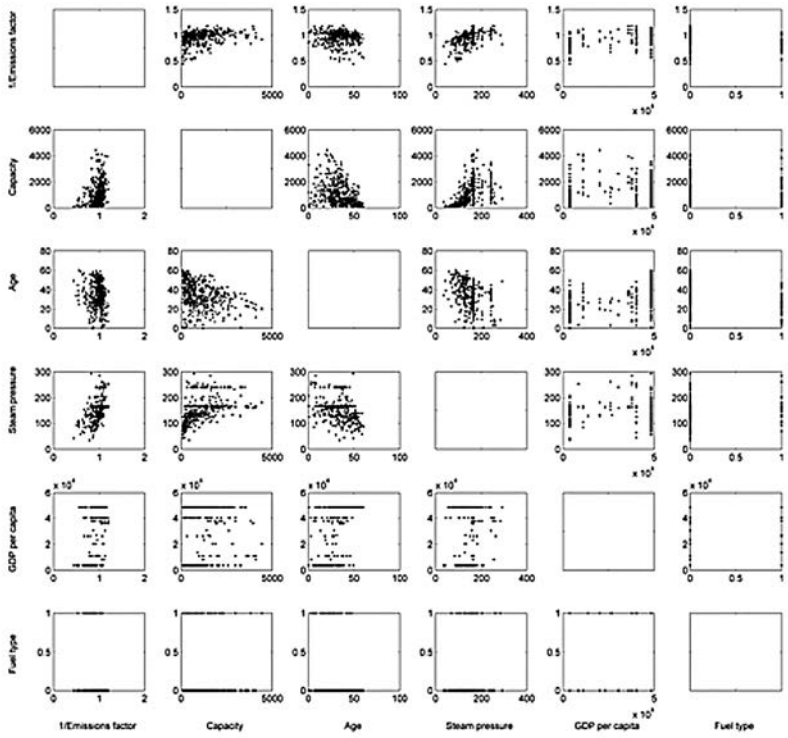

FIGURE S1 Comparison between model predictors and response variables.

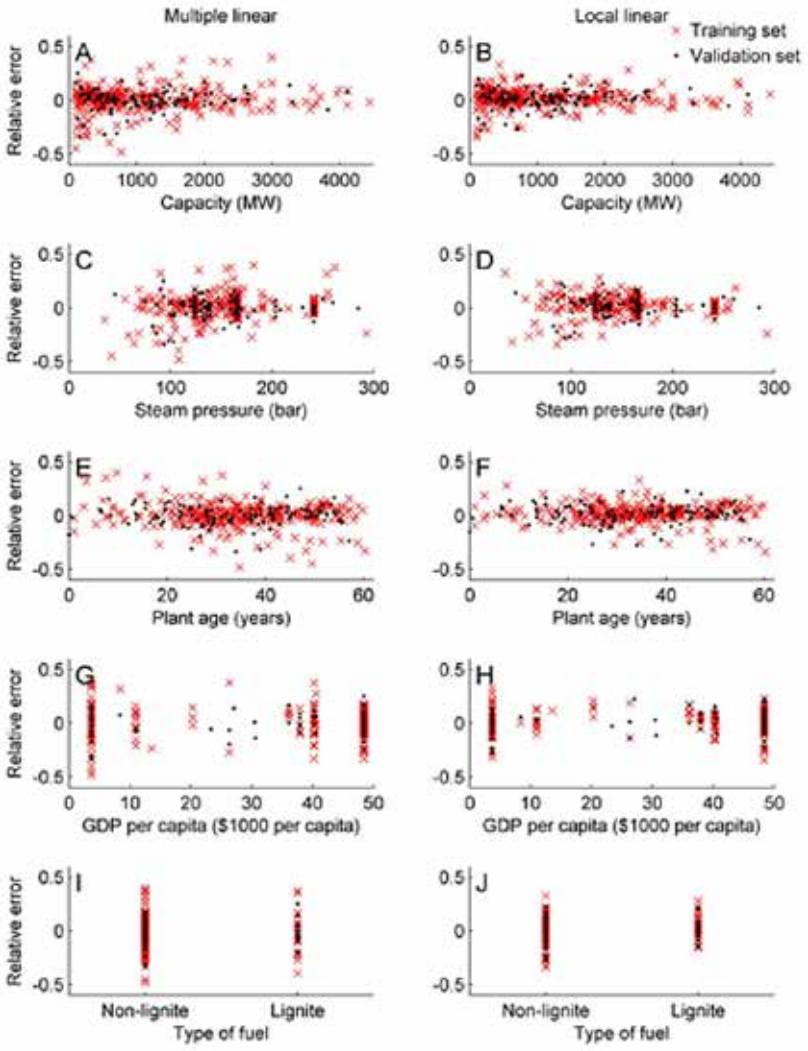

FIGURE S2 Relative errors of the multiple regression model (A, C, E, G, I) and local linear regression model (B, D, F, H, J) without capacity factor plotted against predictor variables

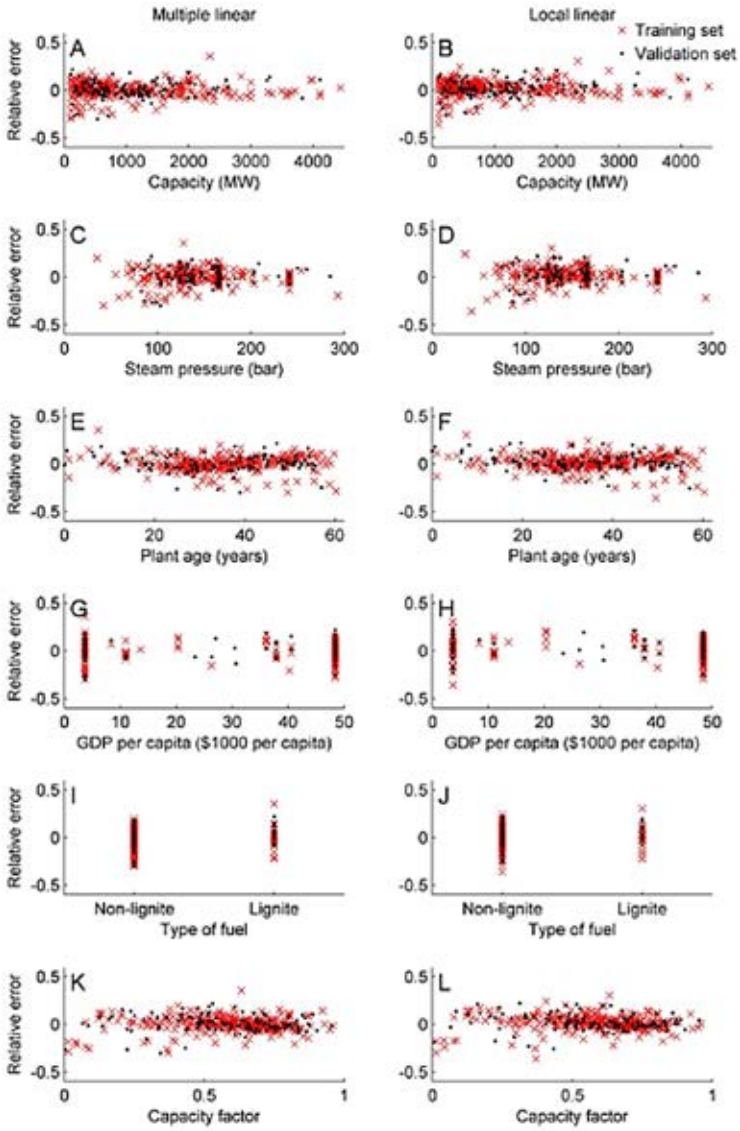

FIGURE S3 Relative errors of the multiple regression model (A, C, E, G, I, K) and local linear regression model (B, D, F, H, J, L) with capacity factor plotted against predictor variables

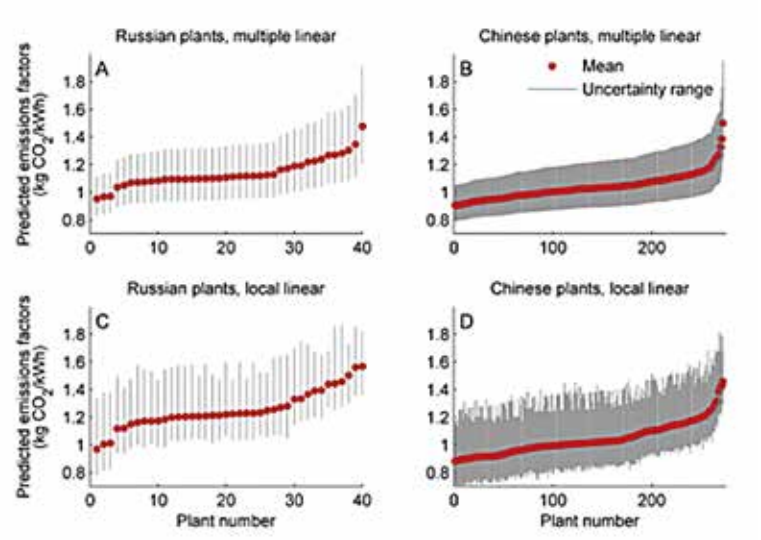

FIGURE S4 Predictions of emissions factors (mean and 95% prediction intervals) of coal power plants in China and Russia from multiple regression model and the local linear regression model. Power plants are sorted from low to high by predicted CO_2 emissions factor.

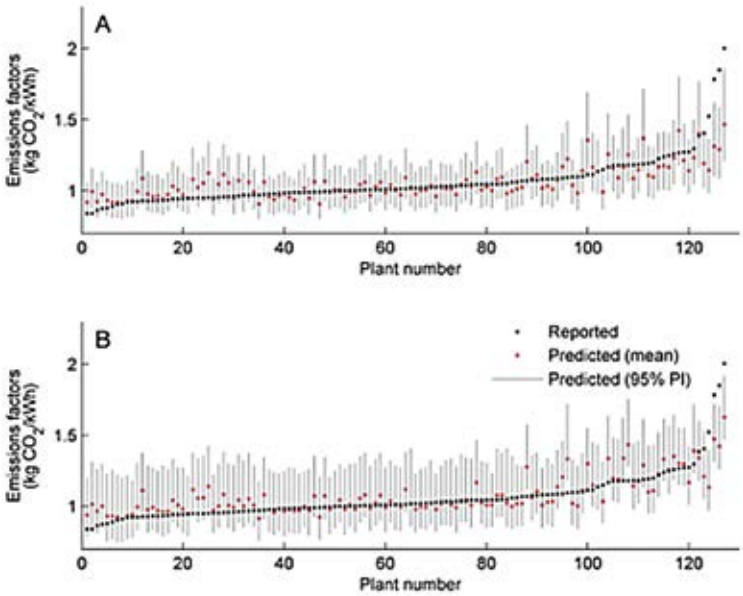

FIGURE S5 (A) Multiple regression and (B) local linear regression model predictions and 95% intervals for the 30% test set with capacity factor (127 power plants). Power plants are sorted from low to high by reported CO_2 emissions factor.

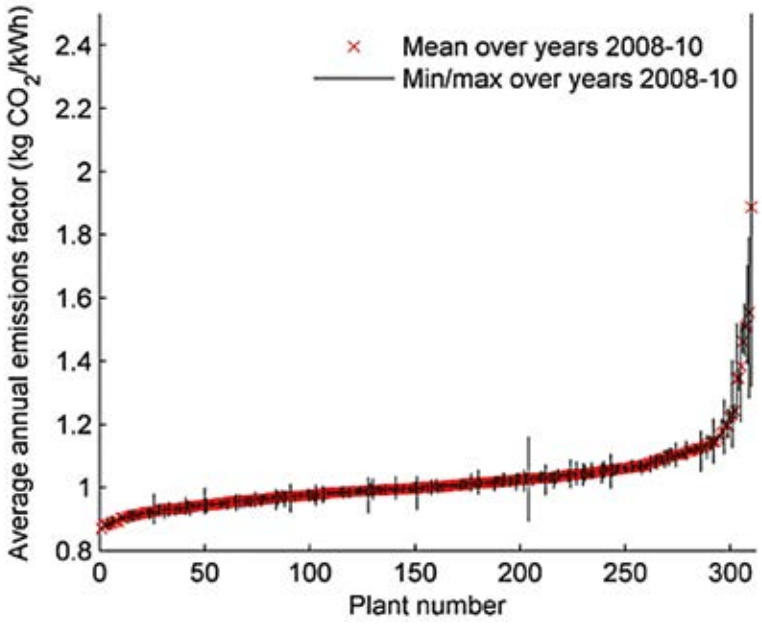

FIGURE S6 Analysis of temporal variability in emission factors for US coal power plants. The figure displays the mean emission factor for the years 2008-2010 and the minimum and maximum of these years. Emission factors are essentially invariable over time for the most plants, except for the plants with the highest emission factors.

Supplementary tables

TABLE S1 Variance inflation factors of predictors

Predictor	VIF (log-transformed model without capacity factor)	VIF (log-transformed model with capacity factor)
log [capacity (in MW)]	1.68	1.81
log [age + 1 (in years)]	1.39	1.46
log [steam pressure (in bar)]	1.95	1.98
log [GDP (in $PPP) per capita]	1.29	1.32
fuel type (1=lignite, 0=non-lignite)	1.09	1.10
Capacity factor	NA	1.41

TABLE S2 See Excel file "Table S2 all model coefficients.xlsx" (available via Journal website)

TABLE S3 Predictor coefficients for the normalized multiple regression models with and without capacity factor

Predictor	Normalized model without capacity factor	Normalized model with capacity factor
Intercept	-2.67E-01	-2.11E-01
log [capacity (in MW)]	1.84E-01	1.58E-01
log [age + 1 (in years)]	-1.31E-01	-4.74E-02
log [steam pressure (in bar)]	7.49E-01	5.76E-01
log [GDP (in $PPP) per capita]	5.39E-01	5.30E-01
fuel type (1=lignite, 0=non-lignite)	-1.49E-01	-1.51E-01
Capacity factor	NA	9.56E-02

TABLE S4 Predictor coefficients for the multiple regression models with and without capacity factor and for the fit with equal amounts of US and non-US plants

Predictor	Model without capacity factor	Model with equal number of US and non-US plants	Model with capacity factor
Intercept	-3.65E-01	-2.62E-01	-3.38E-01
log [capacity (in MW)]	6.38E-02	9.04E-02	5.49E-02
log [age + 1 (in years)]	-8.69E-02	-1.72E-01	-3.14E-02
log [steam pressure (in bar)]	3.46E-01	2.87E-01	2.67E-02
log [GDP (in $PPP) per capita]	1.20E-01	1.37E-01	1.17E-01
fuel type (1=lignite, 0=non-lignite)	-1.49E-01	-1.72E-01	-1.52E-01
Capacity factor	NA	NA	1.66E-01

TABLE S5 See Excel file "Table S5 predictions 764 power plants.xlsx" (available via Journal website)

TABLE S6 Summary of R^2 values for alternate regression models implemented

Model/method	Training set R^2	Test set R^2
k-Nearest neighbors	0.44	0.59
Kernel regression	0.47	0.58
Local linear regression with log transform	0.53	0.54
Partial least squares regression	0.48	0.49

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APPENDIX 3, SUPPORTING INFORMATION FOR:

CHAPTER 4: ESTIMATING THE GREENHOUSE GAS BALANCE OF INDIVIDUAL GAS-FIRED AND OIL-FIRED ELECTRICITY PLANTS ON A GLOBAL SCALE.

