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Process to Planet: A Multiscale Modeling Framework Toward Sustainable Engineering

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To prevent the chance of unintended environmental harm, engineering decisions need to consider an expanded boundary that captures all relevant connected systems. Comprehensive models for sustainable engineering may be developed by combining models at multiple scales. Models at the finest "equipment" scale are engineering models based on fundamental knowledge. At the intermediate "value chain" scale, empirical models represent average production technologies, and at the coarsest "economy" scale, models represent monetary and environmental exchanges for industrial sectors in a national or global economy. However, existing methods for sustainable engineering design ignore the economy scale, while existing methods for life cycle assessment do not consider the equipment scale. This work proposes an integrated, multiscale modeling framework for connecting models from process to planet and using them for sustainable engineering applications. The proposed framework is demonstrated with a toy problem, and potential applications of the framework including current and future work are discussed. *AIChE J*, 61: 3332–3352, 2015
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Introduction

History is replete with examples of technologies that were developed and adopted with the intention of enhancing human well-being but, while meeting this goal, caused unintended and unexpected damage to the environment. Prominent examples include formation of the ozone hole due to the use of chlorofluorocarbons, climate change due to reliance on fossil fuels, and aquatic dead zones due to use of artificial fertilizers. This harm to ecosystem services—the basic life support for humanity—can make human activity unsustainable. The underlying causes for these negative impacts include the narrow boundary of traditional engineering that ignores the broader life cycle environmental implications of engineering decisions, and the practice of ignoring the role of ecosystems in enabling engineering activities.[1]

Life cycle assessment (LCA)[2,3] and related footprint methods[4,5] developed over the last two decades have become popular for considering the broader impacts of engineering activities. These methods consider activities from "cradle to grave" so that environmental impacts across the entire larger system may be assessed. Decisions based on such analyses are less likely to shift the impact outside the narrow boundary of engineering models and analysis. Cradle-to-grave methods, and LCA in particular, have been used to incorporate sustainability considerations into virtually all engineering fields, including product design, process design, supply chain design, planning and logistics, and economic and policy analysis.[6–9] Such methods quantify environmental impacts and incorporate them into the decision-making process, in addition to the more traditional technological and economic criteria such as profitability, safety, and reliability.

Methods for sustainable process and supply chain design use life cycle assessment to quantify environmental interventions, including pollutant production and natural resource consumption, attributable to the system being designed. Life cycle implications of the system are determined based on environmental interventions data for the production and distribution of all inputs to the designed system. The design problem is typically formulated as an optimization with at least two objective functions, one economic and one environmental.[10,11] Usually, the economic objective function is quantified with profit or net present value (NPV) of the system of interest, and the environmental objective function is quantified by an aggregated indicator such as global warming potential[12,13] or Eco-Indicator 99[14,15] based on the system of interest and its life cycle.

Most sustainable engineering methods follow a "bottom up" approach in that they model the system of interest in detail at the smallest relevant scale, using fundamental engineering models or plant- or product-specific data. The larger scale life cycle is modeled in less detail using empirical data that represents regionally average production technology. Such approaches are an appealing way of expanding traditional engineering design methods to incorporate life cycle considerations in engineering decisions, and have been applied to product design,[16,17] process optimization,[18] and supply chain design.[19] However, this approach suffers from some serious

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shortcomings. Using life cycle models from inventory databases requires defining a system boundary, generally by choosing which parts of the life cycle are considered to be most important. This process LCA method accounts for a relatively small proportion of the complete life cycle.[20] Because a large portion of the life cycle is neglected, any design decisions based on inventories used in process LCA are based on *incomplete* life cycle information and may, therefore, be suboptimal. In particular, the narrow process LCA system boundary allows environmental impacts to be shifted to processes outside the life cycle. As a result, impacts within the system boundary decrease but impacts generated outside the boundary may not change at all or may even increase.[21] In order to ensure correct, optimal design decisions and to avoid causing unintended harm, the full life cycle must be accounted for in the sustainable design problem. However, process LCA requires that each life cycle process and each connection between processes be modeled individually. Expanding the life cycle boundary is thus impractical and computationally intractable for moderately large life cycle networks, as the number of connections in any life cycle network is essentially infinite.[22]

In addition to the narrow life cycle boundary, the life cycle itself is modeled with fixed vectors of inputs and outputs that are scaled linearly.[23,24] Environmental interventions generated within the life cycle are modeled with constant emissions factors,[7,8,25] the values of which are assumed to be independent of the life cycle structure and of the system being designed. The life cycle model thus fails to capture effects of interactions between the life cycle and system of interest.

These challenges of using bottom up models also apply to most LCA and footprint studies. In LCA, "top down" methods have also been developed to analyze large systems at the regional, national, and global scales. Top down analyses rely on coarse, simplified models derived from highly aggregated empirical data. Environmentally extended input–output (EEIO) analysis is one example of a top down method,[26–28] and has been applied to sustainability studies up to the global scale.[29] Computable general equilibrium and partial equilibrium models[30,31] are other top down methods applied to macroscale sustainability analyses. Although top down models are comprehensive, particularly compared to process LCA, they lack detail at smaller scales.

LCA researchers have developed methods for integrating process LCA with EEIO models to result in hybrid LCA models.[32] These methods combine models of key life cycle processes with a narrow reach (value chain scale), with data from input–output models that are coarse and highly aggregated but with a broad reach (economy scale).[33–37] To date, sustainability studies using hybrid life cycle methods[38–40] have focused solely on analysis; there have been no applications of hybrid methods to sustainable design problems.

Life cycle studies and methods rely on empirical data from process and input–output LCA databases, and do not benefit from the availability of fundamental models of individual processes and equipment. Consequently, life cycle models, be they process model-based, input–output model-based, or hybrid, treat the constituent processes as fixed and linearly scalable. In practice, industrial processes are influenced by factors such as market conditions and corporate objectives, and benefit from economies of scale. In engineering design and analysis, such changes are captured using fundamental process models, but these benefits currently do not extend to life cycle methods. Conversely, the ability of LCA to consider scales all the way from the value chain to the planet does not extend to sustainable design. Characteristics of the models used in each of these methods are summarized in Figure 1.

This work develops a multiscale "process to planet" (P2P) modeling framework that integrates engineering models, standard life cycle models, and EEIO models to capture systems at multiple spatial scales. The P2P modeling framework connects detailed fundamental models of individual processes and unit operations at the "equipment" scale with linear, empirical models of averaged life cycle processes at the "value chain" scale and input–output models of the regional, national, or global economic system at the "economy" scale. Current hybrid LCA methods connect models at the value chain and economy scales, and the P2P framework expands the reach of these methods to fundamental models at smaller scales. The resulting model is both detailed and comprehensive, and can be used to capture the effects of small-scale decisions on a large-scale system and vice versa: the P2P framework thus combines the advantages of bottom up and top down methods while addressing the shortcomings of both. The framework is also highly versatile and can be used within an optimization formulation to solve virtually any sustainable engineering problem, from process design to multiperiod supply chain planning.[41] The flexibility of the P2P framework also enables design problems to be solved at scales larger than conventional sustainable process and supply chain design; for instance, design variables can be included at the value chain scale for the simultaneous design of a life cycle network and individual plants within the network. In a similar manner, design variables at the economy scale can be used to capture the effects of tax and other policies on the entire system, allowing policies to be designed according to the effect they have at smaller scales.

First, background is given on input-output models, EEIO analysis and life cycle assessment methodologies. The P2P modeling framework is then developed and demonstrated with a toy production system. The article concludes with a discussion of potential applications of the framework, including current and future work.

Background

This section gives a brief introduction to input–output analysis and life cycle assessment, two types of models that are incorporated into the P2P framework beginning in the next section. As each model is introduced, the reader is referred to the relevant portions of the section demonstrating the P2P framework with a toy system for basic examples of the model setup and application, including the data required and necessary calculations.

For the remainder of the article, the following notation will be used to distinguish between different types of models. An overbar $\bar{X}$ indicates models and variables at the economy scale, and an underbar $\underline{X}$ indicates models and variables at the value chain scale. Uppercase boldface quantities indicate matrices, and lowercase boldface quantities indicate vectors. Nonboldface quantities of both upper and lowercase indicate scalars which may be functions, variables, or constants. Subscripts are used to indicate matrix elements, matrix columns, vector elements, and sets of variables. Table 6 contains definitions of the various symbols and annotations used in this and subsequent sections.

