A Methodology for Integrated, Multiregional Life Cycle Assessment Scenarios under Large-Scale Technological Change

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Ⓢ Supporting Information

ABSTRACT: Climate change mitigation demands large-scale technological change on a global level and, if successfully implemented, will significantly affect how products and services are produced and consumed. In order to anticipate the life cycle environmental impacts of products under climate mitigation scenarios, we present the modeling framework of an integrated hybrid life cycle assessment model covering nine world regions. Life cycle assessment databases and multiregional input−output tables are adapted using forecasted changes in technology and resources up to 2050 under a 2 °C scenario. We call the result of this modeling "technology hybridized environmental-economic model with integrated scenarios" (THEMIS). As a case study, we apply THEMIS in an integrated environmental assessment of concentrating solar power. Life-cycle greenhouse gas emissions for this plant range from 33 to 95 g CO_2 eq./kWh across different world regions in 2010, falling to 30−87 g CO_2 eq./kWh in 2050. Using regional life cycle data yields insightful results. More generally, these results also highlight the need for systematic life cycle frameworks that capture the actual consequences and feedback effects of large-scale policies in the long term.
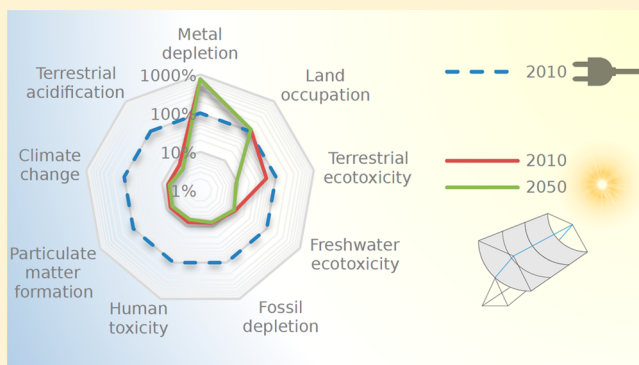
1. INTRODUCTION

A 2 °C global average temperature increase is considered the threshold above which global warming consequences on human health, ecosystems, and resources might be disastrous. Pathways incorporating a combination of a shift toward low-carbon energy technologies, efficiency improvements, and a decrease in final consumption present various ways to reduce greenhouse gas emissions as means to reach climate targets. In effect, climate change mitigation demands large-scale technology change on a global level and, if successful, will significantly affect how products and services are produced and consumed. Understanding the future life cycle implications of this substantial change requires a modeling of technological deployments in the global economy.

In general, life cycle assessment (LCA) studies provide static snapshots of systems at a given moment in the past or in a hypothetical future for a given region. In contrast, energy scenario models trace fuel chains, and do not account for the life cycle aspects related to the energy systems' infrastructure. This paper demonstrates a methodology that combines these approaches to overcome the shortcomings of each. Depending on the large scale impact of a certain technology's deployment, the whole life cycle impact of any given product may be affected. Modifications predicted in climate change mitigation roadmaps address all sectors of the economy, from electricity

generation through transportation to cement production. It is therefore essential to assess these modifications based on a model that contains all life cycle phases of both existing and emerging technologies.

Extending LCA to future scenarios is an arguably effective way to understand the implications of long-term changes such as those planned in climate change mitigation roadmaps. In a review of LCA methodology, Guinée et al.[1] argue: "It may be more realistic [than microscopic consequential product LCAs] to start thinking how more realistic, macroscopic scenarios for land use, water, resources and materials, and energy (top-down) (...) can be transposed to microscopic LCA scenarios." In a review of LCAs of energy technology systems, Masanet et al. emphasize the usefulness of combining LCA with input−output analysis and scenario models.[2] A survey by Reap et al.[3] and a more complete summary of the state of the art in LCA by Finnveden et al.[4] raise concerns that the time dimension in LCA is often overlooked. Attempts to address time dependency and scenarios in LCA have increased over the past decade,[5−9] including with the use of input−output analysis.[10−12] In

scenario modeling, the relevance of including information from LCA is increasingly recognized. The IPCC writes, "By extending scenario analyses to include life cycle emissions and the energy requirements to construct, operate and decommission the different technologies explicitly, integrated models could provide useful information about the future mix of energy systems together with its associated life cycle emissions and the total environmental burden." (see ref 13, p. 729).

Proposed here is a method for assessing the environmental and resource implications of the large-scale adoption of climate change mitigation measures, which includes various scenarios, and present a model implementing this method. We call this model the technology hybridized environmental-economic model with integrated scenarios (THEMIS). We use THEMIS to evaluate technologies from a life cycle perspective by calculating the material and energy inputs and outputs to production, operation and maintenance, and disposal. With the increasing utilization of renewable energy technologies and energy conservation, the importance of quantifying life cycle impacts increases, as relatively fewer impacts take place directly at power stations and relatively more impacts occur upstream in supply chains. The THEMIS framework consists of three main features. (i) A multiregional life cycle assessment framework that hybridizes process LCA and input—output, thereby providing for more complete life cycle inventories, including, for example, the input of services. (ii) The electricity generation and other key activities described in the input—output and life cycle databases reflect the market mixes and production volumes of existing scenario models, including the deployment of novel technologies in specific regions. (iii) The products modeled in the foreground are used in the process LCA and MRIO backgrounds, replacing the production of commodities (e.g., electricity, materials) to the degree foreseen in the scenario. Downstream impacts are thus addressed via linkages between foreground inventories to background processes and sectors. We illustrate this approach in the present paper by applying the resulting model on the life cycle inventory of a concentrating solar power (CSP) plant. Furthermore, THEMIS underpins the results of Hertwich et al., a companion paper that applies its principles to the case of global low-carbon electricity scenarios (including the CSP inventory described here).[14] Other applications have been carried out, taking advantage of the flexibility of the model, using various foreground systems such as lighting[15] or building energy management systems,[16] or even using CEDA (comprehensive environmental data archive[17]) in lieu of EXIOBASE (database originally created for EXIOPOL, externality data and input—output tools for policy analysis[18]) as an input—output background.[19] The present paper focuses on the generic and adaptable framework fundamental to these studies.