TABLE S1 Predictor variables and ranges in and the WEPP database for natural gas fired and oil fired power plants above 100 MW.

Variable	Unit	Total in WEPP database gas fired power plants[A]	Total in WEPP database oil fired power plants[A]
Capacity	MW	100-4800	100-5600
Age	Years	1-71	1-59
Technology Type[B]	-	SC or CC	SC or CC
Type of fuel[C]	-	Natural gas	Oil

[A] Platts (Platts 2012).
[B] SC plants are modeled as 1, while CC plants were assigned a value of 0.
[C] Oil plants are modeled as 1, while natural gas plants were assigned a value of 0.

TABLE S2 Variance inflation factors for each of the predictors Log Capacity, Log Age, fuel type and technology type with all others.

log Capacity	log Age	Technology type	Fuel type
1.05	1.95	2.19	1.43

TABLE S3 Variance inflation factors for each of the predictors Log Capacity, Log Age, fuel type, technology type and log Capacity factor with all others.

log Capacity	log Age	Technology type	Fuel type	log Capacity factor
1.07	2.24	2.78	1.73	1.64

TABLE S4 Plant data training set, sorted from lowest GHG emission factor to highest.

	Capacity	Age	Capacity factor	Country	Oil	Emission factor
1	1147.5	2	0.803	India	FALSE	0.360
2	311	7	0.579	Brazil	FALSE	0.386
3	384	5	0.205	Morocco	FALSE	0.407
4	370	3	0.802	India	FALSE	0.411
5	464	2	0.815	India	FALSE	0.439
6	2728	14	0.259	Hong Kong	FALSE	0.457
7	540	1	0.407	USA	FALSE	0.460
8	400	5	0.397	USA	FALSE	0.464
9	254	7	0.503	USA	FALSE	0.465
10	939	12	0.485	USA	FALSE	0.466
11	655	13.21	0.630	India	FALSE	0.468
12	1132	10	0.610	USA	FALSE	0.468
13	820	17.99	0.725	India	FALSE	0.469
14	1240	7	0.752	USA	FALSE	0.470
15	898	10	0.341	USA	FALSE	0.470
16	580	1	0.436	USA	FALSE	0.470
17	300	4	0.648	USA	FALSE	0.471
18	620	10	0.516	USA	FALSE	0.472
19	750	7	0.645	USA	FALSE	0.473
20	540	11.63	0.562	USA	FALSE	0.474
21	1260	9	0.503	USA	FALSE	0.474
22	520	13.65	0.628	USA	FALSE	0.475
23	510	12	0.418	USA	FALSE	0.475
24	1806	7.59	0.606	USA	FALSE	0.475
25	430	11.67	0.815	India	FALSE	0.475
26	619.4	10	0.707	USA	FALSE	0.475
27	530	2	0.646	USA	FALSE	0.476
28	248	8	0.279	USA	FALSE	0.476
29	1130	11	0.673	USA	FALSE	0.476
30	530	9.57	0.688	USA	FALSE	0.476
31	1240	8	0.460	USA	FALSE	0.476
32	1200	8	0.686	USA	FALSE	0.477
33	1022	9	0.147	USA	FALSE	0.477
34	1880	8.5	0.743	USA	FALSE	0.477
35	559	6.59	0.440	USA	FALSE	0.477
36	480	8	0.204	USA	FALSE	0.478
37	525	9	0.456	USA	FALSE	0.479
38	530	3	0.566	USA	FALSE	0.479
39	515	10	0.547	USA	FALSE	0.479
40	605	7	0.302	USA	FALSE	0.479
41	1309.8	6	0.526	USA	FALSE	0.479
42	510	1	0.441	USA	FALSE	0.480
43	545	11	0.745	USA	FALSE	0.480
44	1470	1.75		Singapore	FALSE	0.480

45	596	10	0.589	USA	FALSE	0.480
46	730	9	0.600	USA	FALSE	0.481
47	370	11	0.743	USA	FALSE	0.482
48	545	10	0.564	USA	FALSE	0.482
49	575	7	0.472	USA	FALSE	0.482
50	315.2	4.94	0.749	India	FALSE	0.482
51	1083	9	0.435	USA	FALSE	0.482
52	755	7	0.440	USA	FALSE	0.482
53	1158	5.5	0.224	USA	FALSE	0.482
54	1032	10	0.472	USA	FALSE	0.483
55	1169	5	0.554	USA	FALSE	0.484
56	939	10	0.201	USA	FALSE	0.485
57	503	8	0.291	USA	FALSE	0.485
58	287	4	0.660	Mexico	FALSE	0.485
59	210	4		Australia	FALSE	0.485
60	610	10	0.579	USA	FALSE	0.486
61	348.9	3	0.735	USA	FALSE	0.486
62	900	9	0.341	USA	FALSE	0.486
63	833	10	0.684	USA	FALSE	0.486
64	508	10	0.767	USA	FALSE	0.487
65	810	9	0.459	USA	FALSE	0.487
66	591	9	0.242	USA	FALSE	0.487
67	870	9	0.489	USA	FALSE	0.487
68	559	9.54	0.463	USA	FALSE	0.487
69	520	6	0.766	USA	FALSE	0.487
70	2200	9	0.373	USA	FALSE	0.488
71	330.38	8.63	0.784	India	FALSE	0.488
72	241	17	0.329	USA	FALSE	0.488
73	795	10	0.313	USA	FALSE	0.488
74	265	12	0.680	USA	FALSE	0.489
75	650	6	0.315	USA	FALSE	0.489
76	500	12.68	0.551	USA	FALSE	0.490
77	850	9	0.326	USA	FALSE	0.490
78	568	5	0.372	USA	FALSE	0.490
79	520	9	0.424	USA	FALSE	0.490
80	771	11	0.551	USA	FALSE	0.490
81	520	11	0.232	USA	FALSE	0.491
82	633.2	11	0.232	USA	FALSE	0.491
83	272	12	0.445	USA	FALSE	0.491
84	717.2	6.22	0.653	India	FALSE	0.491
85	546	10	0.242	USA	FALSE	0.491
86	385	11		Australia	FALSE	0.492
87	1840	8.41	0.429	USA	FALSE	0.492
88	290	5	0.276	USA	FALSE	0.492
89	983	2	0.388	Mexico	FALSE	0.492
90	939	11	0.396	USA	FALSE	0.492
91	500	12	0.628	USA	FALSE	0.493

92	840	10	0.717	USA	FALSE	0.493
93	1280	3	0.651	USA	FALSE	0.493
94	570	11	0.418	USA	FALSE	0.493
95	182.9	14	0.711	India	FALSE	0.493
96	1280	10	0.260	USA	FALSE	0.494
97	2045	12.55	0.606	USA	FALSE	0.495
98	550	9	0.210	USA	FALSE	0.495
99	570	10	0.235	USA	FALSE	0.495
100	578	8	0.774	USA	FALSE	0.495
101	520	11	0.335	USA	FALSE	0.495
102	640	9	0.319	USA	FALSE	0.495
103	574	8	0.713	USA	FALSE	0.496
104	658	10	0.335	USA	FALSE	0.496
105	1143	8	0.193	USA	FALSE	0.497
106	150	9.67	0.730	India	FALSE	0.497
107	570	10	0.219	USA	FALSE	0.497
108	610	4	0.149	USA	FALSE	0.497
109	614	11.97	0.144	USA	FALSE	0.499
110	1060	10	0.385	USA	FALSE	0.499
111	564.5	6.51	0.484	USA	FALSE	0.500
112	521	12.67	0.558	USA	FALSE	0.500
113	2120	9.5	0.592	USA	FALSE	0.501
114	119.8	6	0.781	India	FALSE	0.501
115	1250	10	0.273	USA	FALSE	0.502
116	945	8	0.523	USA	FALSE	0.503
117	1370	9	0.264	USA	FALSE	0.503
118	532	10	0.356	USA	FALSE	0.503
119	595	3	0.396	USA	FALSE	0.503
120	1052	6.5	0.503	USA	FALSE	0.504
121	584	8	0.521	USA	FALSE	0.505
122	2348	9	0.157	USA	FALSE	0.505
123	720	8	0.579	USA	FALSE	0.505
124	646	11	0.120	USA	FALSE	0.506
125	656	18.31	0.662	India	FALSE	0.506
126	585	10.55	0.155	USA	FALSE	0.507
127	816	10	0.184	USA	FALSE	0.507
128	588	10.1	0.263	USA	FALSE	0.507
129	677	2	0.353	USA	FALSE	0.507
130	240	11	0.342	USA	FALSE	0.508
131	737	11.2	0.424	USA	FALSE	0.511
132	1000	12	0.490	USA	FALSE	0.511
133	292	10	0.202	USA	FALSE	0.512
134	594	9	0.128	USA	FALSE	0.513
135	256	8	0.689	USA	FALSE	0.513
136	780	6.5	0.600	Italy	FALSE	0.513
137	515	9.7	0.269	USA	FALSE	0.514
138	562	11	0.164	USA	FALSE	0.515

139	912	24.66	0.676	India	FALSE	0.515
140	488	10	0.534	USA	FALSE	0.516
141	413	21.64	0.659	India	FALSE	0.516
142	1000	11	0.243	USA	FALSE	0.516
143	1650	11.17	0.285	USA	FALSE	0.516
144	1783.8	9	0.531	USA	FALSE	0.517
145	584.3	10	0.487	USA	FALSE	0.517
146	511	3	0.133	USA	FALSE	0.518
147	672	7.63	0.212	USA	FALSE	0.518
148	514	4	0.690	USA	FALSE	0.519
149	300	4	0.452	USA	FALSE	0.519
150	679	5	0.074	USA	FALSE	0.519
151	636	11	0.171	USA	FALSE	0.520
152	1000	11	0.263	USA	FALSE	0.521
153	569	8	0.398	USA	FALSE	0.522
154	120	7	0.612	USA	FALSE	0.523
155	652	21.69	0.732	India	FALSE	0.526
156	867.9	21.1	0.438	USA	FALSE	0.527
157	420	10	0.473	USA	FALSE	0.529
158	435	4		Australia	FALSE	0.529
159	164	18	0.738	USA	FALSE	0.529
160	1478	10.88	0.572	USA	FALSE	0.529
161	1249.2	14.2	0.532	USA	FALSE	0.529
162	258	6	0.494	USA	FALSE	0.530
163	290	3	0.239	USA	FALSE	0.531
164	256	15	0.541	USA	FALSE	0.532
165	445	1.63	0.605	India	FALSE	0.532
166	570	9	0.164	USA	FALSE	0.535
167	1000	9.36	0.467	USA	FALSE	0.539
168	526	4.5	0.333	USA	FALSE	0.558
169	655	15.21	0.050	India	FALSE	0.558
170	550	10	0.211	USA	FALSE	0.578
171	501	12.33		Australia	FALSE	0.578
172	526	4.5	0.148	USA	FALSE	0.581
173	1030	8.06	0.510	Italy	FALSE	0.596
174	599.56	22.95	0.691	Mexico	FALSE	0.599
175	578	19.55	0.329	USA	FALSE	0.613
176	456	39.5	0.298	USA	FALSE	0.620
177	285	38.6	0.317	USA	FALSE	0.622
178	185	15		Australia	FALSE	0.680
179	1271.8	48.61	0.108	USA	FALSE	0.700
180	282	13		Australia	FALSE	0.709
181	122.5	13	0.772	USA	FALSE	0.712
182	445.5	37	0.221	USA	FALSE	0.713
183	750	39.5	0.485	USA	FALSE	0.718
184	510	10	0.179	USA	FALSE	0.720
185	510	10	0.179	USA	FALSE	0.720

186	613	54.29	0.156	USA	FALSE	0.724
187	654	29.61	0.334	USA	FALSE	0.725
188	519.2	32.02	0.249	USA	FALSE	0.732
189	450	51	0.282	USA	FALSE	0.732
190	314	5	0.154	USA	FALSE	0.732
191	745.8	3.54	0.067	USA	FALSE	0.734
192	1660	31.5	0.185	USA	FALSE	0.738
193	116	15.09	0.616	USA	TRUE	0.740
194	1190	26.46	0.076	USA	FALSE	0.740
195	844.1	46.24	0.327	USA	FALSE	0.741
196	1052.6	31.67	0.214	USA	FALSE	0.741
197	850	9	0.048	USA	FALSE	0.747
198	1960	41.47	0.256	USA	FALSE	0.748
199	1530	41	0.143	USA	FALSE	0.748
200	926.7	46.91	0.196	USA	FALSE	0.750
201	2051.1	41.41	0.267	USA	FALSE	0.752
202	727	40.14	0.093	USA	FALSE	0.752
203	1074	36.6	0.094	USA	FALSE	0.753
204	542.8	41.5	0.362	USA	FALSE	0.757
205	285	48.58	0.372	USA	FALSE	0.760
206	881.5	42.82	0.176	USA	FALSE	0.761
207	328.5	38.87	0.232	USA	FALSE	0.762
208	781.5	38	0.215	USA	FALSE	0.762
209	320	7		Australia	FALSE	0.763
210	983	34.47	0.139	USA	FALSE	0.766
211	504	7		Australia	FALSE	0.767
212	519	4		Australia	FALSE	0.767
213	1042.5	10.81	0.156	USA	FALSE	0.780
214	701.6	47.6	0.172	USA	FALSE	0.780
215	1327.6	43.05	0.238	USA	FALSE	0.797
216	434.4	21.04	0.308	USA	FALSE	0.798
217	383.5	37.35	0.256	USA	FALSE	0.798
218	927.5	40.28	0.079	USA	FALSE	0.804
219	852.3	48.19	0.084	USA	FALSE	0.808
220	900.7	31.97	0.096	USA	FALSE	0.812
221	501	44.15	0.134	USA	FALSE	0.815
222	823.2	44.15	0.107	USA	FALSE	0.815
223	1302.6	47.76	0.039	USA	FALSE	0.818
224	664	5		Australia	FALSE	0.826
225	616	27.05	0.685	Mexico	TRUE	0.830
226	134	39.25	0.499	India	FALSE	0.833
227	148	40.45	0.353	USA	FALSE	0.835
228	320	14	0.822	Mexico	TRUE	0.840
229	632	18	0.635	Mexico	TRUE	0.840
230	619	37.37	0.163	USA	FALSE	0.843
231	406	11.43	0.021	USA	TRUE	0.850
232	680	10	0.124	USA	FALSE	0.877