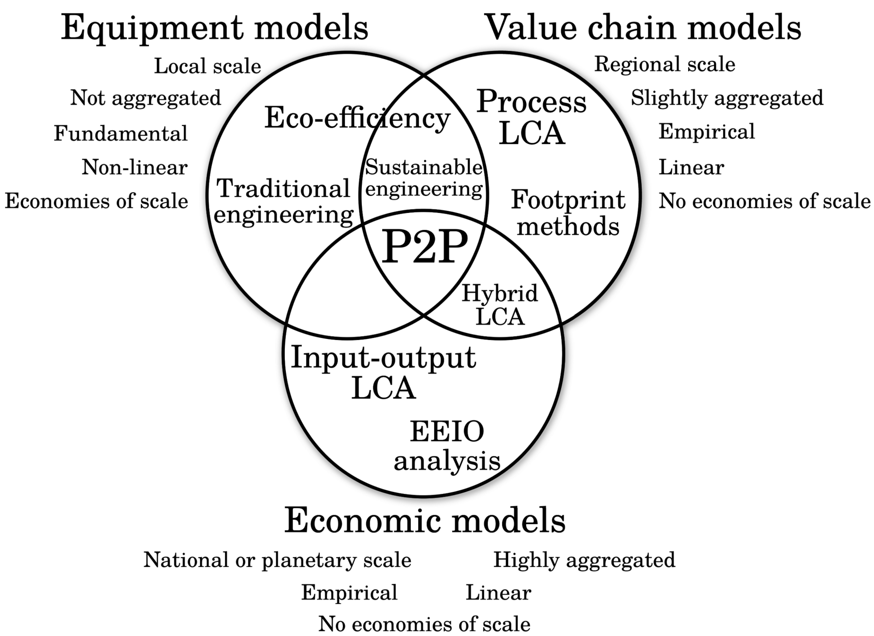

Figure 1. Methods, models, and characteristics.

Input–output analysis

Input–output models represent interdependencies within a large-scale economic system at a highly aggregated level.[42,43] An economic input–output (EIO) model is derived from a transactions matrix $\overline{\mathbf{X}}$, a vector or matrix of value added $\overline{\mathbf{v}}$, and a vector of final demand $\overline{\mathbf{f}}$. The transactions matrix contains commodity exchanges measured in monetary units between economic sectors for a specific time period, usually 1 year. Value added are inputs to production that are not produced by a sector within the economic system, such as labor. Final demand consists of commodities that are sold to purchasers that are not consuming sectors. A transactions matrix, value added and final demand for a two-sector economic system are given in Table 1.

A typical economic sector is highly aggregated, consisting of many processes and production technologies that produce similar products. The EIO model is much coarser than a typical life cycle model and represents sectors within a regional, national, or global economic system.

From the information in Table 1, the direct requirements matrix $\overline{\mathbf{A}}$ is calculated by normalizing the columns of $\overline{\mathbf{X}}$ by the total output $\overline{\mathbf{x}}$ of each sector, as follows[44]

$$\overline{\mathbf{A}} = \overline{\mathbf{X}}\hat{\overline{\mathbf{x}}}^{-1} \tag{1}$$

The elements of $\overline{\mathbf{A}}$ are technical coefficients. $\bar{a}_{ij}$ represents the amount of commodity input in dollars required from the ith producing sector per dollar output of the jth consuming sector. A fundamental assumption of input–output analysis is that the technical coefficients are fixed. This implies that (1) the amount of each commodity input required by a sector is directly proportional to the amount of output produced by that sector and (2) sectors consume commodities in constant proportions regardless of the amount of output being produced.

The total output of each sector is equal to the commodities consumed by other sectors within the economy, $\overline{\mathbf{A}}\overline{\mathbf{x}}$, plus the commodities sold as final demand, $\overline{\mathbf{f}}$. This relationship is an economy-wide balance on monetary flows, expressed as

$$\overline{\mathbf{x}} = \overline{\mathbf{A}}\overline{\mathbf{x}}+\overline{\mathbf{f}} \tag{2}$$

which is solved for $\overline{\mathbf{x}}$ by rearranging as follows

$$\overline{\mathbf{x}} = \left(\overline{\mathbf{I}}-\overline{\mathbf{A}}\right)^{-1}\overline{\mathbf{f}} \tag{3}$$

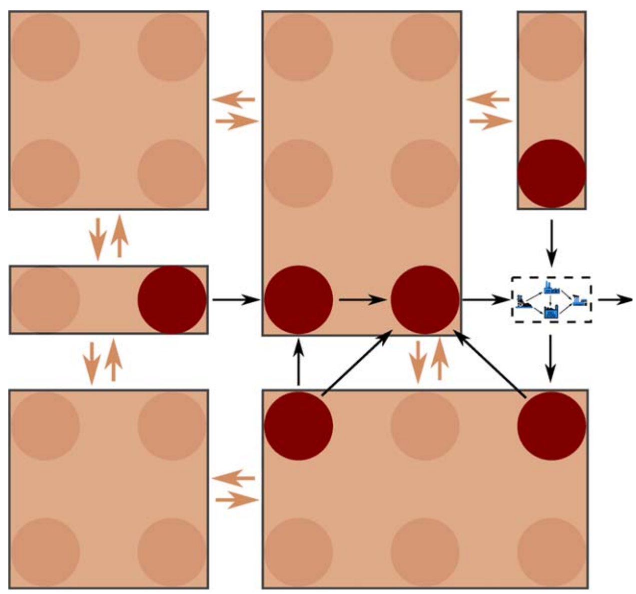

Figure 2. Hybrid life cycle assessment combines coarse, highly aggregated models (rectangles) with more specific models of key life cycle processes (dark circles).

The coarser models capture contributions from life cycle processes not included in process LCA (light circles). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 1. Transactions, Value Added, Final Demand, and Environmental Interventions for a Two-Sector Economic System

Producing Sectors ($)	Consuming Sectors ($)		Final Demand ($)	Total Output ($)
	Sector 1	Sector 2		
Sector 1	$\bar{x}_{11}$	$\bar{x}_{12}$	$\bar{f}_1$	$\bar{x}_1=\bar{x}_{11}+\bar{x}_{12}+\bar{f}_1$
Sector 2	$\bar{x}_{21}$	$\bar{x}_{22}$	$\bar{f}_2$	$\bar{x}_2=\bar{x}_{21}+\bar{x}_{22}+\bar{f}_2$
Value Added ($)	$\bar{v}_1$	$\bar{v}_2$		
Total Input ($)	$\bar{x}_1=\bar{v}_1+\bar{x}_{11}+\bar{x}_{21}$	$\bar{x}_2=\bar{v}_2+\bar{x}_{12}+\bar{x}_{22}$		
Environmental Interventions	$\bar{b}_{11}$ ⋮ $\bar{b}_{r1}$	$\bar{b}_{12}$ ⋮ $\bar{b}_{r1}$		

The matrix $\left(\bar{\mathbf{I}}-\bar{\mathbf{A}}\right)^{-1}$ is the total requirements matrix or the Leontief inverse.

Input-output data can also be represented in make and use matrices. Unlike the transactions matrix of Table 1, make and use matrices distinguish between sector inputs and outputs. The use matrix $\bar{\mathbf{U}}$ describes the consumption of commodities by sectors and has dimensions of $I \times J$, where I is the number of commodities and J the number of sectors. The make matrix $\bar{\mathbf{V}}$ describes the production of commodities by sectors and has dimensions of $J \times I$. When $I=J$, the use matrix is equivalent to the transactions matrix and the make matrix is equivalent to the diagonalized total outputs vector $\hat{\bar{\mathbf{x}}}$.[44]

The direct and total requirements matrices can be derived from $\bar{\mathbf{U}}$ and $\bar{\mathbf{V}}$, but the reverse is not true. $\bar{\mathbf{U}}$ and $\bar{\mathbf{V}}$ separate the flows given in the transactions matrix into inputs, represented in the use matrix, and outputs, represented in the make matrix. Data for $\bar{\mathbf{U}}$ and $\bar{\mathbf{V}}$ must be obtained separately from the transactions data; in general, where data for a transactions matrix is available, make and use matrix data will also be available.

In the EIO model in Eq. 3, flows from sectors i to j are assumed to consist of sector i's primary commodity product. This model, known as the industry–industry approach, does not account for sectors that produce more than one commodity. Sectors in the system may produce multiple commodities, but that information is not captured in the transactions matrix or in the requirements matrices. The make-use approach, also known as the commodity–industry approach, offers greater flexibility when dealing with secondary production.