2. MATERIALS AND METHODS

2.1. General Outline. In this paper, we present an approach for scenario modeling in LCA as suggested by Guinée et al.[1] We embed a process LCA database in a multiregional input—output (MRIO) description of the global economy[18] using a hybrid LCA framework.[20−23] An LCA database contains physical information regarding the material and energy flows occurring over the life cycle phases of given processes, as well as their associated environmental emissions and natural resource use ("stressors"). An MRIO table is generally defined as a symmetric input—output table containing

the domestic monetary transactions of a set of regions, as well as the trade data between these regions. The MRIO database used in this study is extended with environmental stressor data for each economic sector. The frequently cited advantage of hybrid LCA is a more comprehensive coverage of inputs from the use of input—output tables while retaining the detailed process descriptions from process LCA. The current work also provides an additional advantage by embedding process LCA in an MRIO model, giving us the opportunity to capture the structure of regional electricity production under different energy policy scenarios, as illustrated in Lenzen and Wachsmann's study on the geographical variability of the life cycle impacts from wind turbines.[24] Market shares, energy conversion efficiencies and capacity factors are also adjusted to follow regional variations. Furthermore, we link the functional units of the foreground life cycle inventories back into the input—output description of the economy, thus achieving the closure that has been suggested for integrated hybrid LCA.[25] In this way, we also capture the downstream use of the product system by other parts of the economy and its feedback to the economy itself.[26] To note, in this work, we assume a symmetric LCI database; in comparison, Suh provides a general framework for both symmetric and nonsymmetric (but invertible) databases.[25]

In LCA, a distinction is often made between a foreground system, which describes the assessed product system and contains the data collected for most direct inputs, and a background system, which is commonly a generic life cycle inventory (LCI) database.[15,20] In a hybrid LCA, the foreground system typically requires both physical inputs from the process LCI database and economic inputs from the input—output database. We adopt the following notation[22] to describe the technology matrix and its associated variables:

$$
A_t = \begin{pmatrix} A_{ff,t} & A_{fp,t} & A_{fn,t} \\ A_{pf,t} & A_{pp,t} & A_{pn,t} \\ A_{nf,t} & A_{np,t} & A_{nn,t} \end{pmatrix}
\tag{1}
$$

$$
F_t = \begin{pmatrix} F_{f,t} & F_{p,t} & F_{n,t} \end{pmatrix}
\tag{2}
$$

Here, A and F are the technology and stressor (or factor) matrices, respectively. The index f denotes the set of foreground processes, or the direct inputs to the technology being studied, p indicates the set of physical background processes, and n the set of sectors of the economic input—output system. For example, $A_{fp,t}$ denotes the matrix of coefficients from foreground f to physical background processes p in year t. $A_{ff,t}$, $A_{pp,t}$, and $A_{nn,t}$ are therefore square and symmetrical. $A_{pp,t}$ and $A_{nn,t}$ may be multiregional, and all subsequent equations apply both to single-region or multiregional matrices, unless otherwise mentioned. Since there is no linkage between physical and economic databases ($A_{pp,t}$ and $A_{nn,t}$, respectively), $A_{np,t} = A'_{pn,t} = 0$, an appropriately sized null matrix. Prospective LCA scenario modeling is achieved by integrating the foreground into the background, bringing forth nonzero values in $A_{fp,t}$ and $A_{fn,t}$. When nonzero values are introduced in $A_{fp,t}$ and $A_{fn,t}$, adjustments to the background matrices are needed to avoid double-counting: the background inputs and emissions to the corresponding sector or process are zeroed out, as shown later in eqs 8 and 9. In the following, $\tilde{A}$ denotes a version of a technology matrix that has undergone
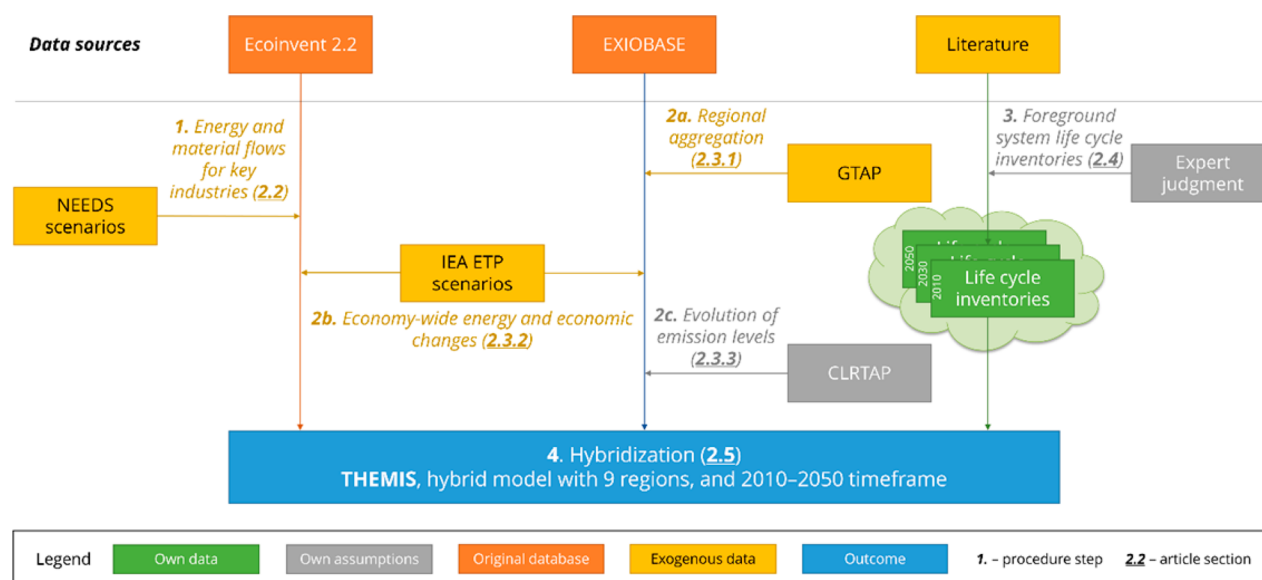
Figure 1. Structure of the model, and interactions between the various data sources. Main data sources are the International Energy Agency's (IEA's) Energy Technology Policy (ETP) scenarios, the *ecoinvent* life cycle inventory database, the *EXIOBASE* multiregional input—output database, and the New Energy Externalities Development for Sustainability (NEEDS) scenarios for life cycle inventories, the Global Trade Analysis Project (GTAP), and the European Convention on Long-Range Transboundary Air Pollution (CLRTAP).