233	1701	36	0.039	USA	FALSE	0.879
234	490	31.95	0.316	Canada	TRUE	0.880
235	484	27.43	0.339	Mexico	TRUE	0.880
236	750	42.5	0.251	USA	TRUE	0.880
237	172.7	39.71	0.477	USA	FALSE	0.894
238	322	50.47	0.368	USA	TRUE	0.900
239	891	37	0.131	USA	FALSE	0.904
240	1590	35.5	0.123	USA	TRUE	0.930
241	1200	18.54	0.836	Mexico	TRUE	0.940
242	414.7	40	0.003	USA	TRUE	0.940
243	700	18.5	0.529	Mexico	TRUE	0.950
244	882	37	0.009	USA	TRUE	0.950
245	402.1	44	0.169	USA	TRUE	0.950
246	150	11		Australia	FALSE	0.966
247	767.9	44.02	0.027	USA	TRUE	0.970
248	294	11		Australia	FALSE	0.971
249	414	10.65		Australia	TRUE	1.010
250	213.6	36		Australia	FALSE	1.017
251	235.2	33		Australia	FALSE	1.017
252	480	45.25		Australia	FALSE	1.035
253	1112.4	36	0.175	USA	TRUE	1.050
254	326.4	50.5	0.008	USA	TRUE	1.050
255	902	32	0.008	USA	TRUE	1.060
256	117	42	0.577	Mexico	TRUE	1.070
257	150	28.25	0.555	Mexico	TRUE	1.080
258	100	35	0.003	USA	TRUE	1.120
259	212.4	40.75	0.012	USA	TRUE	1.160
260	489.9	43.6	0.007	USA	TRUE	1.170
261	165	34	0.008	USA	TRUE	1.170
262	252	34	0.008	USA	TRUE	1.200
263	104.4	56.44	0.053	USA	TRUE	1.210
264	202.2	34	0.017	USA	TRUE	1.210
265	600	38.33	0.033	Canada	TRUE	1.220
266	567	37.5	0.010	USA	TRUE	1.240
267	126	40.63	0.003	USA	TRUE	1.370
268	1546	27.4	0.645	Mexico	TRUE	1.420
269	846	38.17	0.008	USA	TRUE	1.540
270	782	37	0.007	USA	TRUE	1.740

TABLE S5 Plant data validation set, sorted from carbon footprint to highest GHG emission factor.

	Capacity	Age	Capacity factor	Country	Oil	GHG emission factor
1	375	1	0.670	India	FALSE	0.395
2	184.4	5.7	0.246	India	FALSE	0.440
3	144.5	3.6		Australia	FALSE	0.455
4	819	2.5	0.435	USA	FALSE	0.462
5	3750	2.33	0.645	USA	FALSE	0.463
6	1185.9	5.45	0.543	USA	FALSE	0.464
7	270	11	0.356	USA	FALSE	0.466
8	180	17.33	0.973	India	FALSE	0.467
9	418	10	0.563	USA	FALSE	0.469
10	235	12	0.772	USA	FALSE	0.469
11	287	9	0.280	USA	FALSE	0.470
12	500	6	0.769	USA	FALSE	0.471
13	706	2	0.674	USA	FALSE	0.472
14	525	11	0.686	USA	FALSE	0.475
15	219.4	5.95	0.442	India	FALSE	0.475
16	565	9	0.654	USA	FALSE	0.476
17	712.4	2	0.317	USA	FALSE	0.478
18	896	9	0.534	USA	FALSE	0.478
19	613.4	6.7	0.294	USA	FALSE	0.479
20	852	9	0.260	USA	FALSE	0.480
21	677	9	0.560	USA	FALSE	0.481
22	1240	3.5	0.365	USA	FALSE	0.481
23	1150	8	0.400	USA	FALSE	0.482
24	1240	9	0.535	USA	FALSE	0.483
25	248.5	15	0.467	USA	FALSE	0.484
26	1640	9	0.643	USA	FALSE	0.485
27	1060	10	0.187	USA	FALSE	0.486
28	525	10	0.590	USA	FALSE	0.487
29	759	9	0.719	USA	FALSE	0.488
30	900	8	0.704	USA	FALSE	0.488
31	1150	7	0.555	USA	FALSE	0.488
32	939	9	0.371	USA	FALSE	0.488
33	630	3		Australia	FALSE	0.489
34	520	12	0.390	USA	FALSE	0.489
35	520	12	0.551	USA	FALSE	0.489
36	540	8	0.517	USA	FALSE	0.492
37	1186	6	0.509	USA	FALSE	0.493
38	600	9	0.445	USA	FALSE	0.494
39	765	11	0.708	USA	FALSE	0.494
40	570	1	0.295	USA	FALSE	0.497
41	893.2	10	0.532	USA	FALSE	0.497
42	795	8.99	0.232	USA	FALSE	0.498
43	533	8	0.262	USA	FALSE	0.498
44	1279	9	0.436	USA	FALSE	0.502
45	688	10	0.469	USA	FALSE	0.503

46	620	10	0.208	USA	FALSE	0.503
47	1168	10	0.215	USA	FALSE	0.504
48	1068	6.5	0.207	USA	FALSE	0.505
49	295	2	0.412	USA	FALSE	0.510
50	679	2	0.344	USA	FALSE	0.510
51	330	3.67	0.668	India	FALSE	0.512
52	1096	8	0.051	USA	FALSE	0.514
53	1724.6	39.03	0.224	USA	FALSE	0.518
54	730	9	0.390	USA	FALSE	0.522
55	836.1	12	0.258	USA	FALSE	0.522
56	1250	9	0.550	USA	FALSE	0.522
57	247	12	0.607	USA	FALSE	0.524
58	1326	16.38	0.203	USA	FALSE	0.526
59	555	1	0.265	USA	FALSE	0.526
60	450	32.78	0.609	USA	FALSE	0.529
61	650	10	0.109	USA	FALSE	0.530
62	470	10.64	0.607	USA	FALSE	0.531
63	169	13	0.662	USA	FALSE	0.535
64	580	2	0.536	USA	FALSE	0.536
65	541	9	0.275	USA	FALSE	0.536
66	586.6	8	0.090	USA	FALSE	0.550
67	1042.6	29.45	0.552	USA	FALSE	0.552
68	135	18.67	0.555	India	FALSE	0.552
69	264.6	22	0.307	USA	FALSE	0.558
70	926	17.31	0.210	USA	FALSE	0.568
71	264.6	21	0.318	USA	FALSE	0.594
72	124.4	30.37	0.548	USA	FALSE	0.595
73	250	4	0.601	Mexico	FALSE	0.607
74	300	35	0.318	USA	FALSE	0.617
75	212.2	21.18	0.839	USA	FALSE	0.618
76	119.4	12	0.605	India	FALSE	0.630
77	165	12.78	0.090	India	TRUE	0.640
78	110.5	10.59	0.292	India	FALSE	0.655
79	580	35.38	0.170	USA	FALSE	0.677
80	470	42	0.199	USA	FALSE	0.694
81	510	33		Australia	FALSE	0.713
82	1050	28.67	0.494	Canada	TRUE	0.720
83	1062.4	11.5	0.827	USA	FALSE	0.724
84	550	1		Australia	FALSE	0.728
85	845	7.2	0.100	USA	FALSE	0.736
86	305	41.49	0.171	USA	FALSE	0.750
87	1146	47.11	0.097	USA	FALSE	0.758
88	1586	40.58	0.102	USA	FALSE	0.770
89	1043.7	46.97	0.190	USA	FALSE	0.773
90	982.2	46.21	0.173	USA	FALSE	0.779
91	266.5	45.44	0.300	USA	FALSE	0.786
92	474.7	47.35	0.244	USA	FALSE	0.787
93	871.5	10.06	0.067	USA	FALSE	0.792
94	639	42.48	0.099	USA	FALSE	0.808

95	1250.9	45.93	0.164	USA	FALSE	0.826
96	667	4		Australia	FALSE	0.826
97	1982.4	49.08	0.059	USA	FALSE	0.829
98	320	13.07	0.696	Mexico	TRUE	0.830
99	2100	11.33	0.573	Mexico	TRUE	0.850
100	610	40.12	0.563	USA	TRUE	0.860
101	1314.8	39.66	0.051	USA	FALSE	0.873
102	300	27.39	0.483	Mexico	TRUE	0.880
103	120	21.79	0.686	India	FALSE	0.885
104	220	7.52		Australia	FALSE	0.892
105	882	38	0.012	USA	TRUE	0.900
106	800	35.5		Australia	FALSE	0.952
107	376	53	0.118	USA	TRUE	0.980
108	176.4	38	0.004	USA	TRUE	1.040
109	156	40		Australia	FALSE	1.077
110	120	35.5	0.159	USA	TRUE	1.080
111	226.8	38.25	0.051	USA	TRUE	1.140
112	414	38	0.020	USA	TRUE	1.140
113	220.6	12		Australia	FALSE	1.162
114	112.5	24	0.525	Mexico	TRUE	1.230
115	270	44	0.003	USA	TRUE	1.480
116	102.6	39	0.005	USA	TRUE	1.630

TABLE S6 Model coefficients from the 90-10 cross-validated, R^2_{CV} was 0.89.

Intercept	log Capacity	log Age	Fuel type is Oil	Technology is Single Cycle
-0.24	-0.03	0.04	0.13	0.16
-0.24	-0.04	0.04	0.13	0.17
-0.27	-0.03	0.05	0.14	0.17
-0.25	-0.03	0.04	0.14	0.17
-0.25	-0.03	0.04	0.12	0.17
-0.25	-0.03	0.04	0.14	0.16
-0.28	-0.02	0.04	0.13	0.17
-0.26	-0.03	0.04	0.14	0.17
-0.25	-0.03	0.05	0.13	0.16
-0.25	-0.03	0.04	0.14	0.16

TABLE S7 Standardized coefficients for normalized predictors for the best models with and without capacity factor.

Model	Intercept	Log Capacity	Log Age	Fuel type is OIL	Technology is Single Cycle	Log Capacity factor
Without Capacity Factor	-0.29	-0.01	0.02	0.14	0.17	NA
With capacity factor	-0.29	-0.01	0.02	0.12	0.15	-0.02

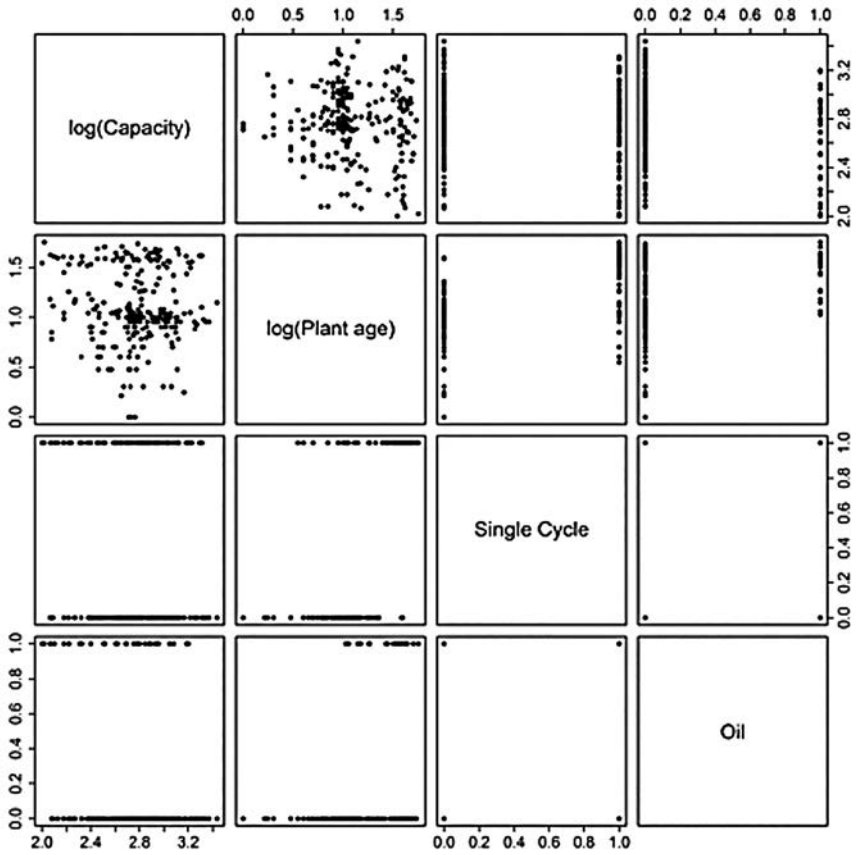

FIGURE S1 Model predictors plotted against each other (pairplots).

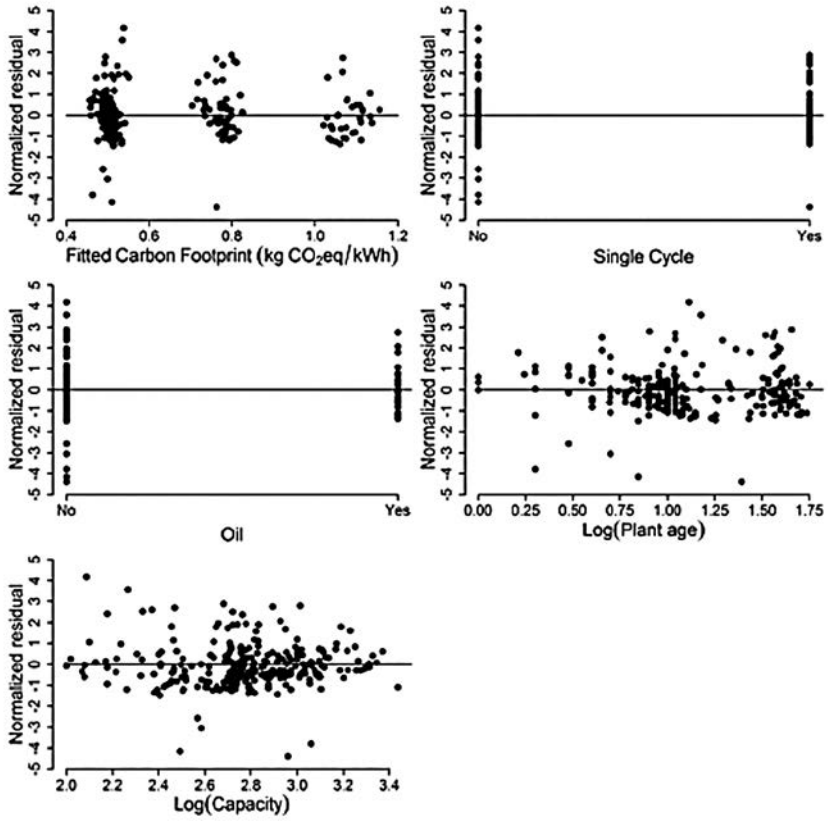

FIGURE S2 Relation between normalized residuals from training model estimates and fitted values and between normalized residuals and predictor variables.