When secondary production exists in the economic system, the industry–industry and commodity–industry approaches are not equivalent. In contrast to the single direct requirements matrix $\bar{\mathbf{A}}$ of the industry–industry approach, under the commodity–industry approach, there are several direct requirements matrices that can be derived from $\bar{\mathbf{U}}$ and $\bar{\mathbf{V}}$. These direct requirements matrices differ in their dimensions, which can be either $I \times I$ or $J \times I$, and in the technology assumption used in the derivation. There are two technology assumptions that make statements about the basic structure of the economy. The commodity–technology assumption states that a commodity is always produced from the same combination of commodity inputs regardless of the sector that produces it. In contrast, the industry–technology assumption states that all commodity outputs from a sector are produced from the same combination of commodity inputs regardless of the commodity type.[44]

The P2P modeling framework requires a commodity–commodity direct requirements matrix, but does not require one technology assumption over the other.[35] Although neither of the technology assumptions hold for a real economic system, it is our opinion that the commodity–technology assumption is slightly more realistic and is, therefore, better suited to design applications. For these reasons, only the commodity–commodity direct requirements matrix under the commodity–technology assumption is derived here.

The commodity–technology assumption defines a relationship between $\bar{\mathbf{U}}$ and $\bar{\mathbf{V}}$, that is used to derive the total requirements matrix. Consider the matrix $\bar{\mathbf{U}}\hat{\bar{\mathbf{x}}}^{-1}$, the columns of which give the mix of commodity inputs to each sector per dollar sector output. The mix of commodity outputs produced by each sector are given by the columns of $\bar{\mathbf{V}}^{\mathrm{T}}\hat{\bar{\mathbf{x}}}^{-1}$. Let $\bar{\mathbf{A}}_c$ be the commodity–commodity direct requirements matrix under the commodity–technology assumption. The jth column of $\bar{\mathbf{A}}_c$ gives the combination of commodity inputs required to produce a dollar's worth of commodity j. Under the commodity–technology assumption, the jth column of $\bar{\mathbf{U}}\hat{\bar{\mathbf{x}}}^{-1}$ is equal to a linear combination of the columns of $\bar{\mathbf{A}}_c$, weighted by the elements in the jth column of $\bar{\mathbf{V}}^{\mathrm{T}}\hat{\bar{\mathbf{x}}}^{-1}$. In other words, the mix of commodity inputs consumed by sector j are equal to a linear combination of the different mixes of commodities required to produce each of sector j's commodity outputs. In this linear combination, the weights of each commodity mix are the proportion of sector j's output that consists of a particular commodity. This relationship is expressed as

$$\bar{\mathbf{U}}\hat{\bar{\mathbf{x}}}^{-1}=\bar{\mathbf{A}}_c\bar{\mathbf{V}}^{\mathrm{T}}\hat{\bar{\mathbf{x}}}^{-1} \tag{4}$$

and is solved to yield the commodity–commodity direct requirements matrix as follows

$$\bar{\mathbf{A}}_c=\bar{\mathbf{U}}\left(\bar{\mathbf{V}}^{\mathrm{T}}\right)^{-1} \tag{5}$$

Because we previously assumed that the number of sectors and the number of commodities are equal, $\bar{\mathbf{A}}_c$ has the same dimensions as the industry–industry direct requirements matrix $\bar{\mathbf{A}}$. However, the elements of $\bar{\mathbf{A}}_c$ are in general not equal to the elements of $\bar{\mathbf{A}}$. Throughout the rest of the article, the direct requirements matrix referred to will be the commodity–commodity model derived from make and use matrices using Eq. 5.

EEIO models

EEIO models combine an EIO model with data on emissions or resource use in each sector to calculate the environmental interventions generated by the economic activity required to produce $\bar{\mathbf{f}}$.[26,27] This data is given in the environmental interventions matrix $\bar{\mathbf{B}}$, also shown in Table 1, as intervention amount in physical units by sector per dollar of output. The inventory vector of economy-wide interventions $\bar{\mathbf{g}}$ caused by producing $\bar{\mathbf{f}}$ is calculated by postmultiplying $\bar{\mathbf{B}}$ with the vector of sector outputs $\bar{\mathbf{x}}$

$$\overline{\mathbf{g}} = \overline{\mathbf{B}}\overline{\mathbf{x}} \tag{6}$$

which can also be written as

$$\overline{\mathbf{g}} = \overline{\mathbf{B}}\left(\overline{\mathbf{I}} - \overline{\mathbf{A}}\right)^{-1}\overline{\mathbf{f}} \tag{7}$$

using Eq. 3 to expand $\overline{\mathbf{x}}$. With the assumption of fixed $\bar{a}_{ij}$ and $\bar{b}_{rj}$, the total economic activity $\overline{\mathbf{x}}$ and total environmental interventions $\overline{\mathbf{g}}$ required to produce the final demand $\overline{\mathbf{f}}$ can be calculated for an arbitrary $\overline{\mathbf{f}}$. Equations 46 – 53 contain the data and calculations, involved in the derivation and application of an EEIO model.

Process life cycle assessment

Life cycle assessment is a systematic method intended to account for all material and energy inputs required throughout a product or service's production, use and end of life, as well as all associated environmental impacts. A life cycle is defined with respect to the functional unit, a measure of the function provided by a product or service that serves as a basis for comparison between life cycles. A typical life cycle includes the process that directly produces the functional unit as well as upstream and downstream processing stages, the use stage, and end of life activities such as disposal and materials recycling.[45,46]

There are three common LCA methodologies: process-based, input–output, and hybrid. These methodologies differ primarily in the level of aggregation of the life cycle inventory and in the scope of the system boundary, as shown in Figure 1.[47]

Process-based LCA is the life cycle method of choice for most applications, including virtually all sustainable engineering applications. Many common LCA tools, including SimaPro, openLCA, and the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation fuel cycle model, rely on this method.[48–50] The inventory for a process LCA is assembled one process at a time until including more processes is determined to have a negligible effect on the inventory.[51] Exactly where to draw the system boundary is a subjective decision made based on the purpose of the life cycle study and on the accuracy required of the results. Systematic methods of drawing the system boundary have been developed, but even among similar functional units, similar system boundaries do not guarantee the same accuracy in results.[52,53]

The network of processes in a process-based inventory is represented with a $K \times L$ technology matrix $\underline{\mathbf{X}}$, in which each column represents a process in the life cycle and each row represents the production and consumption of one product. Column l of $\underline{\mathbf{X}}$ is a model of life cycle process l, assumed to be linearly scalable and derived from empirical data obtained from a life cycle inventory database[54,55] or from literature sources. Each element $\underline{x}_{kl}$ is the amount of product k produced or consumed by process l. Consumption of a product is indicated by a negative element and production is indicated by a positive element. If process l neither produces nor consumes product k then $\underline{x}_{kl}$ is zero. $\underline{\mathbf{X}}$ can be divided into a $K \times L$ make matrix $\underline{\mathbf{V}}$ and a $L \times K$ use matrix $\underline{\mathbf{U}}$, similarly to the economy scale make and use matrices $\overline{\mathbf{V}}$ and $\overline{\mathbf{U}}$, such that the following equation holds

$$\underline{\mathbf{X}} = \underline{\mathbf{V}}^{\mathrm{T}} - \underline{\mathbf{U}} \tag{8}$$

A process-based inventory also includes data on exchanges between the life cycle processes and the environment, represented by an $R \times L$ environmental interventions matrix $\underline{\mathbf{B}}$. Column l of $\underline{\mathbf{B}}$ contains data on R flows between the environment and process l; such flows include natural resources consumed and pollutants produced. As in $\underline{\mathbf{X}}$, consumption is indicated by a negative element and production by a positive element.

One of the objectives of life cycle assessment is to calculate the total environmental interventions generated by a life cycle as a consequence of producing the functional unit $\underline{\mathbf{f}}$. Assuming that $\underline{\mathbf{X}}$ is both square and invertible, the inventory vector $\mathbf{g}$ for a process-based inventory is calculated as follows[56]

$$\underline{\mathbf{g}} = \underline{\mathbf{B}}\underline{\mathbf{X}}^{-1}\underline{\mathbf{f}} \tag{9}$$

Equations 54 – 58 demonstrate the application of Eq. 9.

Input–output and hybrid life cycle assessment

Another application of EEIO models is input–output model-based LCA (IO-LCA).[57] Unlike process LCA, in which the life cycle is built process by process, IO-LCA includes the entire economy in the life cycle boundary. IO-LCA is, therefore, more comprehensive than process LCA but can also be less precise due to the coarseness of the EEIO model. IO-LCA also generally neglects the use and end of life stages in the life cycle, as such activities tend to be outside the scope of EEIO models. To calculate the IO-LCA inventory vector, the final demand vector is specified to be the functional unit of the IO-LCA study and Eq. 7 is applied.