such adjustments. Index t denotes time as matrices are derived for years 2010, 2030, and 2050.

When assessing new energy technologies that are penetrating a market, feedback effects arise. In the case of electricity generation, foreground systems that describe the production of power plants and fuels must become part of the background electricity, which in turn is part of the energy mix used to build future power plants. In the following, *technology* refers to a distinctive category of electricity generating systems using a specific pathway from an energy source to electricity generation (e.g., photovoltaic (PV) technology). A *system* refers to a technology variant (e.g., ground-mounted cadmium-telluride PV system).

The design of THEMIS consists of four steps, shown in Figure 1, and which are described in the next sections. First, we implement technological efficiency improvements of key sectors, such as metals and construction material production and transportation, in the databases in a manner consistent with the scenario. As efficiencies are likely to improve over time, we produce separate tables for each time step (2010, 2030, 2050) that reflect each of the model years according to the nine model regions. Second, we incorporate parameters from the energy scenario in the background LCI and MRIO databases, and adjust the background databases to represent production and consumption in the model years. We also implement separate scenario information for the potential reduction of conventional emissions in the MRIO database following the European Convention on the Long-Range Transboundary Air Pollution (CLRTAP).[27] Third, we compile life cycle inventories for the foreground processes. We model electricity generation specifically, as a change in electricity generation technology will be most radical under climate change mitigation and will have the largest impacts on the life cycle of other products. Inputs to the foreground system can be either physical inputs from the process LCI database or economic inputs from the input—output database. Fourth, we link the foreground life cycle inventories back to the background by replacing technologies already represented in the background, or

appending new ones and changing the production mixes of the background with each time step. The model thus becomes fully integrated. The exogenous scenarios altering the original databases are applied in a complementary manner. The NEEDS inventories mainly address industrial processes, whereas the IEA scenarios describe electricity sectors. They are therefore not consistent with each other in a strict sense; however they align with the same target (i.e., a 2 °C global warming by 2050).

The hybrid LCA setup is similar to earlier scenario work for CO_2 capture and storage[28] and wind power.[29] A commonly used process-level LCI database, *ecoinvent* 2.2,[30] serves as $A_{pp,0}$ while a multiregional input—output database, *EXIOBASE*, in its first version,[18] serves as $A_{nn,0}$ in eq 1. Their respective environmental extensions, once harmonized, serve as $F_{p,0}$ and $F_{n,0}$ in eq 2. The BLUE Map and Baseline scenarios of the International Energy Agency's (IEA) Energy Technology Perspectives (ETP)[31] are used to explore two different futures: one with aggressive climate change mitigation, or the BLUE Map scenario, and one without coordinated efforts to reduce greenhouse gas emissions, or the Baseline scenario.

2.2. Adjustments to Process LCI Database. *Ecoinvent* 2.2[30] is used as the background process LCI database. The use of a preallocated database is a prerequisite for the following adjustments, which are only valid for a square matrix. In this matrix, electricity mixes are adjusted to align with the respective energy scenarios. These adjusted mixes are presented in the Supporting Information (SI). Likewise, key industrial production processes are altered to represent the projected average technology of 2030 and 2050. These processes are namely aluminum, copper, nickel, iron, and steel, metallurgical grade silicon, flat glass, zinc, and clinker. These processes and their forecasted values are also available in the SI.

We create versions of the *ecoinvent* 2.2 database for each region and time period by changing the electricity mix using matrix multiplication. Let J be an identity matrix of the same size as the *ecoinvent* database's original matrix, A_{orig}. Let k be the index of any power generation technology contributing to the original electricity mix, and l the index of any technology

contributing to the new electricity mix. Now let $j_{kk} = 0$ (instead of 1, those being the diagonal elements of J) and $j_{lk} = 1$ (instead of 0). The new database is obtained multiplying the pseudoidentity matrix J with A_{orig}: $A_{new} = JA_{orig}$. This method can be generalized in order to adjust process LCI databases to any set of scenario assumptions.