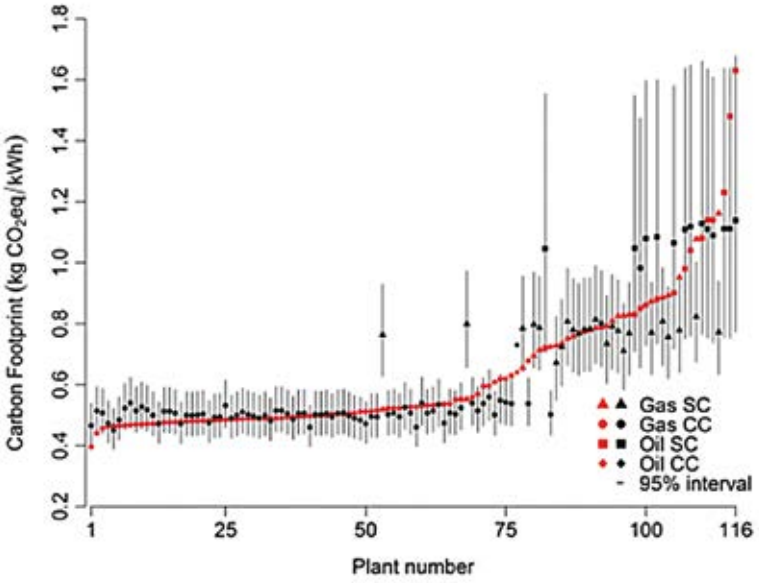

FIGURE S3 Reported (red) and estimated (black) and reported (red) carbon footprints and 95% prediction intervals (grey lines) for single cycle gas plants (triangles) combined cycle gas plants (circles), single cycle oil plants (squares) and combined cycle oil plant (diamond) for the model validation set. Power plants observations are sorted by increasing emission factors. Note that the prediction interval of the combined cycle oil plant is absent because the residual standard error for this category cannot be estimated reliably due to lack of data (1 plant in the training set).

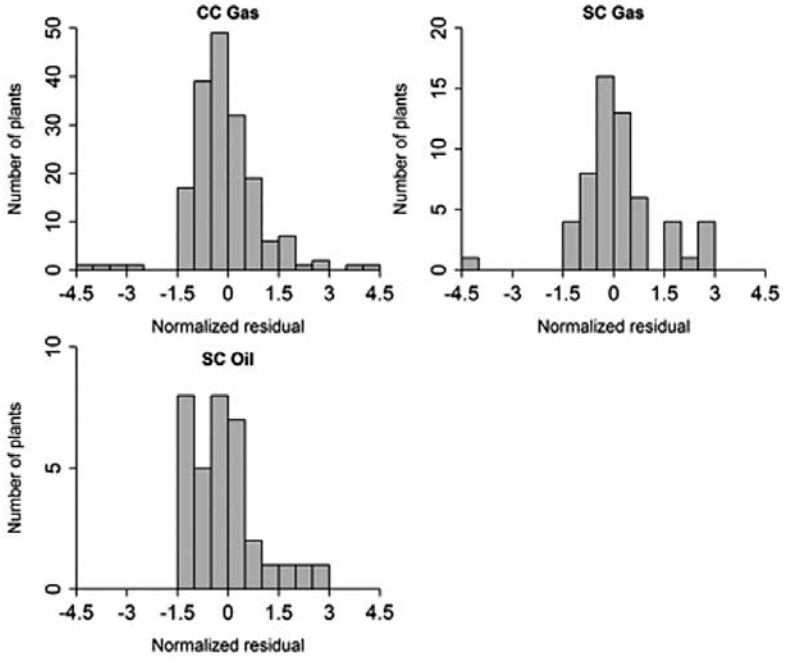

FIGURE S4 Histograms of normalized residuals for CC Gas (n=178) SC Gas (n=57) and SC Oil (n=34).

APPENDIX 4: SUPPORTING INFORMATION FOR:

CHAPTER 5. HOW MANY ENVIRONMENTAL IMPACT INDICATORS ARE NEEDED IN THE EVALUATION OF PRODUCT LIFE CYCLES?

SI 1: Indicator loadings

The loadings of all 135 indicators on the first four principal components are displayed on Figures S1 and S2. All indicators have positive correlations, meaning that the first component can be seen as representative of overall impact. The stronger the loading of an indicator on a component the more this component is representative of that particular type of impact. 28 indicators have almost identical (< 1% difference) loadings on the first component (see also table S1). These indicators are almost all related to freshwater of marine ecotoxicity. A group of indicators of climate change, human toxicity and acidification is not far behind (1%-2% lower absolute loadings). The most extreme scores on the second component can be observed for indicators of land use, high loadings are also seen for indicators of terrestrial ecotoxicity and water use, making this component indicative of the amount of land used. On the third component indicators of eutrophication are separated from indicators of ozone depletion and ionizing radiation, while the fourth component mostly separates the indicators of ozone depletion from all other indicators except one indicator of aquatic eutrophication.

SI 2: Resource footprints

We quantified four resource footprints for each product: non-renewable energy demand, raw material use, land use and freshwater consumption in the following way:

1 Energy demand (MJ) was quantified as the total amount of fossil energy required, including energy from oil, coal, gas and peat. This footprint is reported directly by ecoinvent.
2 Raw material use was calculated as the total amount of all raw materials extracted from the earth and reported in kilograms, thereby excluding the fossil fuels that were already covered by the energy demand calculations and also excluding organic carbon in soil or biomass. Metal extractions as reported in ecoinvent were converted to ore extractions by dividing by the metal-specific ore grades, as reported in ecoinvent. In case of multiple metals derived from the same ore (e.g., silver and gold), we used the maximum ore extraction needed to obtain the required amount of any of the metals, in order to avoid double counting of ore produced.
3 Land use ($m^2 \cdot yr$) was quantified as the total area of land used over time, irrespective of the type of land use.
4 Freshwater consumption (m^3) was defined as the amount of evaporated water plus the amount of water that is incorporated in the products. The freshwater consumption was approximated by the total amount of freshwater extracted (specified in ecoinvent as cooling and non-cooling water from unspecified natural origin, water for turbine

use, and water extracted from ground wells, lakes and rivers), minus the total amount of water returned to the environment (specified in ecoinvent as 'to: surface water, ground water, the ocean or unspecified sources)'. In some cases the water evaporation (calculated by summing all emissions of water to the air) exceeded the amount of extracted water minus the amount of returned water. In these cases (245 out of 976) the evaporation was used as approximation of the water consumption.

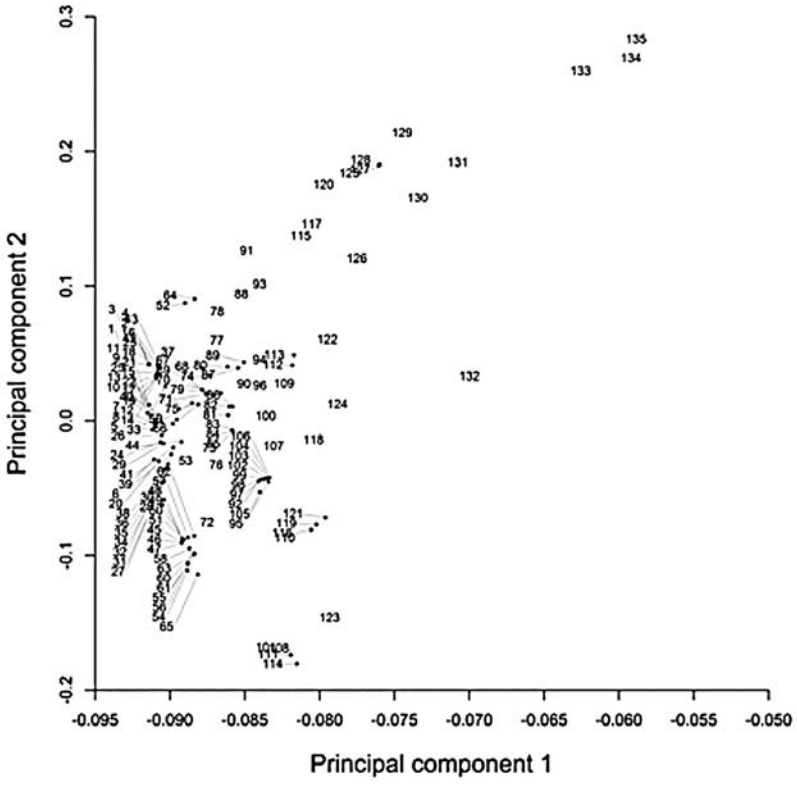

FIGURE S1 Loadings of all methodologies on the first and second principal component. The names of the indicators are given in table S1. Numbers range from 1 (highest absolute score on first principal component) to 135 (lowest absolute score on first principal component).

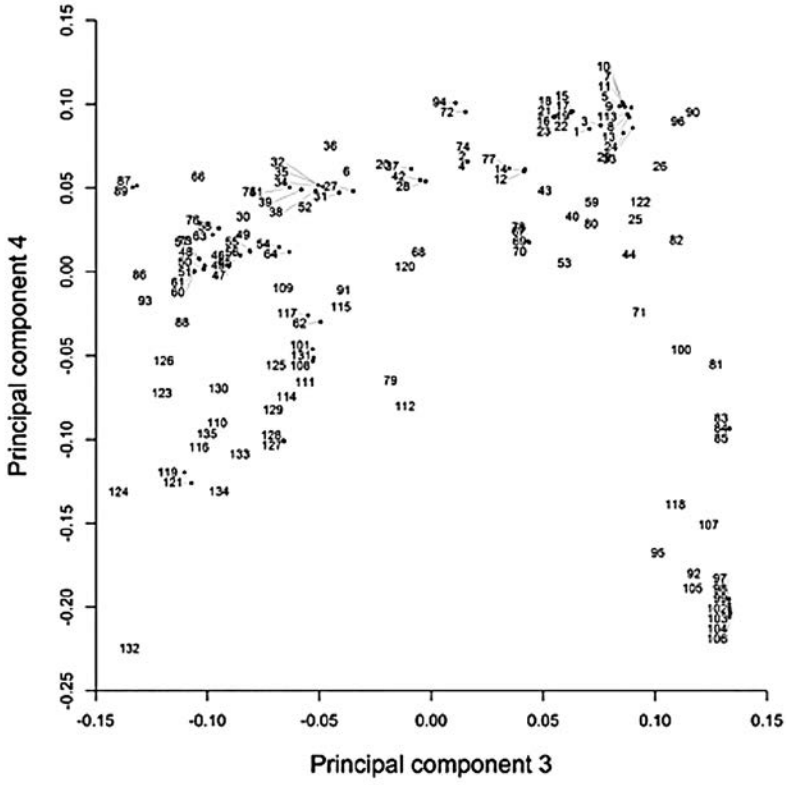

FIGURE S2 Loadings of all methodologies on the third and fourth principal components. The names of the indicators are given in table S1. Numbers range from 1 (highest absolute score on first principal component) to 135 (lowest absolute score on first principal component).

TABLE S1 Included indicators and their loadings on the first four components, ranked from highest to lowest absolute score on component 1.

#	Indicator category	Method: full name of indicator	Loadings per component			
			1	2	3	4
1	Marine ecotoxicity	ReCiPe: METP100a (I)	-0.091	0.006	0.071	0.085
2	Freshwater ecotoxicity	ReCiPe: FETPinft (E)	-0.091	0.042	0.016	0.066
3	Marine ecotoxicity	ReCiPe: METPinft (H)	-0.091	0.012	0.076	0.087
4	Freshwater ecotoxicity	ReCiPe: FETPinft (H)	-0.091	0.042	0.016	0.066
5	Marine ecotoxicity	ReCiPe: METPinft (E)	-0.091	-0.007	0.084	0.099
6	Respiratory effects & PM	Impact2002: human health:respiratory effects (inorganics)	-0.091	-0.029	-0.038	0.060
7	Marine ecotoxicity	CML2001: MAETP 100a	-0.091	-0.002	0.086	0.100
8	Marine ecotoxicity	CML2001: MAETP 20a	-0.091	-0.004	0.088	0.094
9	Marine ecotoxicity	CML2001: MSETP 100a	-0.091	0.001	0.087	0.098
10	Marine ecotoxicity	CML2001: MAETP 500a	-0.091	-0.002	0.085	0.101
11	Marine ecotoxicity	CML2001: MSETP 500a	-0.091	0.001	0.086	0.100
12	Freshwater eutrophication	ReCiPe: FEPt (H)	-0.091	0.034	0.041	0.060
13	Marine ecotoxicity	CML2001: MSETP 20a	-0.091	-0.001	0.088	0.092
14	Eutrophication	EDIP2003: eutrophication:separate P potential	-0.091	0.032	0.042	0.061
15	Freshwater ecotoxicity	CML2001: FSETP infinite	-0.091	0.036	0.063	0.096
16	Freshwater ecotoxicity	CML2001: FAETP infinite	-0.091	0.041	0.055	0.092
17	Freshwater ecotoxicity	CML2001: FSETP 500a	-0.091	0.034	0.063	0.096
18	Freshwater ecotoxicity	CML2001: FAETP 500a	-0.091	0.039	0.056	0.093
19	Freshwater ecotoxicity	CML2001: FSETP 100a	-0.091	0.034	0.063	0.095
20	Endpoint: single score	ReCiPeend: ReCiPeend(E,A)	-0.091	-0.030	-0.022	0.064
21	Freshwater ecotoxicity	CML2001: FAETP 100a	-0.091	0.039	0.056	0.093
22	Freshwater ecotoxicity	CML2001: FSETP 20a	-0.091	0.034	0.062	0.095
23	Freshwater ecotoxicity	CML2001: FAETP 20a	-0.091	0.039	0.055	0.092
24	Marine ecotoxicity	CML2001: MSETP infinite	-0.091	-0.016	0.090	0.086
25	Aquatic ecotoxicity	EDIP2003: ecotoxicity:chronic, in water	-0.091	-0.001	0.091	0.031
26	Human Toxicity	ReCiPe: HTPinft (E)	-0.091	-0.011	0.102	0.063
27	Acidification	EDIP2003: acidification:acidification	-0.091	-0.046	-0.035	0.048
28	Respiratory effects and PM	TRACI: human health:respiratory effects, average	-0.091	-0.063	-0.002	0.054
29	Marine ecotoxicity	CML2001: MAETP infinite	-0.090	-0.017	0.086	0.083
30	Photochemical ozone formation	TRACI: environmental impact:photochemical oxidation	-0.090	-0.059	-0.084	0.033