Hybrid LCA methods capture processes and inputs neglected in process-based LCA by combining detailed data for key life cycle processes with an EEIO model that captures the macroeconomic system within which the processes operate.[58] A hybrid inventory, therefore, combines the level of detail and specificity of a process based inventory with the completeness of an economy scale system boundary. Hybrid LCA also allows for inclusion of both the use and end of life stages through use of the process based LCA data. Equations 62 – 66 demonstrate two forms of hybrid LCA, tiered hybrid and integrated hybrid.

P2P Modeling Framework

The P2P modeling framework represents a life cycle with components at three distinct scales: equipment, value chain, and economy. Conventional models and modeling techniques have been developed at all three scales. The P2P approach integrates these separate models into a single cohesive multi-scale model representing a national or planetary system that can encompass production, use and end-of-life stages.

At the equipment scale, the smallest scale, system components are individual industrial processes, such as a chemical plant or a factory. Traditional process, product, and supply chain design takes place at this scale using models that are completely disaggregated and highly specific to the process, product, or supply chain being considered. The more detailed equipment scale models are derived from fundamental knowledge of unit operations and involve design variables at this unit operation level.

The largest scale in the framework is the economy scale, at which input–output and EEIO analysis takes place. System components at this scale are industrial sectors, aggregates of many production technologies, within a macroeconomic system. Mining, grain farming, and power generation are examples of economic sectors. National economy scale models are available from tools such as EIO-LCA[57] and Eco-LCA[59] as well as from governmental sources for some countries.[60] Planetary scale economy models have also been developed that use multiregional input–output (MRIO) models to represent the global economy.[61,62]

In between the economy and equipment scales is the value chain scale. Value chain scale models represent an activity, an aggregate of several processes of a particular type such as passenger vehicle manufacturing. An averaged production technology, such as those modeled in process LCA, is one example of a value chain activity. Activity models are thus more aggregated than equipment scale models in that they do not represent specific plants, but are less aggregated than economy scale models. The exact scale of value chain activity models is variable but generally corresponds to a geographic area smaller than that represented by an economy scale model. In the United States, an activity model can represent average technology within one or several states; in smaller countries, an activity model can represent average technology for one or several countries. Activity models are empirical, assumed to be linearly scalable, and are obtained from life cycle inventory databases such as ecoinvent[54] and the US NREL database.[55] The combination of the value chain and equipment scales represents the usual scope for conventional sustainable process design problems.

For the remainder of the article, the overbar notation will continue to indicate models and variables at the economy scale, and the underbar notation will continue to indicate value chain scale models. No bars on a quantity indicates the equipment scale. A combined over- and underbar, $\underline{\overline{X}}$, is used to indicate the complete P2P system. A superscript star * denotes a component model that has been disaggregated. Other subscripts and superscripts used in the notation will be defined as they occur. Table 6 contains a list of terms along with their definitions and first appearance in the article.

An illustrative P2P system is shown in Figure 3. System components are sectors ($\bar{S}_1$, $\bar{S}_2$, and $\bar{S}_3$) modeled at the economy scale, activities ($\underline{S}_4$ and $\underline{S}_5$) at the value chain scale and processes (S_6) at the equipment scale. In Figure 3, S_6 represents a single production facility, but in general equipment scale models may represent single processes, a supply chain, or other types of industrial systems. Product flows (solid arrows) exist within system components at each scale and between components at different scales. Flows are usually in physical units at the equipment scale and in monetary units at the economy scale. Value chain scale flows may be in either monetary or physical units, although physical units are more common. Flows originating at the economy scale consist of commodities, which are aggregates of many products. At the value chain scale, products are more distinct but still represent aggregates of similar products produced by several distinct production technologies. Equipment scale flows consist of individual products from specific processes. Flows are converted from one scale to another, using information on the aggregation of products into value chain products and commodities as well as price data for value chain products and individual products. In addition to interactions between technological components, the system in Figure 3 involves the interaction of each component with the environment (dotted arrows), which consist of emissions produced and resources consumed, among other quantities. The units for environmental interventions vary based on the type of intervention, but are consistent for all three scales. The remainder of this section details the types of models that are used at different scales and how these models are integrated to form a cohesive modeling framework.

System component models

In Figure 3, all of the system components save S_6, the equipment scale component, are shown as filled circles with no internal structure. This representation indicates the different types of models being used: the activities and sectors are modeled linearly, with inputs and outputs related by fixed proportions that are derived from empirical data. Each sector and activity model is a vector of inputs and outputs, $\overline{\mathbf{x}}_j$* and $\underline{\mathbf{x}}_l$ respectively. $\overline{\mathbf{x}}_j$ and $\underline{\mathbf{x}}_l$ are the columns of matrices $\overline{\mathbf{X}}$ and $\underline{\mathbf{X}}$

$$\overline{\mathbf{X}} = [\overline{\mathbf{x}}_1 | \overline{\mathbf{x}}_2 | \cdots | \overline{\mathbf{x}}_J] \tag{10}$$

$$\underline{\mathbf{X}} = [\underline{\mathbf{x}}_1 | \underline{\mathbf{x}}_2 | \cdots | \underline{\mathbf{x}}_L] \tag{11}$$

Each row of these matrices represents production of a particular commodity or product and each column consists of one sector or activity model. The direct requirements matrix $\overline{\mathbf{A}}$ and Leontief inverse are derived from $\overline{\mathbf{X}}$, the transactions matrix, as discussed in the Input–Output Analysis section of the Background. $\underline{\mathbf{X}}$, the value chain technology matrix, contains product flows in physical units and is called the value chain technology matrix from the process LCA technology matrix discussed in Process Life Cycle Assessment section.

Environmental interventions for both scales are specified as vectors of exchanges with the environment. $\overline{\mathbf{b}}_j$ contains interventions in physical units per dollar of output from sector j, while $\underline{\mathbf{b}}_l$ contains interventions per the level of production specified in $\underline{\mathbf{x}}_l$. $\overline{\mathbf{b}}_j$ and $\underline{\mathbf{b}}_l$ are collected into interventions matrices $\overline{\mathbf{B}}$ and $\underline{\mathbf{B}}$

$$\overline{\mathbf{B}} = \left[\overline{\mathbf{b}}_1 | \overline{\mathbf{b}}_2 | \cdots | \overline{\mathbf{b}}_J\right] \tag{12}$$

$$\underline{\mathbf{B}} = [\underline{\mathbf{b}}_1 | \underline{\mathbf{b}}_2 | \cdots | \underline{\mathbf{b}}_L] \tag{13}$$

As the sector, activity, and process models will be integrated into a single framework, homogeneity between models at different scales is a necessity. Both the economy and value chain scales are represented with an input–output-type model, thus it is necessary that the equipment scale is represented with a similar model.

The equipment scale model for process n consists of a set of fundamental technology or unit operation models $\mathbf{h}_n(\mathbf{z}_n)$ that are usually nonlinear. The set of models $\mathbf{h}_n(\mathbf{z}_n)$ is unique to process n, as are the variables $\mathbf{z}_n$. $\mathbf{h}_n(\mathbf{z}_n)$ describe the inner workings of process n: how inputs are transformed into outputs, how the proportions between different inputs and between different outputs are affected by design variables, and so on. The information that is needed to connect equipment scale models to the economy and value chain scale is simply process input and output amounts and types—information that is already within the models, but in a form not compatible with the input–output framework used at the larger scales. The incompatibility is resolved by duplicating information from the process models in an input–output vector $\mathbf{x}_n(\mathbf{z}_n)$, which is exactly analogous to those used to model value chain activities. Figure 4 demonstrates this for a process with five design

*Not to be confused with $\overline{\mathbf{x}}$, the vector of total sector outputs used to derive the direct requirements matrix, which does not have a subscript