Life cycle inventories of key industrial processes for 2030 and 2050 are adapted according to the inventories produced by the New Energy Externalities Development for Sustainability (NEEDS) project.[32] The authors of NEEDS developed LCI data fitting to the *ecoinvent* database, using expert judgment and technology roadmaps for various technologies as well as a set of scenarios until 2050 to reflect both assumptions of varying optimism and different policies. We identified NEEDS' realistic-optimistic scenario as the closest match to the BLUE Map scenario assumptions, namely the deployment of best available techniques, and reasonable efficiency trends. We applied these exogenous data in a complementary way.

2.3. Adjustments to Input−Output Database. A nine-region MRIO model is constructed to reflect the nine world regions represented by IEA energy scenarios.[31] These regions are formed by aggregating the countries and regions from the *EXIOBASE* database.[18] To be consistent with the process-based life cycle inventory database, the symmetric commodity-by-commodity input−output tables of *EXIOBASE* are selected for use in the model. Since there is no perfect many-to-one match between the original 44 *EXIOBASE* regions and nine IEA regions, the higher-resolution GTAP MRIO model[33] is used to split the large "rest of world" IEA region, as shown in the SI. Forecasted electricity generation and installed capacity data provided by the IEA are also used to adapt the database to current and future years. Several important parameters implemented in THEMIS are include population; GDP; industry final energy demand; total primary energy demand and final energy consumption (including nonenergy use) of coal, oil, gas, heat, biomass, and waste and other renewables; power generation capacity and actual annual power production for 15 types of electricity generation sectors (section 1 of the SI); investment sums; operation and maintenance costs; efficiency; and learning rate for these technologies. Other parameters and data needed for disaggregation or to adjust parameters in the original data are presented in Sections 4−9 in the SI. Regional aggregation is achieved simultaneously with the disaggregation of electricity sectors, as presented in the next section.

Electricity supply is modeled in the original version of *EXIOBASE* through six electricity sectors: coal, natural gas, nuclear, hydropower, wind power, and a category for all remaining electricity sources, "oil, biomass, waste and nowhere else classified". The total number of sectors is m (here, $m = 129$). We expand this set of electricity supply sectors with eight additional technologies: coal with carbon dioxide capture and storage (CCS), natural gas with CCS, biomass and waste, biomass and waste with CCS, ocean and tidal, geothermal, solar photovoltaics, and concentrating solar power. We further disaggregate the wind power sector into the wind onshore and wind offshore sectors, therefore adding nine electricity sectors. New electricity mixes are applied to the existing database through the modification and disaggregation of electricity sectors in the coefficient matrix. The original number of electricity sectors is k (here $k = 6$), while the new number of sectors is l ($l = 15$). See section 6 of the SI for the redistribution of inputs to each electricity sector. The new electricity share

vectors, v_c, contain $m − k + l$ elements for a given country or region, c. The sum of any row of v_c equals one. The conversion matrix H_{el} has as many columns as the original coefficient matrix (A_{nn}) and as many rows as the new one (defined as $\tilde{A}_{nn}$). The blocks of H_{el} that correspond to domestic electricity-to-electricity flows (of dimensions $k \times l$) are populated with the elements of $v_c i$, with i being a row vector of m ones.

In the case of a multiregional matrix, regional aggregation can be achieved simultaneously with electricity sector disaggregation. In this case, a region-to-region concordance matrix, H_{reg}, of dimensions $r_{orig} \times r_{new}$, with r_{orig} the original number of regions (before aggregation; here, 44) and r_{new} the new number of regions (after aggregation; here, nine) is required. A new concordance matrix $H_{reg,el}$ can then be computed from H_{reg} and H_{el} as follows: $H_{reg,el} = H_{reg} \otimes H_{el}$, where $\otimes$ denotes the matrix direct product, or Kronecker product.[34] $H_{reg,el}$ has dimensions $r_{orig}k \times r_{new}l$. eq 3 describes the simultaneous process of electricity sector disaggregation and regional aggregation for a multiregional matrix.

$$\tilde{A}_{nn} = H_{reg,el}A_{nn}H'_{reg,el} \tag{3}$$

Market shares of new electricity systems are estimated based on a combination of IEA scenario data for the technology market shares, and expert judgment for the system market shares. Detailed market shares can be found in the SI. The input of each foreground system to the background electricity mix, h_{ij}, is therefore a multiplication of two (or three) factors:

$$h_{fp,ij} = \alpha_i \beta_{ij} \tag{4}$$

$$h_{fn,ij} = \alpha_i \beta_{ij} \gamma_{ij} \tag{5}$$

The values $h_{fp,ij}$ and $h_{fn,ij}$ are the flows of the foreground-to-background quadrant of the technology matrix for the process-LCA and the input−output parts, respectively. Inventories are constructed and scaled to a functional unit, the mathematical quantity of product delivered by a system, typically one plant or one kWh. Additional factors are introduced to scale this flow appropriately. In eqs 4 and 5, α_i is the inventory scaling factor, in kWh per functional unit, that is, "one plant" or "one kWh" in a specific region, at row i. The value β_{ij} is the share of functional unit i in process or product j, that is, the physical share of each electricity generating system's functional unit entering a corresponding background's electricity process. Finally, in eq 5 only, where a conversion to monetary unit is required, γ_{ij} is the price of one scaled functional unit, in euro per kWh in the present case. Prices are derived from an IEA report on the levelized costs of electricity (LCOE) and presented in the SI.[35]