31	Acidification	CML2001: acidification:average European	-0.090	-0.045	-0.041	0.047
32	Acidification	TRACI: environmental impact:acidification	-0.090	-0.037	-0.051	0.052
33	Human Toxicity	ReCiPe: HTPinft (H)	-0.090	0.026	0.080	0.067
34	Acidification	Impact2002: ecosystem quality:aquatic acidification	-0.090	-0.036	-0.049	0.051
35	Acidification	CML2001: acidification:generic	-0.090	-0.036	-0.048	0.051
36	Respiratory effects and PM	ReCiPe: PMFPt (I)	-0.090	-0.035	-0.045	0.075
37	Freshwater ecotoxicity	ReCiPe: FETP100a (I)	-0.090	0.051	-0.009	0.061
38	Acidification	ReCiPe: TAP20a (I)	-0.090	-0.032	-0.052	0.048
39	Acidification	ReCiPe: TAP100a (H)	-0.090	-0.025	-0.058	0.049
40	Ecotoxicity	EDIP2003: ecotoxicity:in sewage treatment plants	-0.090	-0.002	0.063	0.033
41	Acidification	ReCiPe: TAP500a (E)	-0.090	-0.020	-0.063	0.050
42	Endpoint: Human health	Impact2002end: Impact2002humanhealth	-0.090	0.001	-0.005	0.055
43	Human toxicity	CML2001: HTP infinite	-0.089	0.009	0.051	0.049
44	Aquatic ecotoxicity	EDIP2003: ecotoxicity:acute, in water	-0.089	-0.016	0.088	0.010
45	Climate change	Impact2002: climate change:total	-0.089	-0.090	-0.091	0.004
46	Climate change	CML2001: GWP 500a	-0.089	-0.090	-0.091	0.004
47	Climate change	ReCiPe: GWP500a (E)	-0.089	-0.091	-0.090	0.003
48	Climate change	CML2001: upper limit of net GWP	-0.089	-0.087	-0.101	0.004
49	Photochemical ozone formation	ReCiPe: POFPt (H)	-0.089	-0.088	-0.084	0.022
50	Climate change	CML2001: GWP 100a	-0.089	-0.088	-0.102	0.002
51	Climate change	ReCiPe: GWP100a (H)	-0.089	-0.088	-0.102	0.001
52	Eutrophication	EDIP2003: eutrophication:combined potential	-0.089	0.088	-0.056	0.039
53	Human toxicity	EDIP2003: human toxicity:via surface water	-0.089	-0.029	0.059	0.005
54	Climate change	EDIP2003: global warming:GWP 500a	-0.089	-0.111	-0.068	0.015
55	Climate change	TRACI: environmental impact:global warming	-0.089	-0.106	-0.081	0.013
56	Climate change	EDIP2003: global warming:GWP 100a	-0.089	-0.106	-0.081	0.012
57	Climate change	CML2001: lower limit of net GWP	-0.089	-0.087	-0.104	0.008
58	Photochemical ozone formation	EDIP2003: photochemical ozone formation:impacts on vegetation	-0.089	-0.095	-0.095	0.026
59	Human toxicity	TRACI: human health:carcinogenics	-0.089	0.013	0.072	0.042
60	Climate change	ReCiPe: GWP20a (I)	-0.088	-0.099	-0.106	0.000
61	Climate change	CML2001: GWP 20a	-0.088	-0.099	-0.106	0.001
62	Photochemical ozone formation	CML2001: Summer smog: high NOx POCP	-0.088	-0.085	-0.049	-0.030
63	Photochemical ozone formation	EDIP2003: photochemical ozone formation:impacts on human health	-0.088	-0.098	-0.098	0.022
64	Eutrophication	CML2001: eutrophication:generic	-0.088	0.090	-0.063	0.012
65	Climate change	EDIP2003: global warming:GWP 20a	-0.088	-0.114	-0.085	0.010

66	Acidification& eutrification	Impact2002: ecosystem quality:terrestrial acidification & eutrification	-0.088	0.012	-0.104	0.057
67	Human toxicity	CML2001: HTP 500a	-0.088	0.023	0.043	0.018
68	Human toxicity	EDIP2003: human toxicity:via air	-0.088	0.039	-0.006	0.012
69	Human toxicity	CML2001: HTP 100a	-0.088	0.023	0.044	0.018
70	Human toxicity	CML2001: HTP 20a	-0.088	0.023	0.044	0.017
71	Land fill	EDIP2003: land filling:slag and ashes	-0.088	0.020	0.093	-0.024
72	Endpoint: Single score	EPS2000end: EPS2000Total	-0.088	-0.075	0.015	0.095
73	Endpoint: Single score	ReCiPeend: ReCiPeend(H,A)	-0.087	-0.020	-0.110	0.019
74	Land fill	EDIP2003: land filling:bulk waste	-0.087	0.034	0.014	0.075
75	Endpoint: Single score	ecological scarcity 2013: EcoscarcityTotal	-0.087	0.019	-0.081	0.048
76	Endpoint: Single score	ReCiPeend: ReCiPeend(I,A)	-0.087	-0.032	-0.107	0.031
77	Human Toxicity	TRACI: human health:non-carcinogenics	-0.087	0.060	0.035	0.062
78	Land use	ReCiPe: ULOPt (E)	-0.087	0.081	0.039	0.027
79	Human Toxicity	EDIP2003: human toxicity:via soil	-0.087	0.020	-0.018	-0.065
80	Human Toxicity	Impact2002: human health:human toxicity	-0.086	0.040	0.071	0.029
81	Ionizing radiation/ radio-active waste	ReCiPe: IRP_It (I)	-0.086	0.004	0.127	-0.055
82	Aquatic ecotoxicity	Impact2002: ecosystem quality:aquatic ecotoxicity	-0.086	0.011	0.109	0.019
83	Ionizing radiation/ radio-active waste	ReCiPe: IRP_HEt (H)	-0.086	-0.007	0.133	-0.093
84	Ionizing radiation/ radio-active waste	Impact2002: human health:ionising radiation	-0.086	-0.007	0.133	-0.094
85	Ionizing radiation/ radio-active waste	CML2001: ionising radiation	-0.086	-0.007	0.133	-0.094
86	Endpoint: single score	EI99end: EI99(H,A)	-0.086	0.011	-0.130	-0.001
87	Eutrophication	CML2001: eutrophication:average European	-0.085	0.039	-0.132	0.051
88	Eutrophication	ReCiPe: MEPt (I)	-0.085	0.094	-0.111	-0.030
89	Eutrophication	EDIP2003: eutrophication:terrestrial eutrophication	-0.085	0.044	-0.133	0.050
90	Water/resource depletion	Impact2002: resources:mineral extraction	-0.085	0.028	0.117	0.095
91	Terrestrial ecotoxicity	ReCiPe: TETPinft (E)	-0.085	0.127	-0.039	-0.011
92	Ozone depletion	CML2001: ODP steady state	-0.084	-0.045	0.117	-0.180
93	Eutrophication	EDIP2003: eutrophication:separate N potential	-0.084	0.102	-0.128	-0.017
94	Endpoint: single score	EI99end: EI99(I,I)	-0.084	0.046	0.011	0.101
95	Ozone depletion	ReCiPe: ODPinft (H)	-0.084	-0.053	0.101	-0.167
96	Water/resource depletion	ReCiPe: MDPt (H)	-0.084	0.027	0.110	0.090
97	Ozone depletion	CML2001: ODP 5a	-0.084	-0.044	0.133	-0.195
98	Ozone depletion	CML2001: ODP 10a	-0.084	-0.043	0.133	-0.198
99	Ozone depletion	CML2001: ODP 15a	-0.084	-0.043	0.133	-0.200

100	Land fill	EDIP2003: land filling:hazardous waste	-0.084	0.004	0.112	-0.046
101	Water/resource depletion	CML2001: depletion of abiotic resources	-0.084	-0.168	-0.053	-0.046
102	Ozone depletion	CML2001: ODP 20a	-0.084	-0.043	0.133	-0.202
103	Ozone depletion	CML2001: ODP 25a	-0.083	-0.042	0.134	-0.203
104	Ozone depletion	CML2001: ODP 30a	-0.083	-0.042	0.133	-0.204
105	Ozone depletion	TRACI: environmental impact:ozone depletion	-0.083	-0.045	0.117	-0.189
106	Ozone depletion	CML2001: ODP 40a	-0.083	-0.042	0.133	-0.206
107	Ionizing radiation/ radio-active waste	EDIP2003: land filling:radioactive waste	-0.083	-0.018	0.124	-0.151
108	Endpoint: resources	Impact2002end: Impact2002resources	-0.083	-0.169	-0.053	-0.053
109	Endpoint: single score	EI99end: EI99(E,E)	-0.082	0.028	-0.066	-0.010
110	Photochemical ozone formation	CML2001: Summer smog: low NOx POCP	-0.082	-0.086	-0.096	-0.090
111	Water/resource depletion	Impact2002: resources:non-renewable energy	-0.082	-0.174	-0.056	-0.066
112	Respiratory effects and PM	CML2001: malodours air	-0.082	0.041	-0.012	-0.080
113	Ecotoxicity	TRACI: environmental impact:ecotoxicity	-0.082	0.049	0.089	0.098
114	Water/resource depletion	ReCiPe: FDPt (E)	-0.082	-0.181	-0.065	-0.074
115	Terrestrial ecotoxicity	CML2001: TAETP infinite	-0.081	0.138	-0.041	-0.021
116	Photochemical ozone formation	CML2001: Summer smog: EBIR	-0.081	-0.081	-0.104	-0.104
117	Terrestrial ecotoxicity	CML2001: TAETP 500a	-0.081	0.146	-0.055	-0.026
118	Land use	ReCiPe: NLTPt (I)	-0.080	-0.014	0.109	-0.139
119	Photochemical ozone formation	CML2001: Summer smog: MOIR	-0.080	-0.077	-0.110	-0.120
120	Endpoint: ecosystems	Impact2002end: Impact2002ecosystemquality	-0.080	0.176	-0.012	0.003
121	Photochemical ozone formation	CML2001: Summer smog: MIR	-0.080	-0.072	-0.107	-0.126
122	Terrestrial ecotoxicity	Impact2002: ecosystem quality:terrestrial ecotoxicity	-0.079	0.061	0.093	0.042
123	Photochemical ozone formation	Impact2002: human health:photochemical oxidation	-0.079	-0.146	-0.120	-0.072
124	Eutrophication	TRACI: environmental impact:eutrophication	-0.079	0.013	-0.140	-0.131
125	Terrestrial ecotoxicity	CML2001: TAETP 100a	-0.078	0.184	-0.070	-0.056
126	Human toxicity	ReCiPe: HTP100a (I)	-0.078	0.121	-0.120	-0.053
127	Terrestrial ecotoxicity	ReCiPe: TETPinft (H)	-0.076	0.190	-0.066	-0.101
128	Terrestrial ecotoxicity	ReCiPe: TETP100a (I)	-0.076	0.190	-0.066	-0.101
129	Terrestrial ecotoxicity	CML2001: TAETP 20a	-0.074	0.214	-0.071	-0.082
130	Ecotoxicity	EDIP2003: ecotoxicity:chronic, in soil	-0.073	0.166	-0.095	-0.069

131	Water/resource depletion	ReCiPe: WDPt (I)	-0.071	0.192	-0.053	-0.051
132	Eutrophication	Impact2002: ecosystem quality:aquatic eutrophication	-0.070	0.033	-0.135	-0.224
133	Land use	CML2001: land use:competition	-0.063	0.260	-0.086	-0.109
134	Land use	ReCiPe: ALOPt (E)	-0.059	0.270	-0.095	-0.131
135	Land use	Impact2002: ecosystem quality:land occupation	-0.059	0.284	-0.100	-0.096

Abbreviations of the methods: METP: Marine EcoToxicity Potential, FETP: Freshwater EcoToxicity Potential, MAETP: Marine Aquatic Ecotoxicity Potential, MSETP: Marine Sediment Ecotoxicity Potential, FEP: Freshwater EutroPhication, FSETP: Freshwater Sediment Ecotoxicity Potential, FAETP: Freshwater Aquatic Ecotoxicity Potential, HTP: Human Toxicity Potential, PMFP: Particulate Matter Formation Potential, FETP: Freshwater Ecotoxicity Potential, TAP: Terrestrial Acidification Potential, GWP: Global Warming Potential, POFP: Photochemical Ozone Formation Potential, POCP: Photochemical Ozone Creation Potential ,ULOP: Urban Land Occupation Potential, IRP: Ionizing Radiation Potential, MEP: Marine Eutrophication Potential, TAETP/TETP: TerrestriAl Ecotoxicity Potential, ODP: Ozone Depletion Potential, MDP: Mineral/Metal Depletion Potential, MOIR: Maximum Ozone Incremental Activity, FDP: Fossil Depletion Potential, EBIR: Equal Benefit Incremential Reactivity, NLTP: Natural Land Transformation Potential, MIR: Maximum Incremental Reactivity, WDP: Water depletion potential, ALOP: Agricultural Land Occupation Potential.

500a/100a/20a: Time Horizons of 500, 100 and 20 years respectively
(I): Individualist perspective, (E): Egalitarian perspective, (H): Hierarchist perspective

TABLE S2 is available as Excel file via the Journal website

APPENDIX 5: SUPPORTING INFORMATION FOR:

CHAPTER 6: HEADLINE ENVIRONMENTAL INDICATORS REVISITED WITH THE GLOBAL MULTI-REGIONAL INPUT-OUTPUT DATABASE EXIOBASE

Section S1 Interpretation of the principal components

All correlations between the indicators were positive, which can be seen from the fact that all indicators have the same sign (i.e. they are all negative) on the first component. On the second component, the toxicity indicators were separated from other indicators of land use, combined endpoint indicators and indicators of eutrophication. The third component separated the toxicity indicators from indicators of climate change and energy use. A distinction between terrestrial and human toxicity indicators on the one hand and freshwater ecotoxicity related indicators was made on the fourth principal component. Note that there are intrinsic differences between the included toxicity indicators for different ecosystems. While the ecotoxic effects are often calculated through extrapolation from one ecosystem to another (freshwater, marine and terrestrial), the characterization factors between the different types of toxicity indicators are not very strongly correlated. This is because the fate part of the characterization factor is specific to the receiving compartments (marine vs freshwater vs terrestrial environment), which results in characterization factors for chemical impacts in different ecosystems that are intrinsically different. This effect is illustrated by the correlations presented in Supporting Table S2, which show, for example, that indicators of marine ecotoxicity are highly related to each other, but only moderately correlated to indicators of freshwater ecotoxicity. All indicator loadings on the first six components are shown in the Supporting Table S3.