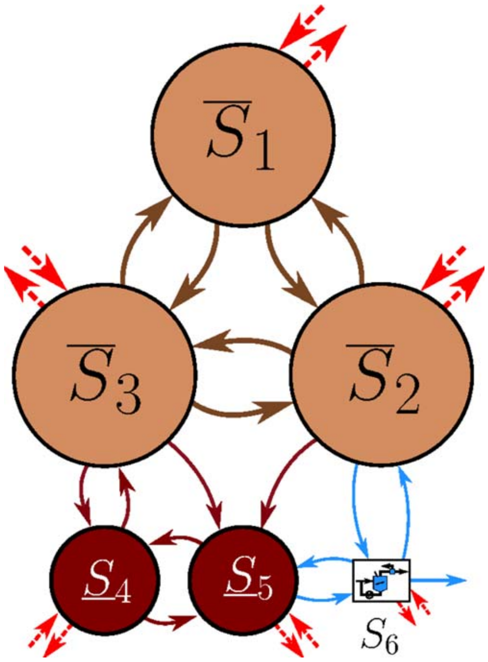

Figure 3. The framework represents large integrated process systems that involve components at the local equipment scale (S_6), intermediate value chain scale ($\underline{S}_4$ and $\underline{S}_5$), and national or planetary economy scale ($\bar{S}_1$, $\bar{S}_2$, and $\bar{S}_3$).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

variables, in which $\mathbf{z}_n = [z_{n1}, z_{n2}, z_{n3}, z_{n4}, z_{n5}]$. For process n in Figure 4, the input–output vector $\mathbf{x}_n(\mathbf{z}_n)$ is

$$\mathbf{x}_n(\mathbf{z}_n) = \begin{bmatrix} -x_{n1}(\mathbf{z}_n) \\ -x_{n2}(\mathbf{z}_n) \\ +x_{n3}(\mathbf{z}_n) \\ +x_{n4}(\mathbf{z}_n) \end{bmatrix} \tag{14}$$

and the associated fundamental models, which constrain $\mathbf{z}_n$ to feasible values, are

$$\begin{aligned} h_{n1}(z_{n1}, z_{n2}) &\geq 0 \\ h_{n2}(z_{n3}) &\geq 0 \\ h_{n3}(z_{n4}, z_{n5}) &\geq 0 \\ h_{n4}(z_{n3}, z_{n4}) &\geq 0 \end{aligned} \tag{15}$$

$\mathbf{x}_n(\mathbf{z}_n)$ differs from $\underline{\mathbf{x}}_l$ in that the elements of $\mathbf{x}_n(\mathbf{z}_n)$ are *variable* and dependent on the values of process n's design variables $\mathbf{z}_n$. No information is lost in using this vector notation, as the fundamental models $\mathbf{h}_n(\mathbf{z}_n)$ are still associated with the process. They are specified externally to the input–output vector that connects the equipment scale to the other scales of the modeling framework and form a set of constraints on the unit operation variables. The equipment scale model then consists of the equipment scale technology matrix $\mathbf{X}(\{\mathbf{z}\})$, in which any or all of the elements may be functions, *and* a set of fundamental models for each process, as follows

$$\begin{aligned} \mathbf{X}(\{\mathbf{z}\}) &= [\,\mathbf{x}_1(\mathbf{z}_1) \quad \cdots \quad \mathbf{x}_N(\mathbf{z}_N)\,] \\ \mathbf{H}(\{\mathbf{z}\}) &\geq \mathbf{0} \end{aligned} \tag{16}$$

$\mathbf{H}(\{\mathbf{z}\})$ denotes the entire set of fundamental models: $\mathbf{H}(\{\mathbf{z}\}) = \{\mathbf{h}_1(\mathbf{z}_1), \ldots, \mathbf{h}_N(\mathbf{z}_N)\}$. $\{\mathbf{z}\}$ denotes the entire set of unit operation variables for all N equipment scale processes: $\{\mathbf{z}\} = \{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$.

The environmental intervention matrix for the equipment scale is likewise dependent on the unit operation variables $\{\mathbf{z}\}$

$$\mathbf{B}(\{\mathbf{z}\}) = [\,\mathbf{b}_1(\mathbf{z}_1) \quad \cdots \quad \mathbf{b}_N(\mathbf{z}_N)\,] \tag{17}$$

Interactions between scales

Thus far the component models have described only exchanges between system components at the same scale. Exchanges between components at different scales are captured in upstream and downstream cutoff matrices. Throughout this discussion and the rest of the article, the descriptors "upstream" and "downstream" are always used with respect to the smaller of the two scales involved in a particular exchange. For instance, commodities produced at the economy scale and consumed at the value chain scale are referred to as value chain upstream cutoff flows. Similarly, products produced at the equipment scale and consumed at the value chain scale are referred to as equipment-value chain downstream cutoff flows.

The value chain's upstream cutoff flows are inputs to value chain activities that are produced by economic sectors. Data on value chain upstream cutoffs are obtained from the same sources as exchanges within the value chain, and are generally in physical units. Cutoff flows are converted to monetary units using market price data and are scaled to the destination activity's level of production. Upstream cutoffs are only different from other inputs to the value chain activity in that their production is modeled at the larger economy scale rather than at the value chain scale. In other words, the production of any given input to a value chain activity can be modeled at either the value chain or the economy scale. Choosing to model some inputs as value chain upstream cutoffs means that activity models for the production of these inputs do not need to be included in the value chain, thus reducing the data required to

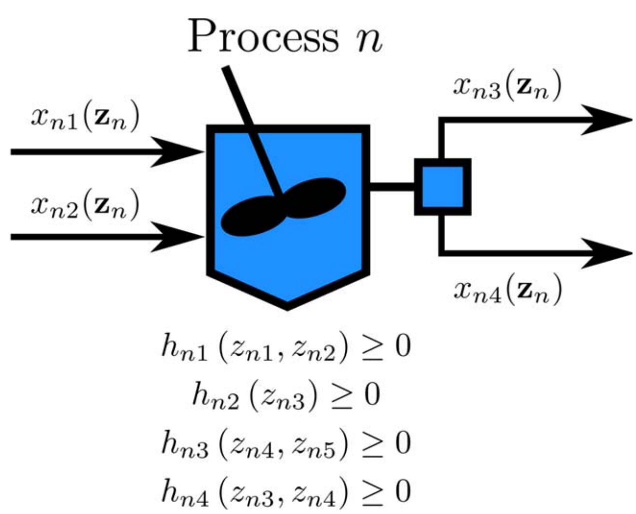

Figure 4. Process model n consists of a set of fundamental unit operation models $\mathbf{h}_n$ involving design variables $\mathbf{z}_n$.

Inputs and outputs of process n are written as functions of $\mathbf{z}_n$, $\mathbf{x}_n(\mathbf{z}_n)$. $\mathbf{z}_n$ are constrained to feasible values by $\mathbf{h}_n(\mathbf{z}_n)$. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

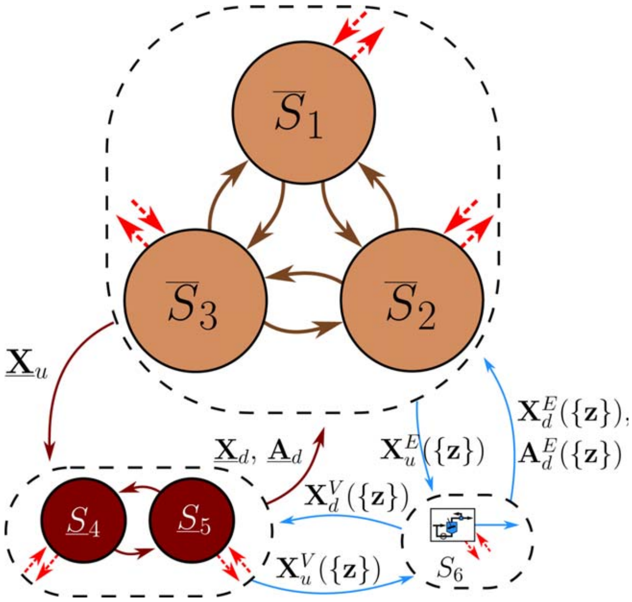

Figure 5. Upstream and downstream cutoff matrices shown as flows connecting system components at different scales.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

build the P2P model. The value chain upstream cutoff matrix $\underline{\mathbf{X}}_u$ has L columns, one for each value chain activity, and I rows, one for each economic commodity. Figure 5 shows $\underline{\mathbf{X}}_u$ in the context of the entire P2P system.

Downstream cutoff flows for the value chain scale are activity outputs that are consumed by economic sectors. These cutoff flows are typically useful by-products of value chain activities; including such flows in the modeling framework captures the effect of displacing a substitutable product by the by-product. In contrast to upstream cutoffs, downstream cutoffs are specified in physical units. Flows in the downstream cutoff matrix are normalized by the total monetary output of the destination sector (found in the total output vector $\bar{\mathbf{x}}$ of input–output analysis) before being incorporated into the P2P model. This normalized value chain downstream cutoff matrix is denoted $\underline{\mathbf{A}}_d$. However, when the downstream cutoff matrix is used in the disaggregation calculations of Model disaggregation, it is *not* normalized and is denoted $\underline{\mathbf{X}}_d$. The relevant flow in Figure 5 is thus labeled as both $\underline{\mathbf{X}}_d$ and $\underline{\mathbf{A}}_d$. Both value chain downstream cutoff matrices have J columns, one for each economic sector, and K rows, one for each value chain product.