Atmospheric emissions intensities per sector are also likely to change due to improved efficiency and pollution control policy. The atmospheric emissions considered in *EXIOBASE* include greenhouse gases, heavy metals and particulate matter. These substances are controlled, reported, and regulated. To estimate the future evolution of national emissions, we have assumed continuity with the historical evolution of most of these pollutants in Europe. The model thus relies on the assumption that future emissions per euro will decrease as pollution control technologies improve and regulations become stricter worldwide, and that it will do so at the same pace as it has in Europe for two decades. To project these potential changes in the model, we adapt existing trends of certain pollutants from 1990 to 2009 in the EU27 from the Convention on Long-Range Transboundary Air Pollution (CLRTAP) historical data for the
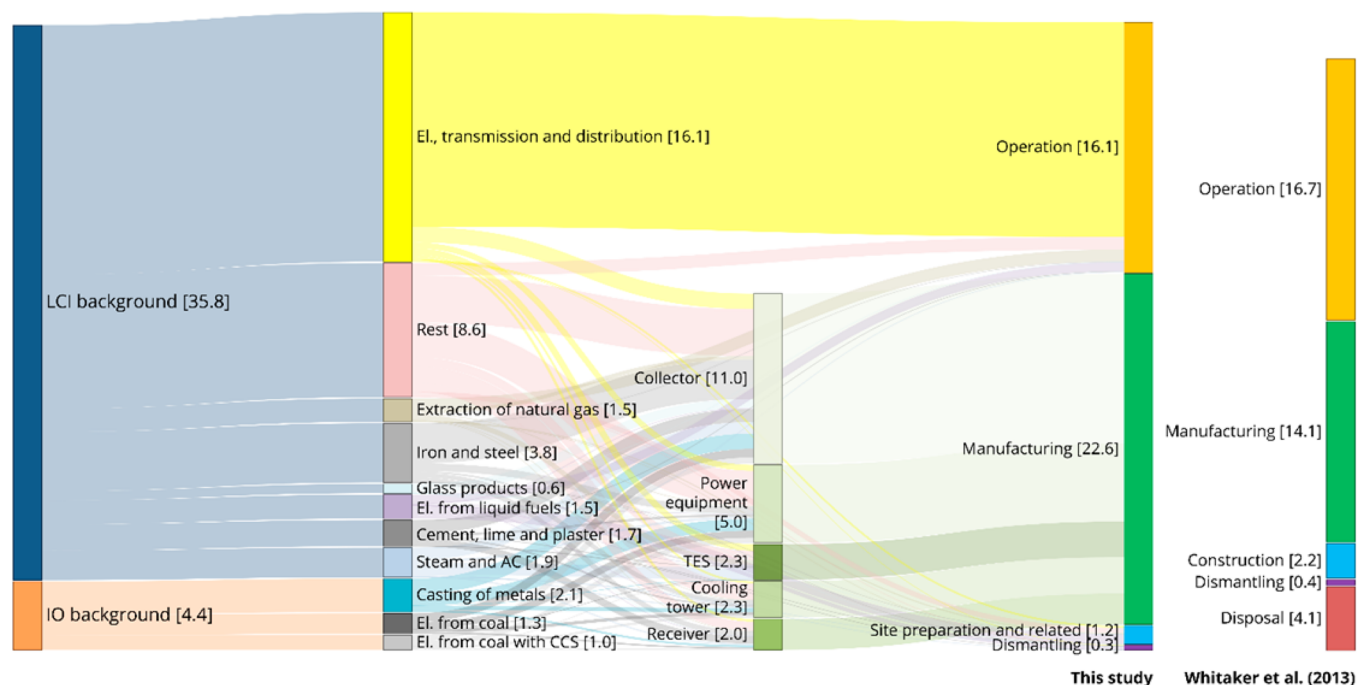
Figure 2. Contribution analysis of the impact on climate change of hybrid LCA results for 1 MWh of electricity produced by a concentrating solar power plant, central tower, in the North America region, in kg CO_2 eq Right hand side: foreground contribution analysis in this study vs Whitaker et al.[37] TES = thermal energy storage, El. = electricity.

EU27 for the following pollutants: Cd, CO, dioxins, HCB, HCH, mercury, NH_3, NMVOC, NO_x, lead, PCB, PM_{10}, $PM_{2.5}$, SO_x, and total PAH.[27] With the notable exception of copper emissions and arsenic emissions, these pollutants cover the most important environmental stressors used in *EXIOBASE* that contribute to the selected impact categories. We take the following approach to adapt these data to our model: pollutant emissions are normalized by the total GDP of the EU27 countries during the time period of 1990−2009 in order to adjust for changes in economic output that could increase or decrease overall emissions. For each substance, a linear ordinary least-squares regression is used to model the trend in emission levels in the 1990−2009 time period and, on this basis, extrapolated to 2050. Finally, improvement factors are derived from this extrapolation. This method is a first approximation of what can be achieved under continued efforts in pollutant control. Regressions are shown in the SI. Best estimates are used to reallocate inputs after disaggregation; Section 6 of the SI shows how economic sectors were linked to each electricity sector.

2.4. Foreground System LCI. Emerging and future technologies such as coal- and gas-fired power plants with carbon capture and storage, large onshore wind turbines, or concentrating solar power plants are underrepresented in *ecoinvent* 2.2; we have therefore built life cycle inventories for missing or misrepresented processes. Data sources for these life cycle inventories are listed in the SI. A key feature of this modeling framework is the use of foreground systems; in this implementation, we use the inventories compiled in Hertwich et al.[14]

2.5. Hybrid Integration. Upstream requirements include all flows from background sectors to the foreground life cycle inventories. All flows from either process or economic background to foreground are provided for each technology. Both process-to-economic (A_{pn}) and economic-to-process

(A_{np}) backgrounds are represented by zero matrices. In other words, economic sectors are assumed to give a complete representation of the economy, and process life cycle inventories are not hybridized. Double-counting is assumed to be avoided at the data collection stage.