Section S2 Principal component scores

Figure S1 displays the distributions of the principal component scores on the first four principal components. From studying these scores we can learn which components are linked to which kind of indicator. The products are divided into eight product categories (agricultural & food products, electricity, fossil fuels, metals & electronics, minerals, chemicals & plastics, non-food bio-based products, services, waste & recycling). For the first component, the highest scores are observed for the category 'services' while the 'metals & electronics' and the 'minerals, chemicals & plastics' categories have the lowest values. Because the loadings of the first component are all negative, this reflects the fact that in general the services category is the least impact-intensive per million euro. The scores on the second component separate the metal products and electronics category from the agricultural and food products sector. Agricultural products have relatively high land-related impacts per million euro and low combustive and toxic emissions, while for metal products and electronics this pattern is reversed. While not unexpected, these findings indicate that a ranking of the impact of agricultural products is best made according to their land use per million euro while for metal products and electronics this would have limited added value. The third component distinguishes impacts related to energy use (including climate change) from toxic impacts. This is reflected through the

highest and lowest scores for fuels and electricity generation products on the one hand and metal products and electronics on the other.

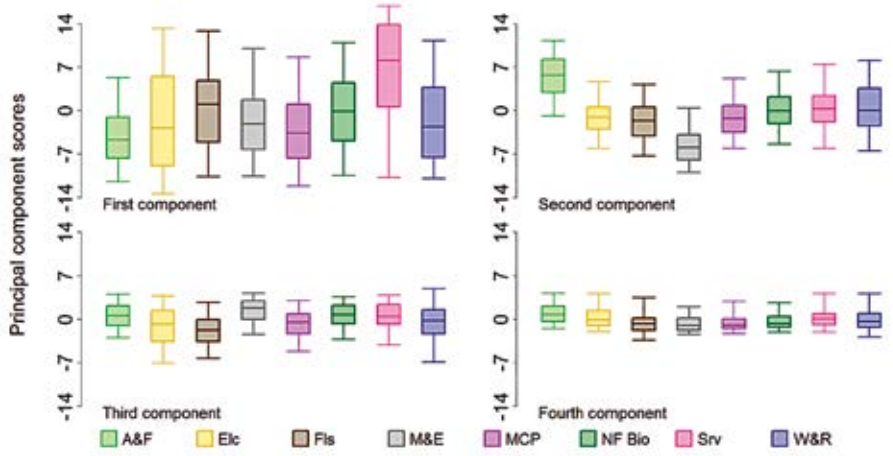

FIGURE S1 Principal component scores of the first four principal components for the impact indicators per product category. Boxes denote the medians and interquartile ranges, whiskers extend to the 5th and 95th percentiles. Abbreviations: A&F = Agricultural and food products, Elc = Electricity generation, Fls = Fossil Fuels, M&E = Metal products and Electronics, MCP = Minerals, Chemicals and Plastics, NF Bio = Non-food biobased products, Srv = Services, W&R = Waste treatment and Recycling.

TABLES S1 TO S4 are available as Excel files via the journal website

TABLE S5 Numerically best indicator sets of sizes 1 to 6.

Numerically best indicator set		Method	Explained variance
1	Particulate matter formation (Hierarchist)	ReCiPe 2008	50.1%
2	Particulate matter formation (Hierarchist)	ReCiPe 2008	74.3%
	Freshwater aquatic ecotoxicity (infinite time horizon)	CML 2001	
3	Particulate matter formation (Hierarchist)	ReCiPe 2008	84.0%
	Freshwater aquatic ecotoxicity (infinite time horizon)	CML 2001	
	Marine ecotoxicity (infinite time horizon)	ReCiPe 2008	
4	Particulate matter formation (Hierarchist)	ReCiPe 2008	90.0%
	Freshwater aquatic ecotoxicity (infinite time horizon)	CML 2001	
	Marine ecotoxicity (infinite time horizon)	ReCiPe 2008	
	Global warming (100 year time horizon)	EDIP 2003	
5	Particulate matter formation (Hierarchist)	ReCiPe 2008	92.5%
	Freshwater aquatic ecotoxicity (infinite time horizon)	CML 2001	
	Marine ecotoxicity (infinite time horizon)	ReCiPe 2008	
	Global warming (100 year time horizon)	EDIP 2003	
	Terrestrial ecotoxicity (100 year time horizon, Individualist)	ReCiPe 2008	
6	Particulate matter formation (Hierarchist)	ReCiPe 2008	93.9%
	Freshwater aquatic ecotoxicity (infinite time horizon)	CML 2001	
	Marine ecotoxicity (infinite time horizon)	ReCiPe 2008	
	Global warming (100 year time horizon)	EDIP 2003	
	Terrestrial ecotoxicity (100 year time horizon, Individualist)	ReCiPe 2008	
	Photochemical oxidation (Maximum Increment Reactivity)	CML 2001	

APPENDIX 6: SUPPORTING INFORMATION FOR:

CHAPTER 7: RESOURCE FOOTPRINTS ARE GOOD PROXIES OF ENVIRONMENTAL DAMAGE

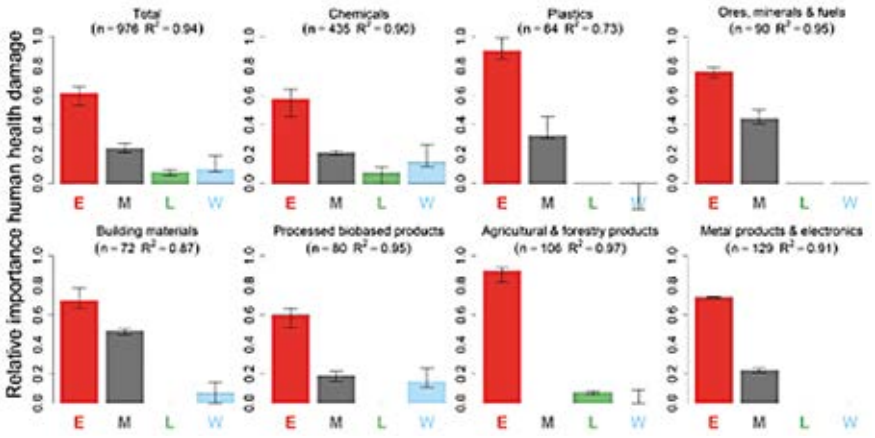

FIGURE S1 Associations between human health damage and four resource footprints per product group. E=Energy, M=Material, L=Land, W=Water, values are expressed as standardized coefficients of log-linear regression models based on 976 products, for all products combined and per product group. Boxplots (quartiles and 90% interval) reflect spatial variability in damage associated with land use and water consumption. R^2 was calculated as the mean value over the 156 country-specific regression models.

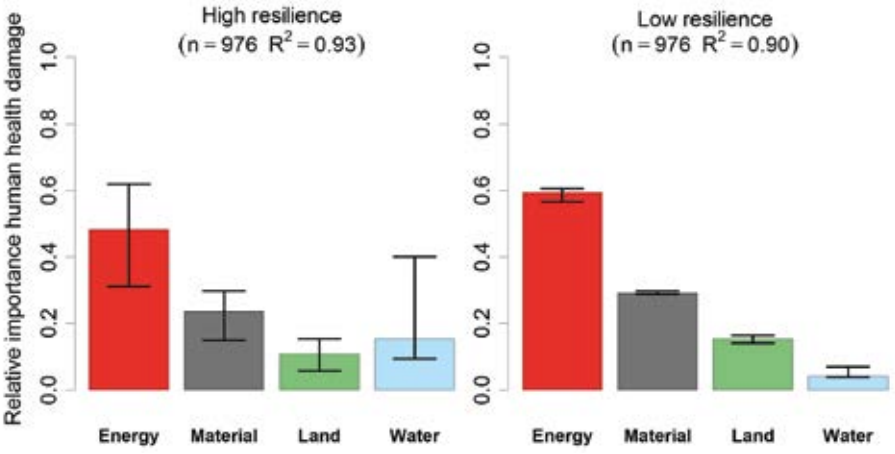

FIGURE S2 Associations between human health damage and four resource footprints for two alternative sets of characterization factors, based on high resilience and low resilience. Values are expressed as standardized coefficients of log-linear regression models based on 976 products. The error bars reflect spatial variability (90% interval) in damage. R^2 was calculated as the mean value over the 156 country-specific regression models.

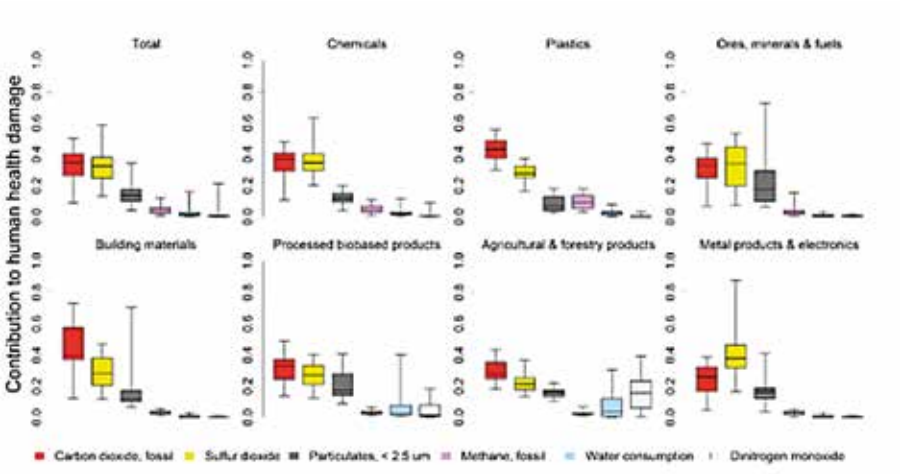

FIGURE S3 Contributions to human health damage (per product group) of most important contributors. All resource extraction or substance emissions with a contribution of >5% for >5% of the total set of products are displayed. Boxplots represent quartiles and 90% intervals encompassing the 976 products.

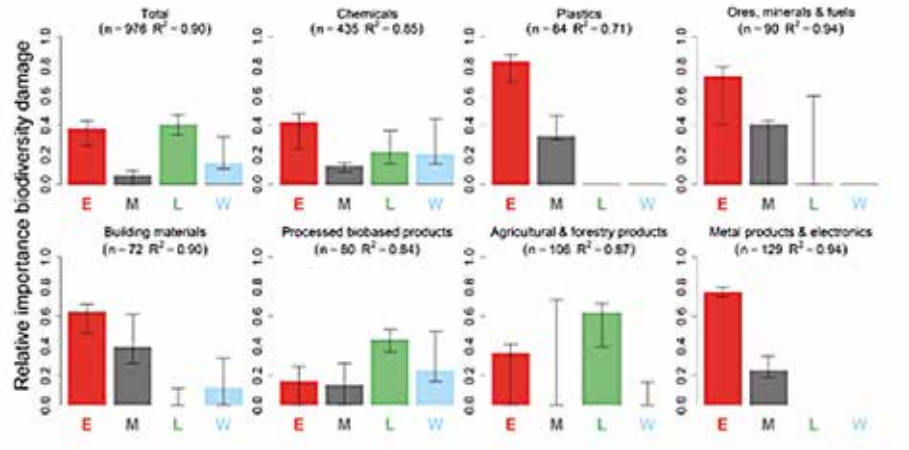

FIGURE S4 Associations between biodiversity damage and four resource footprints per product group. E=Energy, M=Material, L=Land, W=Water, values expressed as standardized coefficients of log-linear regression models based on 976 products, per product group. The error bars reflect spatial variability (90% interval) in damage. R^2 was calculated as the mean value over the 156 country-specific regression models.

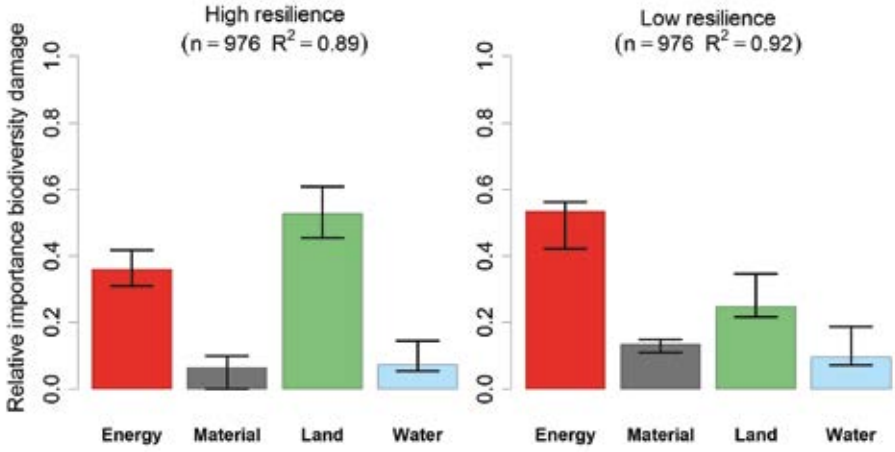

FIGURE S5 Associations between biodiversity damage and four resource footprints for two alternative sets of characterization factors, based on high resilience and low resilience. Values are expressed as standardized coefficients of log-linear regression models based on 976 products. The error bars reflect spatial variability (90% interval) in damage. R^2 was calculated as the mean value over the 156 country-specific regression models.

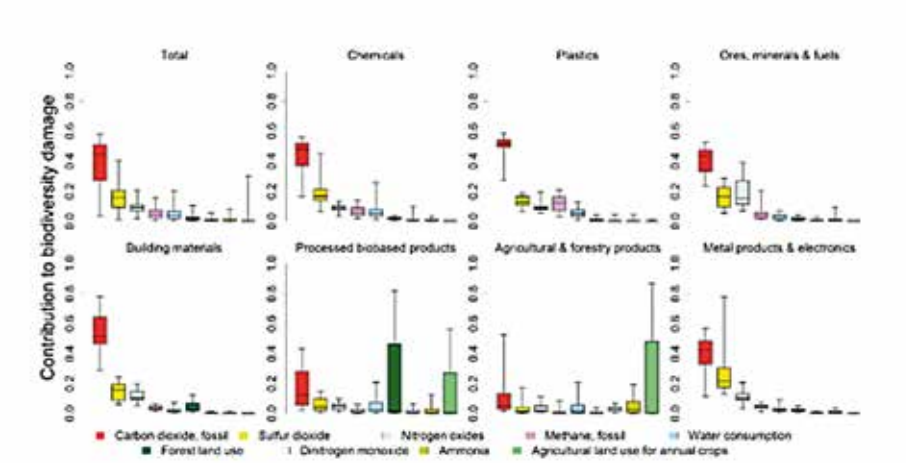

FIGURE S6 Contributions biodiversity damage (per product group) of most important contributors. All resource extraction or substance emissions with a contribution of >5% for >5% of the total set of products are displayed. Boxplots represent quartiles and 90% intervals encompassing the 976 products.