Equipment scale cutoff matrices are analogous, although a superscript ^{E} or ^{V} is added to indicate whether the cutoff flows connect to the economy or the value chain scale. Any or all of the equipment scale cutoff flows may be functions of design variables. The equipment-economy upstream cutoff matrix $\mathbf{X}_u^E(\{\mathbf{z}\})$ contains flows in monetary units and has N columns, one for each process at the equipment scale, and I rows, one for each economic commodity. The equipment-value chain upstream cutoff matrix $\mathbf{X}_u^V(\{\mathbf{z}\})$ contains flows in physical units, assuming that the value chain models are also in physical units, and has N columns and K rows, one for each value chain product. Both equipment scale downstream cutoff matrices have M rows, one for each equipment scale product. The equipment-economy downstream cutoff matrix has J columns and the equipment-value chain downstream cutoff matrix has L columns. The elements of $\mathbf{A}_d^E(\{\mathbf{z}\})$, like $\underline{\mathbf{A}}_d$, are normalized by the total output of each destination sector; the equipment-economy downstream cutoff matrix used in disaggregation, $\mathbf{X}_d^E(\{\mathbf{z}\})$, is not normalized just as $\underline{\mathbf{X}}_d$ is not normalized. However, the elements of the equipment-value chain downstream cutoff matrix, $\mathbf{X}_d^V(\{\mathbf{z}\})$, are *not* normalized by the total output of the destination activity in the P2P model. The relevant flows are labeled in Figure 5.

Model disaggregation

The multiscale nature of the system in Figure 3 leads to inevitable overlap between models. Because the economy scale represents an entire economy, and the value chain and equipment scales represent systems that operate within that economy, activity models and process models are captured by models of corresponding sectors. It is also possible for process models to be similarly captured by value chain activity models. In this situation, the smaller scale models are represented twice in the P2P modeling framework—once explicitly and once implicitly—leading to the smaller scale's technological and environmental exchanges being counted twice. The inputs and outputs of sector $\bar{S}_3$ in Figure 6a, for instance, also contain inputs and outputs of activity $\underline{S}_4$. To avoid double-counting, the parent component is split into two or more subcomponents: the constituent component(s) that are modeled separately at the smaller scale(s), and the remainder of the parent component which remains as part of the parent scale model.

In Figure 6a, $\underline{S}_4$ represents constituent value chain activity(ies) and $\bar{S}_3$ represents the parent industrial sector such that $\underline{S}_4 \in \bar{S}_3$. Figure 6b illustrates the system after disaggregation; $\bar{S}_{3^*}$, the adjusted sector, represents the remainder of $\bar{S}_3$. The relationship between $\bar{S}_3$, $\bar{S}_{3^*}$, and $\underline{S}_4$ is

$$\bar{S}_3 = \bar{S}_{3^*} \cup \underline{S}_4 \tag{18}$$

As an example, suppose $\bar{S}_3$ represents the power generation sector and $\underline{S}_4$ represents a coal electricity generating activity, for which more detailed empirical data is available. To model $\bar{S}_3$ and $\underline{S}_4$ without overlap, the power generation sector is divided into a coal-burning electricity generation activity $\underline{S}_4$ and all other electricity generating activities, $\bar{S}_{3^*}$. $\underline{S}_4$ is then modeled separately from the EEIO model at the value chain scale using the more detailed data.

Suppose that $\underline{S}_4$ also has a constituent process, S_7 (not shown in Figure 6). Two disaggregations would be needed in this case, one for $\bar{S}_{3^*}$ and one for $\underline{S}_{4^*}$; the relationship between $\bar{S}_3$ and its constituents is expressed as

$$\bar{S}_3 = \bar{S}_{3^*} \cup \underline{S}_{4^*} \cup S_7 \tag{19}$$

where $\underline{S}_4$ in Eq. 18 has been disaggregated as follows

$$\underline{S}_4 = \underline{S}_{4^*} \cup S_7 \tag{20}$$

Standalone components that do not overlap with any larger scale system component are less common than constituent components. Standalone processes may represent newly developed technology that cannot be classified into existing sectors or value chain activities. Value chain activities that are standalone can arise from recently implemented commercial technologies not represented in the EEIO model, which is derived from economic data that may be several years out of date. In Figure 6, $\underline{S}_5$ is a standalone activity. $\underline{S}_5$, like the constituent activity $\underline{S}_4$, interacts with other system components, but as it does not have a parent component no disaggregation need be performed.

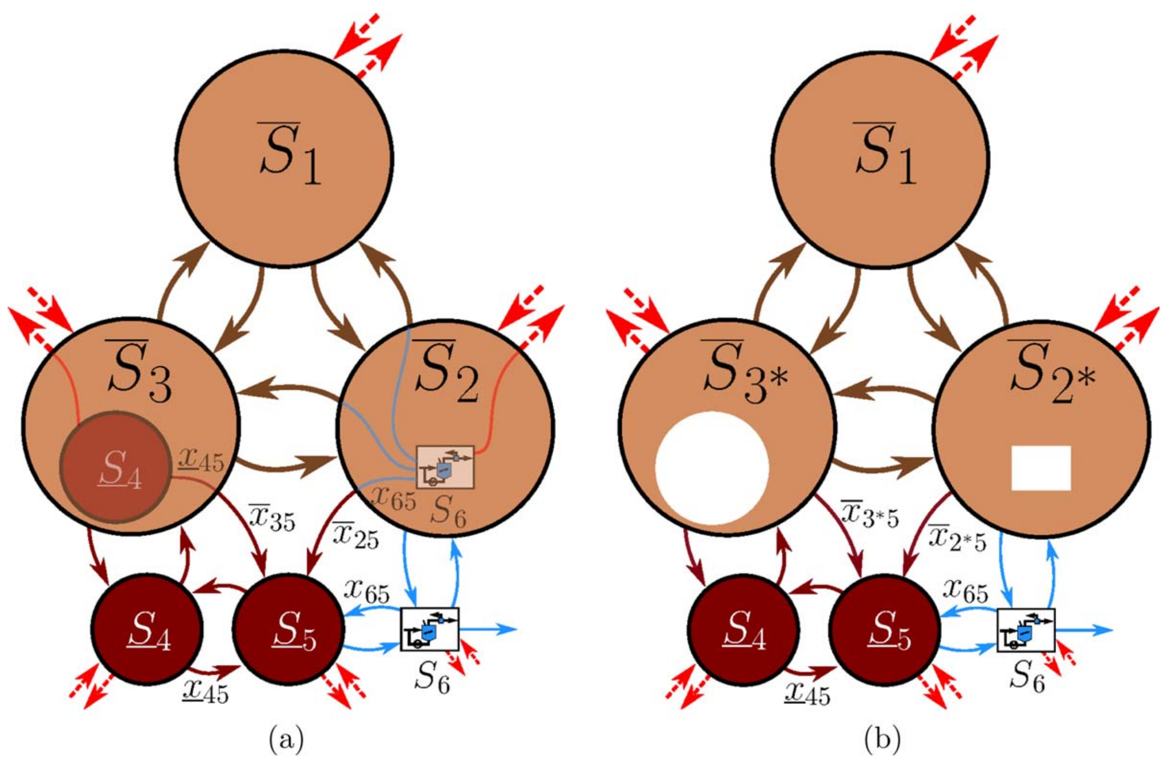

Figure 6. When smaller scale system components overlap with larger scale components as shown on the left, the parent components ($\bar{S}_3$ and $\bar{S}_2$) must be disaggregated into constituent activities and/or processes ($\underline{S}_4$ and S_6), which are modeled in detail at smaller scales, and adjusted components ($\bar{S}_{3^*}$ and $\bar{S}_{2^*}$), which remain in the original parent model as shown on the right.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Disaggregation is performed by subtracting the inputs and outputs of the constituent components from the inputs and outputs of the parent component, leaving only those flows that are both produced and consumed at the parent scale in the parent scale model. The disaggregation of $\bar{S}_3$ and $\bar{S}_2$ shown in Figure 6 is accomplished by subtracting off flows originating in the constituent components