Downstream flows comprise all flows from the foreground systems to any background sector. In our case, downstream flows stem from the modeled electricity generation systems in the foreground to the appropriate electricity generation mixes or sectors in the backgrounds. Their inclusion can be regarded as the key operation that completes the integration.

$$A_{fp} = H_{fp} \quad\quad\quad (6)$$

$$A_{fn} = H_{fn} \quad\quad\quad (7)$$

where H_{fp} and H_{fn} are matrices containing $h_{fp,ij}$ and $h_{fn,ij}$, respectively, from foreground process to life cycle inventory database and input−output database. These two matrices are structurally sparse, with only a few elements linking the foreground and background.[35]

Adjustments are required in the process-to-process background technology matrix:

$$\tilde{A}_{nn} = A_{nn}\widehat{\overline{i'H_{fn}}} \qu\quad\quad (8)$$

where i is an appropriately sized vector of ones, $'$ denotes transposition, $^-$ denotes the logical complementary operator (that changes nonzero values into zeros and vice versa), and $^\wedge$ denotes diagonalization. eq 8 zeroes out the sectors of A_{nn} that are already addressed by a market mix of foreground systems. It is equivalent to assuming that hybrid foreground systems are considered representative of an entire sector.

The same operation is applied to the stressor matrix, in which we assume that all direct emissions and direct requirements to and from the environmental compartments are covered by the foreground systems.
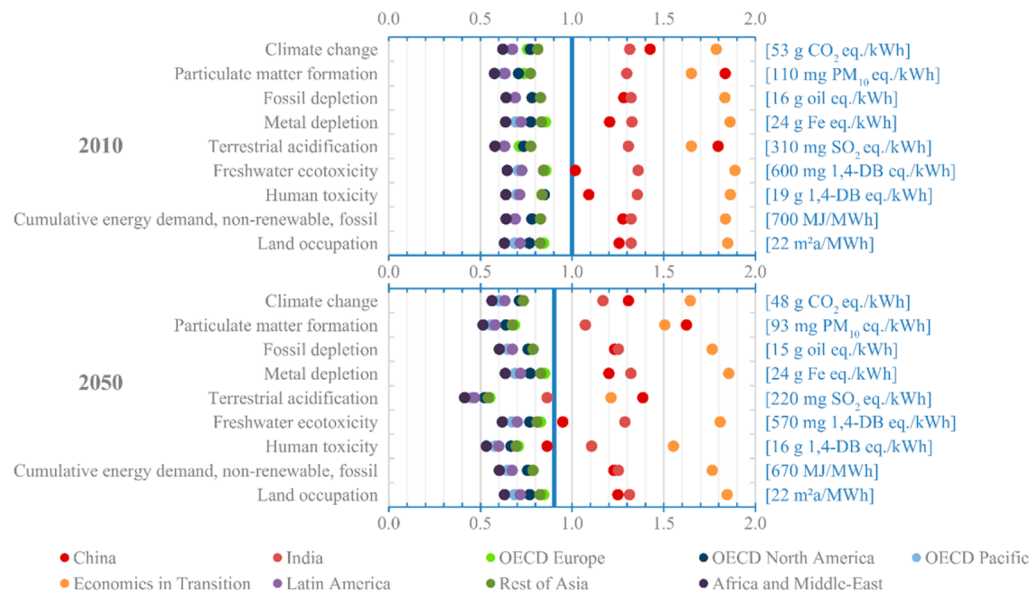
Figure 3. Comparison of selected life cycle impact assessment results of a concentrating solar power plant installed in each of the nine world regions for 2010 and 2050. The world average in 2010, weighted by regional expected production in 2050, is set to 1, with the absolute values on the right-hand side, in blue.

$$\tilde{F}_n = F_n \widehat{i' H_{fn}} \tag{9}$$

2.6. Impact Assessment. Once adapted, the model yields impact assessment results following eqs 10a and 10b.

$$d_t = CF_t(I - A_t)^{-1} y_t = CF_t x_t \tag{10a}$$

$$d_t = C \begin{pmatrix} F_{f,t} & F_{p,t} & F_{n,t} \end{pmatrix} \left(I - \begin{pmatrix} A_{ff,t} & A_{fp,t} & A_{fn,t} \\ A_{pf,t} & A_{pp,t} & A_{pn,t} \\ A_{nf,t} & A_{np,t} & A_{nn,t} \end{pmatrix} \right)^{-1} \begin{pmatrix} y_{f,t} \\ y_{p,t} \\ y_{n,t} \end{pmatrix} \tag{10b}$$

where d_t is the vector of environmental impacts at year t; C is a characterization matrix containing factors from ReCiPe 1.08;[36] F_t is the stressor matrix of the model, designed as described in section 2.3, at year t; A_t is the hybridized technology matrix at year t; and x_t and y_t are the total output and final demand at year t. Contribution analysis can be performed at the consumption level eq 11), production level eq 12, or through the advanced contribution analysis approach (eqs 15 and 16. The diagram shown in Figure 2 uses eq 16.