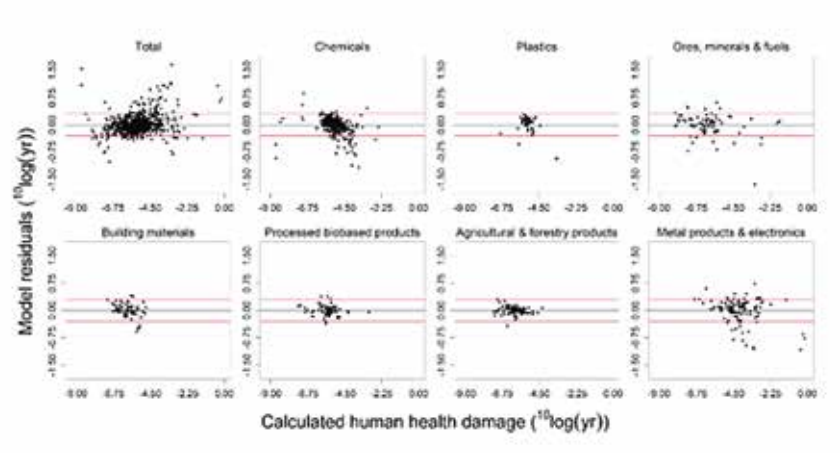

FIGURE S7 Residuals of the regression models for human health damage for all the products and per product category. Results are based on default characterization factors. Horizontal red lines represent a factor of 2 over- and underestimation. Overall, the damage as predicted from the resource footprints was within a factor of 2 from the actual values for 85% of the products. Using separate models for each product category increases this fraction to 90%.

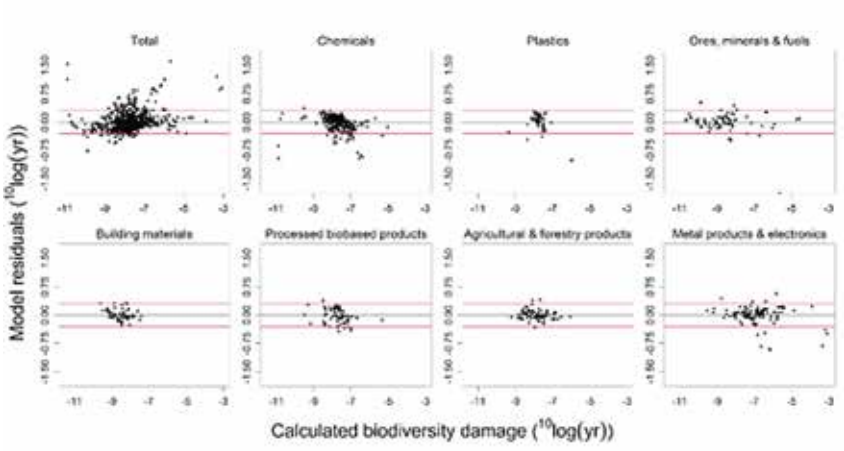

FIGURE S8 Residuals of the regression models for biodiversity damage for all the products and per product category. Results are based on the default characterization factors. Horizontal red lines represent a factor of 2 over- and underestimation. Using the overall model, the damage as predicted from the resource footprints was within a factor of 2 from the actual values for 87% of the products. Using separate models for each product category increases this fraction to 94%.

TABLE S1 Included impact categories in ReCiPe, covered areas of protection and damage pathways

Impact category	Area of protection	Fate and exposure pathways	Damage pathways
Climate change	Human health	Time-integrated increase in global mean temperature due to an increase in GHG emissions *(1, 2)*	Years of life lost and disabled due related to increased malaria, diarrhea, malnutrition and natural disasters due to increased global mean temperature *(3, 4)*
	Ecosystems (terrestrial)	Time-integrated increase in global mean temperature due to an increase in GHG emissions *(1)*	Species loss related to changing biome distributions due to increased global temperature *(5)*
	Ecosystems (freshwater)	Time-integrated change in water discharge due to an increase in GHG emissions *(6)* Based on *(7, 8)*	Fish species loss due to decrease river discharge(6) Based on *(7, 8)*
Stratospheric ozone depletion	Human health	Increase in Equivalent Effective Stratospheric Chlorine (EESC) *(9)*	Years of life lost and disabled related to increased skin cancer and cataract due to UV-exposure *(10)*
Ionizing radiation	Human health	Fate modelled via emissions to air, rivers and seas to estimate the collective exposure dose of a hypothetical world population of 10 billion people	Years of life lost and disabled related to an increase in cancer and hereditary diseases due to exposure to radiation *(11)*
Particulate matter formation	Human health	Change in ambient PM2.5 concentration after emission of PM or a precursor. On a 1°x1° grid scale *(12)*	Years of life lost related to an increase in respiratory diseases caused by primary and secondary aerosols *(13)*
Photochemical ozone formation	Human health	Change in ambient tropospheric ozone concentration after emission of NO_x or NMVOC. On a world-region scale *(12)*	Years of life lost related to an increase in respiratory diseases caused by exposure to ozone *(13, 14)*
	Ecosystems (terrestrial)	Change in cumulative tropospheric ozone exposure after emission of NO_x or NMVOC. On a 1°x1° receiving grid scale *(14)*	Loss of grassland and forest plants species due to increased ground level ozone exposure *(14)*
Terrestrial acidification	Ecosystems (terrestrial)	Soil specific increase in H+ concentration as a result of an emission of NO_x, NH_3 or SO_2 *(15)* Atmospheric model on a 2°x2.5° scale *(16)*	Loss of plant species due to decrease in soil pH *(17)*
Freshwater eutrophication	Ecosystems (aquatic)	A global fate model for phosphorus to estimate grid cell specific fate factors on a 0.5°x0.5° scale *(18)*	Loss of aquatic species due to increased phosphorus concentrations *(19, 20)*
Toxicity	Human health	Modelled via a multimedia fate and exposure model. Exposure routes include drinking water, 7 different food types and inhalation *(21)*	Years of life lost and disabled due to cancer and non-cancer effects due to ingestion and inhalation of toxic substances *(22)*
	Ecosystems (marine) Ecosystems (terrestrial) Ecosystems (freshwater)	Multimedia fate model to predict change in environmental concentrations *(21)*	Species loss due to chemical exposure in marine waters *(22)* Species loss due to chemical exposure in soils *(22)* Species loss due to chemical exposure in freshwater *(22)*

Water consumption	Human health Ecosystems (terrestrial) Ecosystems (aquatic)	Reduction of water availability in watershed due to water consumption	Malnutrition caused by water shortage *(65)* Decrease in Net Primary Productivity because of water shortage as proxy for total species loss *(23)* Fish species loss due to decrease river discharge *(6)*
Land occupation and transformation	Ecosystems (terrestrial)	Not applicable	Occupation: species loss due to different types of land use (agriculture, forestry, built up) Transformation: species loss caused by transformation of natural land to used land, including the time it takes to back-transform to natural land *(24)*

TABLE S2 Goodness of fit and coefficients of log-linear regression models. Two damage footprints (human health, biodiversity) are related to four resource footprints (energy, materials, land and water) for various product groups. All values outside parentheses belong to the models with the lowest AIC values and the default characterization factors. Between parentheses: 90% intervals of the regression coefficients, R^2 values and residual standard errors based on country specific CFs.

	Product category	Intercept	Energy	Material	Land	Water	R2	Res. SE
Human health damage	All	-5.98 (-6.49~-5.84)	0.59 (0.57~0.71)	0.22 (0.19~0.24)	0.05 (0.05~0.09)	0.17 (0.08~0.19)	0.93 (0.93~0.94)	0.25 (0.23~0.25)
	Chemicals	-5.77 (-6.45~-5.65)	0.50 (0.49~0.69)	0.18 (0.17~0.20)	0.04 (0.00~0.11)	0.24 (0.11~0.26)	0.88 (0.88~0.91)	0.22 (0.21~0.22)
	Plastics	-6.86 (-7.36~-6.79)	0.92 (0.92~1.07)	0.30 (0.27~0.40)	- -	- (-0.17~0.00)	0.74 (0.71~0.77)	0.23 (0.22~0.25)
	Ores, minerals & fuels	-6.81 (-7.13~-6.61)	0.81 (0.78~0.85)	0.40 (0.36~0.44)	- -	- -	0.95 (0.94~0.95)	0.30 (0.30~0.33)
	Building materials	-6.28 (-6.69~-6.23)	0.73 (0.70~0.85)	0.42 (0.41~0.45)	- -	0.13 (0.00~0.14)	0.88 (0.81~0.92)	0.19 (0.15~0.24)
	Processed bio-based products	-5.92 (-6.45~-5.70)	0.59 (0.56~0.69)	0.14 (0.13~0.19)	- -	0.22 (0.11~0.23)	0.96 (0.92~0.97)	0.13 (0.12~0.19)
	Agricultural & forestry products	-6.45 (-6.87~-6.27)	0.90 (0.89~1.00)	- -	0.06 (0.06~0.08)	0.08 (0.00~0.09)	0.97 (0.96~0.97)	0.10 (0.10~0.12)
	Metal products & electronics	-6.39 (-6.64~-6.21)	0.78 (0.77~0.78)	0.21 (0.18~0.21)	- -	- -	0.91 (0.90~0.92)	0.32 (0.28~0.33)
Biodiversity damage	All	-7.90 (-8.13~-7.25)	0.39 (0.28~0.47)	0.04 (0.00~0.08)	0.35 (0.32~0.45)	0.19 (0.10~0.32)	0.92 (0.83~0.93)	0.24 (0.24~0.43)
	Chemicals	-8.00 (-8.38~-7.43)	0.39 (0.26~0.51)	0.10 (0.07~0.13)	0.15 (0.13~0.35)	0.30 (0.14~0.44)	0.91 (0.70~0.91)	0.18 (0.18~0.43)
	Plastics	-9.43 (-9.57~-8.82)	0.92 (0.75~0.95)	0.28 (0.27~0.41)	- -	- -	0.71 (0.68~0.75)	0.24 (0.23~0.28)

	Ores, minerals & fuels	-9.44 (-9.48~-8.18)	0.79 (0.44~0.86)	0.36 (0.00~0.38)	- (0.00~0.58)	- -	0.96 (0.92~0.96)	0.27 (0.27~0.40)
	Building materials	-8.62 (-9.04~-8.11)	0.62 (0.53~0.74)	0.26 (0.25~0.54)	- (0.00~0.11)	0.19 (0.00~0.31)	0.92 (0.84~0.94)	0.13 (0.12~0.23)
	Processed bio-based products	-7.75 (-7.92~-6.72)	0.23 (0.00~0.28)	- (0.00~0.25)	0.39 (0.35~0.49)	0.22 (0.16~0.49)	0.90 (0.71~0.91)	0.19 (0.18~0.47)
	Agricultural & forestry products	-8.13 (-8.15~-7.01)	0.39 (0.00~0.45)	- (0.00~0.63)	0.64 (0.38~0.66)	- (0.00~0.16)	0.96 (0.64~0.96)	0.11 (0.12~0.42)
	Metal products & electronics	-9.26 (-9.40~-8.93)	0.84 (0.79~0.86)	0.19 (0.16~0.29)	- -	- -	0.95 (0.89~0.98)	0.23 (0.15~0.39)

Data files S1 and S2 are available as Excel file via the Journal website

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APPENDIX 7:

RESPONSE TO COMMENT ON "RESOURCE FOOTPRINTS ARE GOOD PROXIES OF ENVIRONMENTAL DAMAGE

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In a recent contribution to this journal we showed that resource footprints provide a good approximation of damage to human health and ecosystems (1). In his correspondence article, Heijungs (2) provides three arguments as to why this may not be the case:

1 Potential of rank reversal in product comparisons by using resource footprints instead of environmental damage.
2 Arbitrary choice of functional unit.
3 Incorrect statistics.

We will argue below why the criticism of Heijungs is not justified.

Rank reversal

Heijungs plotted the rank scores of the 976 products based on human damage footprints against the rank scores based on resource footprints and stated that "every point that is not on the diagonal line forms a possible rank reversal" (2). A **POSSIBLE** rank reversal is, however, not the same as an *actual* rank reversal. To reveal how often rank reversals actually occur, we identified the total number of cases in which a comparison of any two products in our dataset would lead to a different ranking based on the resource as compared to the damage footprints (i.e. product *A* better than product *B* according to the resource footprint proxy but worse according to the damage footprints or vice versa). We checked all 475,800 possible pairwise comparisons and found that resource- and damage-based ranks were identical in 90.6% and 92.4% of the cases for ecosystem and human health damage, respectively. Thus, actual rank reversals are relatively rare, indicating that results for resource footprints and damage footprints do indeed point in the same direction for the vast majority of products.

Functional unit

Heijungs used our initial data set to calculate damage per MJ of fossil energy rather than the common unit of 1 kg of product. He concluded that the remaining variance in environmental damage per MJ between the products is too large to consider resource footprints as sensible proxies. Heijungs missed the main point of our analysis here. In the past, energy as single proxy of damage was promoted by Huijbregts et al. (3) and

later criticized by Laurent et al. (4). In the current analysis we dealt with this criticism by including not only fossil energy, but also land, water and materials as possible proxies of environmental damage. Following the same rescaling procedure as Heijungs, we refitted our model, without fossil energy demand as a predictor (i.e., we used damage per MJ of fossil energy as response variables and the other three resource footprints as predictors). The three remaining resource footprints indeed explained a significant part of the variation in environmental damage (per MJ of fossil energy), i.e. 49.8% of the variation in human health damage and 73.8% of the variation in ecosystem damage. This confirms the importance of combining different resource indicators as proxy of environmental damage.

Statistics

Heijungs argued that statistics such as Variance Inflation Factors (VIFs), Akaike Information Criterion (AIC) and residual standard errors are not valid as the observations (products) in our dataset are a non-random sample. Although we do agree that the ecoinvent database may not provide a random sample of all the products from the world's economy, we consider the sample as representative as possible given that ecoinvent contains a large number of commodities from a wide range of product categories. From this large database we selected 976 products in such a way that as many products as possible were retained, while removing pseudo-duplicates. To demonstrate the robustness of our statistics to possible remaining non-independence/pseudo-replication in the product selection, we refitted the models 10 times based on a random sub-sample of 500 products. Each time this yielded the same set of predictors, as selected based on AIC values and VIFs, for both ecosystem and human health damage. Further, for both ecosystem and human health damage, the residual standard error varied from 0.22 to 0.26 in the random sampling procedure, whereas the residual standard errors we originally calculated from our full dataset of 976 products were 0.24 and 0.25 for ecosystem and human health damage, respectively. This confirms the robustness of the statistics we presented.

In conclusion, we consider the criticism from Heijungs as not justified. Our additional analyses, as presented above, provide further evidence that in the vast majority of product comparisons, resource footprints are indeed good proxies of environmental damage.