$$\bar{x}_{3^*5} = \bar{x}_{35} - \underline{p}\,\underline{y}_{45} \tag{21}$$

$$\bar{x}_{2^*5} = \bar{x}_{25} - p y_{65} \tag{22}$$

in which x refers to flows in monetary units and y to flows in physical units. The terms $\underline{p}$ and p represent the unit market prices of flows $\underline{y}_{kl}$ and y_{mn}, respectively and are used to convert the physical flows into monetary units

$$\underline{x}_{kl} = \underline{p}_{kl}\underline{y}_{kl} \tag{23}$$

Price data for equipment scale flows, p_{mn}, is used analogously

$$x_{mn} = p_{mn} y_{mn} \tag{24}$$

Although products at the value chain and equipment scales may be the same, value chain price data is averaged over a set of products while equipment scale price data is specific to the product of the process being modeled. Returning to the example of coal electricity generation, the value chain scale price of coal electricity is averaged over all coal-burning power plants in a particular region, while the equipment scale price is specific to a single power plant. Environmental interventions are similarly disaggregated:

$$\bar{b}_{3^*} = \bar{b}_3 - \underline{b}_4 \tag{25}$$

Manual disaggregation, as shown in Eqs. 21–25, becomes complex and time-consuming when multiple parent components, each with multiple constituents, exist at various scales. A more efficient way to disaggregate the economy and value chain models is through the make and use matrices discussed in the Background section. Rows of the use matrices correspond to commodities at the economy scale and to products at the value chain and equipment scales; columns of the use matrices correspond to sectors, activities, or processes. Dimensions of the use matrices are as follows: $\overline{\mathbf{U}}$ is $I \times J$, $\underline{\mathbf{U}}$ is $K \times L$ and $\mathbf{U}$ is $M \times N$. Make matrix rows correspond to system components and columns to commodities, value chain products or individual products; the dimensions of the make matrices are $J \times I$ for $\overline{\mathbf{V}}$, $L \times K$ for $\underline{\mathbf{V}}$ and $N \times M$ for $\mathbf{V}$.[44] Price data at the value chain and equipment scales is used to convert product flows to commodity flows at the economy scale. Also required is information on the relationships between all constituent and parent components and their products.[35] Definitions for previously undefined matrices appearing in the following equations are given in Table 6.

The disaggregated economy scale make and use matrices $\overline{\mathbf{V}}^*(\{\mathbf{z}\})$ and $\overline{\mathbf{U}}^*(\{\mathbf{z}\})$ are defined as

$$\overline{\mathbf{V}}^*(\{\mathbf{z}\}) = \overline{\mathbf{V}} - \underline{\hat{\mathbf{p}}}(\underline{\mathbf{P}}_P)^{\mathrm{T}}\underline{\mathbf{V}}(\underline{\mathbf{P}}_F)^{\mathrm{T}} - \hat{\mathbf{p}}(\mathbf{P}_P^E)^{\mathrm{T}}\mathbf{V}(\{\mathbf{z}\})(\mathbf{P}_F^E)^{\mathrm{T}} \tag{26}$$

$$\overline{\mathbf{U}}^{*}(\{\mathbf{z}\}) = \overline{\mathbf{U}} - \left(\hat{\underline{\mathbf{p}}}\,\underline{\mathbf{P}}_F\underline{\mathbf{U}}\underline{\mathbf{P}}_P + \hat{\underline{\mathbf{p}}}\,\underline{\mathbf{P}}_F\underline{\mathbf{X}}_d + \underline{\mathbf{X}}_u\underline{\mathbf{P}}_P\right) - \left(\hat{\mathbf{p}}\mathbf{P}_F^E\mathbf{U}(\{\mathbf{z}\})\mathbf{P}_P^E + \hat{\mathbf{p}}\mathbf{P}_F^E\mathbf{X}_d^E(\{\mathbf{z}\}) + \mathbf{X}_u^E(\{\mathbf{z}\})\mathbf{P}_P^E\right) \quad (27)$$

in which

$$\underline{\mathbf{P}}_F = \{\underline{p}_F\}$$

$$\underline{p}_{Fik} = \begin{cases} 1 & \text{if value chain product } k \text{ belongs to the product set represented by commodity } i \\ 0 & \text{otherwise} \end{cases} \quad (28)$$

$$\underline{\mathbf{P}}_P = \{\underline{p}_P\}$$

$$\underline{p}_{Plj} = \begin{cases} 1 & \text{if value chain activity } l \text{ is constituent to sector } j \\ 0 & \text{otherwise} \end{cases} \quad (29)$$

$$\mathbf{P}_F^E = \{p_F^E\}$$

$$p_{Fim}^E = \begin{cases} 1 & \text{if product } m \text{ belongs to the product set represented by commodity } i \\ 0 & \text{otherwise} \end{cases} \quad (30)$$

$$\mathbf{P}_P^E = \{p_P^E\}$$

$$p_{Pnj}^E = \begin{cases} 1 & \text{if process } n \text{ is constituent to sector } j \\ 0 & \text{otherwise} \end{cases} \quad (31)$$

The permutation matrices defined in Eqs. 28–31 contain information on the relationships between parent sectors and their commodities, and constituent activities and processes and their products. These matrices along with price data vectors $\underline{\mathbf{p}}$ and $\mathbf{p}$ are used to "translate" flows in the various make and use matrices from one scale to another. Superscripts on the equipment scale permutation matrices in Eqs. 30 and 31 are used to specify the scale to which flows are being translated. $\mathbf{P}_F^E$ for instance relates equipment scale products to economic (E) commodities, while $\mathbf{P}_F^V$ in Eq. 34 relates the same equipment scale products to value chain (V) products. Value chain scale permutation matrices all relate the value chain scale to the economy scale, thus no additional superscripts are required as seen in Eqs. 28 and 29. Note that in Eqs. 26 and 27, the *original* value chain make and use matrices are used rather than the disaggregated matrices. This is because, in the situation that a sector-constituent activity also has an activity-constituent process, removing the undisaggregated activity from the parent sector also removes the activity-constituent process. Disaggregation of the value chain scale make and use matrices to $\underline{\mathbf{V}}^*(\{\mathbf{z}\})$ and $\underline{\mathbf{U}}^*(\{\mathbf{z}\})$ is analogous to the economy scale

$$\underline{\mathbf{V}}^*(\{\mathbf{z}\}) = \underline{\mathbf{V}} - \hat{\mathbf{p}}(\mathbf{P}_P^V)^{\mathrm{T}}\mathbf{V}(\{\mathbf{z}\})(\mathbf{P}_F^V)^{\mathrm{T}} \quad (32)$$

$$\underline{\mathbf{U}}^*(\{\mathbf{z}\}) = \underline{\mathbf{U}} - \hat{\mathbf{p}}\mathbf{P}_F^V\mathbf{U}(\{\mathbf{z}\})\mathbf{P}_P^V - \hat{\mathbf{p}}\mathbf{P}_F^V\mathbf{X}_d^V(\{\mathbf{z}\}) - \mathbf{X}_u^V(\{\mathbf{z}\})\mathbf{P}_P^V \quad (33)$$

in which

$$\mathbf{P}_F^V = \{p_F^V\}$$

$$p_{Fkm}^V = \begin{cases} 1 & \text{if product } m \text{ belongs to the product set represented by value chain product } k \\ 0 & \text{otherwise} \end{cases} \quad (34)$$

$$\mathbf{P}_P^V = \{p_P^V\}$$

$$p_{Pnl}^V = \begin{cases} 1 & \text{if process } n \text{ is constituent to value chain activity } l \\ 0 & \text{otherwise} \end{cases} \quad (35)$$

Readers familiar with integrated hybrid LCA will notice similarities between Eqs. 26, 27, 32, and 33 and Eqs. A6 and A7 in [35]. The first two terms in Eqs. 26 and 27 are identical to the disaggregation equations, A7 and A6, respectively, used in integrated hybrid LCA. The final terms in 26 and 27 deal with fundamental models at the engineering scale. As discussed previously, the equipment scale models are dependent on design variables $\{\mathbf{z}\}$; through the disaggregation process, $\{\mathbf{z}\}$ is propagated to the economy scale model, introducing design variables and nonlinearities to this

Table 2. Explanation of Factors Involved in Economy and Value Chain Model Disaggregations Given in Eqs. 26, 27, 32, and 33