$$D_{pro,cons} = CF_t(I - A_t)^{-1}\hat{y}_t \tag{11}$$

$$D_{pro,prod} = CF_t \widehat{(I - A_t)^{-1} y_t} = CF_t \hat{x}_t \tag{12}$$

$$D_{pro,ff,t} = CF_{f,t} \widehat{(I - A_{ff,t})^{-1} y_{f,t}} = CF_{f,t} \widehat{x_{f,t}} \tag{13}$$

$$D_{pro,bf,t} = C \begin{pmatrix} F_{p,t} & F_{n,t} \end{pmatrix} \left(I - \begin{pmatrix} A_{pp,t} & A_{pn,t} \\ A_{np,t} & A_{nn,t} \end{pmatrix} \right)^{-1} \begin{pmatrix} A_{pf,t} \\ A_{nf,t} \end{pmatrix} \widehat{x_{f,t}} \tag{14}$$

$$D_{pro,f,t} = D_{pro,ff,t} + D_{pro,bf,t} \tag{15a}$$

$$= C \begin{pmatrix} F_{f,t} & F_{p,t} & F_{n,t} \end{pmatrix} \left(\begin{pmatrix} \widehat{x_{f,t}} \\ \left(I - \begin{pmatrix} A_{pp,t} & A_{pn,t} \\ A_{np,t} & A_{nn,t} \end{pmatrix} \right)^{-1} \begin{pmatrix} A_{pf,t} \\ A_{nf,t} \end{pmatrix} \widehat{x_{f,t}} \end{pmatrix} \right) \tag{15b}$$

$$= CF_t \begin{pmatrix} I \\ (I - A_{bb,t})^{-1} \begin{pmatrix} A_{pf,t} \\ A_{nf,t} \end{pmatrix} \end{pmatrix} \widehat{x_{f,t}} \tag{15c}$$

$$D_{pro,GWP,f,t} = \widehat{C_{GWP} F_t} \begin{pmatrix} I \\ (I - A_{bb,t})^{-1} A_{bf,t} \end{pmatrix} \widehat{x_{f,t}} \tag{16}$$

3. CASE STUDY

We illustrate the THEMIS model by calculating the life cycle environmental impacts of a concentrated solar power (CSP) plant based on foreground inventory data from Whitaker et al.[37] This inventory is developed in Hertwich et al.,[14] but we use it here to demonstrate the use of the method across the integrated framework. Whitaker et al. state that the original inventory was compiled in a hybrid "top-down" perspective, in which the input−output database was used when "the materials inventory for a specific component was not available," and when they "deemed that the environmental impacts resulting from a product's manufacture could not be accurately evaluated by summing the cumulative impacts of constituent raw materials."[37] The original power tower CSP plant is a 106 MW facility situated in Arizona, equipped with a two-tank thermal energy storage system. We adapted the original inventory to the THEMIS framework and performed an analysis simultaneously for the nine world regions. We performed a contribution analysis and compared the outcome with the original results.

Figure 2 shows the contribution of different processes and economic sectors, components, as well as life cycle stages, to the total greenhouse gas emissions. The life cycle stages are compared to those in the original study,[37] in which the life cycle greenhouse gas emissions of the central tower power plant amount to 37 g CO_2 eq per kWh. The results obtained with THEMIS span from 33 to 95 g CO_2 eq per kWh, for plants built and operated in the Africa and Middle-East region and the Economies in transition regions respectively, in 2010. This range falls to 30−87 in 2050. The main contributions to the life cycle greenhouse gas emissions are from the direct use of electricity from the grid (for auxiliary heating[37]), and iron and steel manufacturing, both from the LCI and the IO backgrounds. The Africa and Middle-East region offers the best direct normal insolation (DNI), 2468 kWh/m^2/year, whereas the Economies in transition region offers a lower insolation of 1991 kWh/m^2/year, as derived from Trieb et al.[38] The DNI assumed in the original LCI is 2400 kWh/m^2/year.[37] The climate change impact of a similar power tower plant therefore varies regionally, namely due to the variability of these aspects across regions: background industrial efficiencies, electricity mixes (especially as the operation and maintenance phase requires a substantial quantity of electricity), and DNI.

The assessment can be extended to other environmental impacts, as illustrated in Figure 3, representing the environmental impacts of 1 kWh of electricity produced at plant, for a set of ten indicators. Figure 3 displays a significant regional variation of impact indicator results, which are due to the regional differences in manufacturing. These regional differences are in turn caused by the differences in background industrial processes and in plant operation parameters resulting from differences in climate and achievable capacity factors. More specifically, the results for land occupation reflect differences in the DNI, while the other indicators reflect differences in both the DNI and in the regional technologies used to manufacture and operate the power plants. We can see, for example, that Latin America has below-average pollution-related environmental indicators, reflecting the larger share of hydropower in its energy mix. The Economies in Transition region has particularly high fossil fuel depletion and greenhouse gas emissions, reflecting both the low efficiency of the employed technologies and the intensive use of coal power. Similarly, China has high pollution-related indicators reflecting both the use of coal and the limited use of pollution control processes. It is worth mentioning that the Chinese coal sector has recently undertaken considerable improvements at the technological and provincial levels that have not been captured here. Henriksson et al. have indeed shown that greenhouse gas emission improvements are 2.5 times higher than *ecoinvent* 2.2's coal-based electricity production process for China.[39]

4. DISCUSSION

4.1. Implications. The application of THEMIS reveals that temporal and regional variations can have a significant impact on life cycle inventory results. In its current implementation, THEMIS focuses on the temporal and regional variation of electricity and key materials, which are responsible for a significant share of overall environmental problems. In the future, more parameters can be incorporated and adjusted by using the approach demonstrated in this paper. Consequently, the range of results yielded for a single technology may increase, and the dependence of impacts on these additional factors can be explored in a comparative analysis.