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Samenvatting

Om de milieuschade van de producten en diensten die onze economie levert te bepalen, zijn diverse methoden ontwikkeld. Bij elk van deze methoden staat het principe centraal dat er over de gehele levenscyclus van een product of dienst gekeken moet worden om afwenteling van milieuproblemen over de productieketen te vermijden. Zo'n levenscyclus bestrijkt alle stappen van het winnen van de ruwe grondstoffen tot aan de uiteindelijke afvalverwerking van het product, inclusief alle benodigde transport- en verwerkingsstappen gedurende deze cyclus. Indicatoren om de milieuschade te kwantificeren, kunnen op verschillende plekken in de oorzaak-effect keten worden afgeleid. Dicht bij de oorzakelijke kant van de keten zitten de grondstofindicatoren die het totale gebruik van een grondstof (respectievelijk energie, land, water en materialen) over de gehele levenscyclus sommeren. Aan het einde van de keten zitten de zogenoemde endpoint-indicatoren die het effect op volksgezondheid of biodiversiteit trachten weer te geven. Midpoint-indicatoren bevinden zich ergens tussen de oorzaak en het uiteindelijke effect in.

Hoe verder in de oorzaak-effect keten, hoe meer data en rekenstappen nodig zijn om de indicatoren af te leiden, hetgeen kan leiden tot toenemende onzekerheid in de berekende milieuschade. Naast onzekerheid zit er ook variabiliteit in de levenscyclusdata, dat wil zeggen daadwerkelijke verschillen tussen bijvoorbeeld technologieën en geografische regio's. Tot slot is er een groot aantal indicatoren en methoden beschikbaar om de milieuschade van producten te bepalen op grondstof-, midpoint- en endpoint-niveau. De vraag is of al deze (typen) indicatoren nodig zijn voor een robuuste analyse van milieu-impacts.

Het doel van dit proefschrift was het reduceren van onzekerheid en mogelijke overtolligheid in de berekening van milieuschade van producten en diensten. De volgende twee onderzoeksvragen stonden hierbij centraal:

1 *In hoeverre kan de onzekerheid gekwantificeerd en gereduceerd worden in milieuschade van producten en diensten, daarbij de nadruk leggend op de klimaatimpact van elektriciteitsproductie op basis van fossiele brandstoffen?*
2 *Wat is de optimale representatieve set aan milieu-indicatoren voor productanalyses?*

In hoofdstuk 2 zijn de onzekerheid en variabiliteit in de klimaatimpact van kolencentrales in de Verenigde Staten onafhankelijk van elkaar gekwantificeerd. Onzekerheid in parameters werd gekwantificeerd door middel van probablitistische simulaties, terwijl de variabiliteit bepaald werd door de verschillende ketens (van kolenmijn tot kolencentrales) apart te houden voor 364 kolencentrales in de VS. De resultaten tonen aan dat de spreiding in klimaatimpact gedomineerd wordt door inherente verschillen tussen centrales, met name in efficiëntie van de elektriciteitsopwekking, met een zeer

geringe bijdrage van onzekerheid. Als de efficiëntie van de 95% slechtst presterende kolencentrales opgehoogd zou kunnen worden naar die van de 5% best presterende centrales dan zou de totale klimaatimpact van de elektriciteitsproductie d.m.v. kolen met 6% verlaagd worden.

Voor veel landen ontbreekt de informatie voor het berekenen van de klimaatimpact veroorzaakt door één specifieke elektriciteitscentrale. Daarom zijn in de hoofdstukken 3 en 4 regressiemodellen gebruikt voor het schatten van klimaatimpact van centrales waar wel technologische data voor beschikbaar was, maar geen specifieke data voor het berekenen van milieuschade. De ontwikkelde regressiemodellen verklaren tussen de 49% en 81% van de variatie in klimaatimpacts. De grootste onzekerheid werd hierbij gevonden voor gas- en oliecentrales met één enkele stoomcyclus, terwijl de klimaatimpact van gascentrales die gebruik maken van een combinatie van een gas- en een stoomturbine met een geringere onzekerheid geschat kon worden. Voor kolencentrales is een onzekerheid gevonden die tussen die van beide typen gascentrales in zit.

Er zijn honderden indicatoren ontwikkeld waarmee de mileuschade van producten bepaald kan worden. In hoofdstuk 5 zijn 135 van deze indicatoren met elkaar vergeleken voor een set van 976 producten uit de LCA database Ecoinvent. Hierbij is gebruik gemaakt van hoofdcomponentenanalyse (PCA), die de onderlinge correlaties tussen de indicatoren in kaart brengt en waarmee een minimale set aan indicatoren gevonden kan worden die een zo groot mogelijke hoeveelheid aan variantie tussen de indicatoren kan verklaren. De gevonden minimale set bestond uit een zestal indicatoren voor respectievelijk klimaatverandering, ozondepletie, verzuring en eutrophiëring, marine ecotoxiciteit en landgebruik. Tezamen verklaarden deze indicatoren 92% van de variantie in de productrangschikking. Een set bestaande uit vier minder ingewikkelde grondstofindicatoren (energie, water, land, materialen) verklaarde 84% van de variantie. In hoofdstuk 6 is gebruikt gemaakt van dezelfde PCA-methode voor een set aan producten uit een Multi Regionaal Input Output model met Milieu-Extensies (EEMRIO) model genaamd EXIOBASE. In totaal werd de milieuschade van 6982 product-regio combinaties gerangschikt aan de hand van 119 indicatoren. Het doel van deze studie was om te kijken in hoeverre een kleine set aan indicatoren die door Eurostat aangewezen zijn als leidende indicatoren voor milieubeleid, namelijk voor klimaat, land, water en materialen, representatief is voor de totale spreiding in rangschikking tussen producten. Een kleine 60% van de variantie werd verklaard met deze set aan vier indicatoren, waarbij reeds 57% werd verklaard door indicatoren voor de klimaatimpact en landgebruik. Het toevoegen van één toxiciteitsindicator verhoogde de verklaarde variantie tot boven de 80%, hetgeen aangeeft dat de toxiciteitsindicatoren in deze dataset niet goed benaderd kunnen worden met de veel gebruikte beleidsindicatoren. Om 95% van de variantie te verklaren was het nodig om de set van vier indicatoren aan te vullen met indicatoren voor marine ecotoxiciteit, terrestrische ecotoxiciteit, fotochemische oxidatie, terrestrische verzuring, en eutrofiëring. Zowel hoofdstuk 5 als hoofdstuk 6 tonen aan dat het overgrote deel van de meer dan 100 verschilllende indicatoren niet strikt noodzakelijk is.

In hoofdstuk 7 is gekeken in hoeverre de schade aan biodiversiteit en volksgezondheid benaderd kan worden door een set bestaande uit vier indicatoren voor respectievelijk energie, land, water en materialen. Meer dan 90% van de variatie in de schade werd verklaard door deze vier relatief simpele indicatoren. Het energieverbruik was de beste voorspeller van schade aan de volksgezondheid, met name door emissies die samenhangen met energiegebruik, zoals fijnstof, koolstofdioxide en zwaveloxides. Voor schade aan biodiversiteit waren zowel het energieverbruik als het landgebruik van belang. De resultaten geven aan dat deze eenvoudige indicatoren kunnen dienen als benadering voor de complexere indicatoren voor schade aan de volksgezondheid en ecosystemen.

Twee hoofdconclusies van dit proefschrift zijn:

1 *Regressieanalyse is een bruikbare methode om de klimaatimpact van elektriciteitscentrales te schatten met relatief geringe onzekerheid voor gascentrales met een gecombineerde gas- en stoomcyclus, gemiddelde onzekerheid voor kolencentrales en een relatief hoge onzekerheid voor gas- en oliecentrales met een enkele stoomcyclus.*
2 *Een gelimiteerde set met indicatoren voor respectievelijk fossiele energie (of broeikasgassen), land en toxiciteit omvat reeds een groot deel van de variatie in milieuimpacts tussen producten.*

Vervolgonderzoek kan zich richten op (i) het ontwikkelen van regressiemodellen voor andere productgroepen waar variabiliteit van belang is en data-schaarste een probleem is, zoals landbouwproducten, (ii) het bepalen van de invloed van temporele variabiliteit in klimaatimpact van hernieuwbare en niet-hernieuwbare energiebronnen, (iii) het nader bepalen van de robuustheid van de simpele indicatorensets wanneer ruimtelijke variabiliteit volledig wordt meegenomen in de berekening van de milieuschade (iv) het toevoegen van belangrijke, maar vooralsnog ontbrekende, mechanismen (zoals bio-invasies of verkeersslachtoffers) die leiden tot schade aan de biodiversiteit of volksgezondenheid aan de huidige methoden voor milieu-analyse van producten.

Summary

A multitude of environmental footprint methods has been developed to determine the environmental impact of products and services provided by our economy. A guiding principle of these footprint methods is that they evaluate the impact over the full life cycle of a product or service to avoid burden shifts from one life cycle stage to another stage. A full life cycle approach covers all relevant stages from extraction of the raw material through manufacture, use and eventually waste disposal. Environmental footprint indicators can be derived at different stages along the cause-and-effect chain, which describes how a human need (driver) for a product or service ultimately leads to environmental damage. Resource-based indicators are located at the start of the chain while endpoint indicators are used to quantify the effect on human health or biodiversity. Midpoint indicators are situated somewhere between the initial emission or resource use and the eventual endpoint impact.

A large amount of life cycle data is required to calculate environmental footprints. The further one progresses along the cause-and-effect chain, the more information about the damage pathway is required. This need for data can result in an increased uncertainty in environmental footprint calculations. Apart from uncertainty, life cycle data also comes with variability, reflecting real-world differences between for example technologies or regions. Further, a large number of footprint indicators has been developed on the level of resources, midpoints and endpoints. It is unclear whether all these indicators are required for a comprehensive environmental footprint assessment.

The goal of this thesis was to reduce uncertainty and redundancy in environmental footprinting. More specifically the following two research questions were addressed:

1 *To what extent can uncertainty be quantified and reduced in environmental footprints, with a focus on the carbon footprint of fossil-fired power plants?*
2 *What is the optimal representative set of impact indicators to be used for environmental footprinting?*

In Chapter 2, the uncertainty and variability in the carbon footprints of coal-fueled power plants in the United States were quantified separately. Parameter uncertainty was quantified via Monte Carlo simulation, while variability was determined by identifying separate life cycle chains (from mine to power plant) for 364 individual coal-fueled power plants in the USA. The results show that the spread in carbon footprints is dominated by variability between the power plants, which in turn is primarily caused by differences in power plant efficiencies. It was also shown that the carbon footprint of coal-fired electricity production in the US can be reduced by 6% increasing the efficiency of the 95% worst-performing power plants to the 95-percentile benchmark efficiency of 35%.

Data required to calculate power plant-specific carbon footprints are lacking for most parts of the world. Regression models were developed in Chapters 3 and 4 to estimate carbon footprints of power plants without empirical data, but with information available on technological characteristics. The models developed had a predictive power of 49% to 81% with steam pressure (for coal) and fuel or plant type as most important predictors of the carbon footprints. The largest uncertainty was found for the carbon footprints of single cycle gas and oil plants, while the carbon footprints of combined cycle gas plants were predicted with less uncertainty. The uncertainty for the coal fueled power plants had an intermediate level.

Hundreds of indicators have been developed to quantify the environmental footprints of products. In Chapter 5, 135 of these indicators were compared for a set of 976 products in the life cycle database Ecoinvent. Principal Component Analysis (PCA) combined with regression analysis was used to identify a minimal set of indicators that covers the maximum amount of variance. This set consisted of six midpoint indicators, representative of climate change, land use, ozone depletion, a combined indicator of acidification & eutrophication, marine ecotoxicity and terrestrial ecotoxicity. Together these six indicators covered 92% of the variance in product rankings. A set of four resource footprints was also tested because these are more easily available, this set (covering energy, water, land and materials) covered 84% of the variance.

In Chapter 6, the same calculation procedure was applied to 119 environmental footprint indicators for 6982 product-region combinations within the Environmentally Extended Multi Regional Input Output (EEMRIO) model EXIOBASE. Eurostat proposes a set of four headline indicators (climate, land, water and material footprints) to be used for sustainability assessment, which can be supplemented with additional indicators if necessary. This headline set covered almost 60% of the variance with the energy and land footprint covering 57%. Adding an indicator of marine ecotoxicity increased the explained variance to more than 80%, indicating that the toxicity-related footprints were not covered well by the headline indicators. To explain 95% of the variance, the headline set of indicators needed to be supplemented with indicators of marine ecotoxicity, terrestrial ecotoxicity, photochemical oxidation, terrestrial acidification and eutrophication. Both Chapters 5 and 6 demonstrate that to adequately rank products only a small subset of the 100+ environmental footprint is needed.

The extent to which endpoint indicators of damage to biodiversity and human health can be approximated by a set of resource footprints (energy, land, water and material) was determined in Chapter 7. The four resource footprints covered 90% of the damage to biodiversity and human health, demonstrating that resource footprints do provide good proxies of environmental damage. The energy footprint was the most important predictor for human health damage, mainly because of emissions that are related to energy use, such as fine particulate matter, carbon dioxide and sulfur oxides. Both the energy and the land footprint were important predictors of damage to biodiversity.

In Chapter 8 the main results of this thesis are discussed and synthesized. The two main conclusions of this thesis are that:

1 *Regression analysis is useful to predict the carbon footprints of fossil-fired power plants with low uncertainty for combined cycle gas plants, intermediate uncertainty for coal fueled power plants and relatively high uncertainties for single cycle gas and oil plants.*
2 *Environmental footprints related to fossil energy (or GHG emissions), land and toxicity embrace a large share of resource, midpoint and endpoint footprints derived via the Ecoinvent and EXIOBASE datasets.*

Future research may include (i) the development of regression models for other product groups in LCA where variability is relevant and predictors are available, such as agricultural products, (ii) the investigation of the influence of temporal variability on life cycle greenhouse gas emissions from both renewable and fossil electricity generation, (iii) a further evaluation of the robustness of the optimal set of environmental indicators with spatially-differentiated impact assessment methods and (iv) to improve life cycle impact assessment methods by including those major drivers of biodiversity and human health damage that are not yet covered and that are attributable to specific life cycle interventions, such as road traffic accidents and the introduction of exotic invasive species.

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About the author

CURRICULUM VITAE

I was born in Nijmegen on June 1st 1986. I moved to Wijchen when I was 8 years old, where I still live today. After graduating in 2004, I briefly studied Natural Sciences and Psychology, before switching to Biology in 2006. I got my bachelor's degree in Biology (cum laude) and my master's degree in Environmental Sciences (*cum laude*) at the Radboud University in Nijmegen. In April 2012, I started to work as a junior researcher at the Department of Enviromental Science at the Radboud University in Nijmegen. Initially I worked on a project funded by ExxonMobil, this project was aimed at quantifying uncertainty and variability in the carbon footprint of fossil energy generation. The work I did for that project was an extension of the work I started as a Master's student. During this project I visited the ExxonMobil research lab in New Jersey for a period of around 10 weeks in the summer of 2012. After that I worked on several other projects, but primarily on a Seventh Framework Programme project called DESIRE (Development of a System of Indicators for a Resource efficient Europe). The combined output of these projects resulted in this PhD thesis. In June 2016, I started to work as a post-doctoral researcher at the Department of Environmental Science at the Radboud University in Nijmegen.

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