A core advantage with THEMIS is that it represents an integrated hybrid LCA of technologies, with the explicit inclusion of regional penetration rates. Traditionally, researchers have seen the reduction of cutoff errors as the main advantage of hybrid LCA, as the input−output table can trace thousands of process chains that are individually small but cumulatively important. The contribution from input−output sectors in Figure 2 shows that this advantage is also realized for concentrating solar power in the present model. The most important feature of THEMIS, however, is that the results of the foreground are fed back to the background system, contrary to most published hybrid LCAs. Thus, THEMIS is an integrated hybrid analysis where electricity from CSP becomes part of the electricity mix used to manufacture new CSP components. In this way, the analysis not only traces the upstream impacts of CSP production but also the effects of CSP use, an aspect seen as important for the prospective assessment of the impact of technologies.[26,40]

We show that the multiregionality of THEMIS is a clear advantage in comparing the implementation of similar systems across various world regions, climate, and other local characteristics. The analysis of a single system may lead to wide variations from region to region, especially for relatively local environmental impacts such as terrestrial ecotoxicity and acidification.

Life cycle assessment of systems in their future context appears to be essential to understand the various environmental impacts of mature and developing technologies. In the context of electricity generation, this remark is all the more important as electricity is an input to every sector in the economy. In this specific case, we observe previously unquantified feedback effects, now captured in THEMIS.[14] THEMIS has been used for various purposes. Bergesen et al. performed a comparative assessment of thin-film photovoltaic (PV) technologies using THEMIS as well as two hybrid life cycle inventories (foregrounds) representing the current and future design of two thin-film PV technologies, without full integration.[19] Hertwich et al. fully integrated foregrounds to the background data, to include assessed inventories in the various background electricity mixes. Hertwich et al. employed vintage capital modeling such that the construction, operation and decommissioning of each foreground system occur at different time points in the prospective model, thereby capturing technological improvements over the lifetime of energy systems.[14] Furthermore, the THEMIS modeling framework is currently being applied in two upcoming reports from the International Resource Panel to the United Nations Environment Programme regarding the cobenefits and adverse side effects of climate change mitigation technologies.[41] The second of these reports will contribute to a special issue of the *Journal of Industrial Ecology*; in this analysis, the THEMIS model is applied to quantify the prospective future impacts of demand-side energy efficiency technologies such as efficient light sources, efficient copper industrial cogeneration, electric vehicles, building envelope technologies, and demand management.

As energy systems develop both qualitatively through the adoption of new technologies, and quantitatively through efficiency gains and increases in installed capacity, their life cycle environmental impacts will change. For long-term decision-making based on sustainability, understanding future impacts of low-carbon technologies in addition to current impacts is necessary, as these technologies will represent the

upstream energy generation used in future materials production and economic activity. The LCA model can be used for prospective analysis of products. An integrated and prospective model, like ours, is essential to properly understand how the environmental impacts of products may change under scenarios of technological change.

4.2. Limitations and Recommended Further Work.

The combination of a heterogeneous set of data sets and their integration to existing databases introduce a number of inherent uncertainties. We have been especially careful to select compatible scenarios (e.g., NEEDS' "realistic-optimistic" and IEA's BLUE Map scenarios) in order to maintain a consistent set of assumptions. In particular, electricity price and cost assumptions, as well as the extrapolations of emissions trends are uncertainties that should be addressed in further research. First, electricity prices are modeling assumptions that link physical inventories with the input–output data, and are therefore part of a technological description of a sector. Quantifying their absolute uncertainty (namely across regions and years) is beyond the scope of this paper, but the price assumptions still allow relative comparison between technologies, regions, and years. Second, applying the emission levels extrapolated from the 1990–2009 European regulation trends for 16 atmospheric pollutants to all regions carries substantial uncertainty. This methodological choice was made based on data availability and on a level of ambition comparable to the NEEDS' and BLUE Map scenarios. As a reference for comparison, note that the emissions level is not adapted in the Baseline scenario.

Investments and capital formation have not been explicitly implemented in the model. Change to the use of capital stock has not been included in the IO part of the model (IO databases generally report annual flows of goods/services, with use of capital stock as an exogenous input). As suggested by Suh, making investments endogenous is a way to tackle that issue.[42] This limitation can be removed with the inclusion of capital consumption in the IO matrix. For present purposes, however, this limitation is a minor one, as inputs from the IO system are not indirectly capital intensive.

Another potential iteration of the THEMIS model would incorporate further integration of energy efficiency technologies into the foreground and background of the model. For example, the changing efficiency and impacts of metals production (e.g., copper) could further influence the long-term impacts of renewable energy technologies, thereby introducing even more feedback effects. Also, the deployment and technological development of electric and hybrid vehicles for both passenger and freight transport would similarly affect the life cycles of many products and services.

While it is impossible to predict which technologies will dominate the electricity market in 2050, it is nevertheless important to integrate all candidates in an existing LCI and input–output database. Additional research is needed to quantify uncertainty in technology adoption (e.g., market shares) and the rate of technological development (e.g., how quickly photovoltaic technologies will reach maturity). Despite these uncertainties, scenario assessment is a key to designing sustainable futures, and the THEMIS model is capable of performing due-diligence studies of long-term, low-carbon energy development scenarios.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.est.5b01558.

Data used to modify the original databases has been gathered in two accompanying files (PDF) (XLSX)

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