Factor	Description
Equation 26	
$\overline{\mathbf{V}}$	Economy scale make matrix: commodities produced by sectors
$\hat{\mathbf{p}}(\underline{\mathbf{P}}_P)^{\mathrm{T}}\underline{\mathbf{V}}(\underline{\mathbf{P}}_F)^{\mathrm{T}}$	Products produced by sector-constituent value chain activities, calculated from value chain scale make matrix $\underline{\mathbf{V}}$
$\hat{\bar{\mathbf{p}}}(\mathbf{P}_P^E)^{\mathrm{T}}\mathbf{V}(\{\mathbf{z}\})(\mathbf{P}_F^E)^{\mathrm{T}}$	Products produced by sector-constituent processes, calculated from equipment scale make matrix $\mathbf{V}(\{\mathbf{z}\})$
Equation 27	
$\overline{\mathbf{U}}$	Economy scale use matrix: commodities consumed by sectors
$\hat{\mathbf{p}}\underline{\mathbf{P}}_F\underline{\mathbf{U}}\underline{\mathbf{P}}_P$	Products consumed and produced by sector-constituent activities, calculated from value chain scale use matrix $\underline{\mathbf{U}}$
$\hat{\bar{\mathbf{p}}}\underline{\mathbf{P}}_F\underline{\mathbf{X}}_d$	Products consumed by sectors and produced by sector-constituent activities, calculated from value chain scale downstream cutoff matrix $\underline{\mathbf{X}}_d$
$\underline{\mathbf{X}}_u\underline{\mathbf{P}}_P$	Products consumed by sector-constituent activities and produced by sectors, calculated from value chain scale upstream cutoff matrix $\underline{\mathbf{X}}_u$
$\hat{\mathbf{p}}\mathbf{P}_F^E\mathbf{U}(\{\mathbf{z}\})\mathbf{P}_P^E$	Products consumed and produced by sector-constituent processes, calculated from equipment scale use matrix $\mathbf{U}(\{\mathbf{z}\})$
$\hat{\mathbf{p}}\mathbf{P}_F^E\mathbf{X}_d^E(\{\mathbf{z}\})$	Products consumed by sectors and produced by sector-constituent processes, calculated from equipment-economy downstream cutoff matrix $\mathbf{X}_d^E(\{\mathbf{z}\})$
$\mathbf{X}_u^E(\{\mathbf{z}\})\mathbf{P}_P^E$	Products consumed by sector-constituent processes and produced by sectors, calculated from equipment-economy upstream cutoff matrix $\mathbf{X}_u^E(\{\mathbf{z}\})$
Equation 32	
$\underline{\mathbf{V}}$	Value chain scale make matrix (not disaggregated): commodities produced by activities
$\hat{\mathbf{p}}(\mathbf{P}_P^V)^{\mathrm{T}}\mathbf{V}(\{\mathbf{z}\})(\mathbf{P}_F^V)^{\mathrm{T}}$	Products produced by activity-constituent processes, calculated from equipment scale make matrix $\mathbf{V}(\{\mathbf{z}\})$
Equation 33	
$\underline{\mathbf{U}}$	Value chain scale use matrix (not disaggregated): commodities consumed by activities
$\hat{\mathbf{p}}\mathbf{P}_F^V\mathbf{U}(\{\mathbf{z}\})\mathbf{P}_P^V$	Products consumed and produced by activity-constituent processes, calculated from equipment scale use matrix $\mathbf{U}(\{\mathbf{z}\})$
$\hat{\mathbf{p}}\mathbf{P}_F^V\mathbf{X}_d^V(\{\mathbf{z}\})$	Products consumed by activities and produced by activity-constituent processes, calculated from equipment-value chain downstream cutoff matrix $\mathbf{X}_d^V(\{\mathbf{z}\})$
$\mathbf{X}_u^V(\{\mathbf{z}\})\mathbf{P}_P^V$	Products consumed by activity-constituent processes and produced by activities, calculated from equipment-value chain upstream cutoff matrix $\mathbf{X}_u^V(\{\mathbf{z}\})$

previously fixed, linear model. As a result, the disaggregated economy scale model is dependent on unit operation design variables. Equations 32 and 33 are directly analogous to A7 and A6, although they are applied to the value chain technology matrices and once again introduce variables and nonlinearities from the equipment scale models.

To summarize, the disaggregated make and use matrices represent production and consumption that takes place within one particular scale. All of the terms subtracted from the original make and use matrices represent products or commodities that are produced and/or consumed by constituent components at other scales. Table 2 gives the physical interpretation of each factor in Eqs. 26, 27, 32, and 33.

Environmental interventions for the parent components must be disaggregated as well to avoid counting the interventions of both the parents and constituents. The interventions matrix used in EEIO models, $\overline{\mathbf{B}}$, is normalized to the total output of each sector, as discussed in Input–Output Analysis section of the Background; $\overline{\mathbf{B}}$ thus represents the average environmental interventions per dollar for all processes and activities that comprise a particular sector. In order to disaggregate the interventions correctly, the calculation must be done relative to the *total interventions* that have not been normalized by sector output. $\overline{\mathbf{R}}$ denotes the total interventions matrix for the economy scale. The value chain interventions $\underline{\mathbf{B}}$ are not normalized by total activity output but represent total environmental interventions for the level of production specified in the activity model. The disaggregated economy scale environmental interventions matrix $\overline{\mathbf{B}}^*(\{\mathbf{z}\})$ is calculated from data in the original and disaggregated make matrices

$$\overline{\mathbf{R}}^*(\{\mathbf{z}\}) = \overline{\mathbf{R}} - \underline{\mathbf{B}}\underline{\mathbf{P}}_P - \mathbf{B}(\{\mathbf{z}\})\mathbf{P}_P^E \tag{36}$$

$$\overline{\mathbf{b}}^*{}_j(\{\mathbf{z}\}) = \frac{1}{(\overline{\mathbf{V}}^{*\mathrm{T}}(\{\mathbf{z}\})\mathbf{1})_j}\overline{\mathbf{r}}^*(\{\mathbf{z}\})_j, \quad j = 1\ldots J \tag{37}$$

Taking the transpose of the matrix before multiplying by $\mathbf{1}$, as in Eq. 37, produces a vector of row sums. The vector $\overline{\mathbf{V}}^{*\mathrm{T}}(\{\mathbf{z}\})\mathbf{1}$, therefore, contains total outputs by sector after disaggregation. $(\overline{\mathbf{V}}^{*\mathrm{T}}(\{\mathbf{z}\})\mathbf{1})_j$ refers to the jth element in $\overline{\mathbf{V}}^{*\mathrm{T}}(\{\mathbf{z}\})\mathbf{1}$, which is the total output of disaggregated sector j. $\overline{\mathbf{r}}_j^*(\{\mathbf{z}\})$ and $\overline{\mathbf{r}}_j$ similarly refer to the jth column of the disaggregated and total interventions matrices $\overline{\mathbf{R}}^*(\{\mathbf{z}\})$ and $\overline{\mathbf{R}}$, respectively. The disaggregated value chain scale interventions matrix $\underline{\mathbf{B}}^*(\{\mathbf{z}\})$ is calculated similarly

$$\underline{\mathbf{B}}^*(\{\mathbf{z}\}) = \underline{\mathbf{B}} - \mathbf{B}(\{\mathbf{z}\})\mathbf{P}_P^V \tag{38}$$

Note that because $\overline{\mathbf{V}}^*(\{\mathbf{z}\})$ and $\underline{\mathbf{V}}^*(\{\mathbf{z}\})$ are dependent on unit operation design variables through the disaggregation calculations, $\overline{\mathbf{B}}^*(\{\mathbf{z}\})$ and $\underline{\mathbf{B}}^*(\{\mathbf{z}\})$ are also dependent on the unit operation design variables.

The disaggregated economy scale make and use matrices are used to calculate the disaggregated direct requirements matrix as in Eq. 5

$$\overline{\mathbf{A}}^*(\{\mathbf{z}\}) = \overline{\mathbf{U}}^*(\{\mathbf{z}\})\left(\overline{\mathbf{V}}^{*\mathrm{T}}(\{\mathbf{z}\})\right)^{-1} \tag{39}$$

If the make and use matrices are rectangular due to the number of commodities and sectors not being equal, $\overline{\mathbf{A}}^*(\{\mathbf{z}\})$ is calculated by solving

$$\overline{\mathbf{A}}^*(\{\mathbf{z}\})\overline{\mathbf{V}}^{*\mathrm{T}}(\{\mathbf{z}\})\left(\widehat{\overline{\mathbf{V}}^*(\{\mathbf{z}\})\mathbf{1}}\right)^{-1} = \overline{\mathbf{U}}^*(\{\mathbf{z}\})\left(\widehat{\overline{\mathbf{V}}^*(\{\mathbf{z}\})\mathbf{1}}\right)^{-1}, \tag{40}$$

a system of linear equations in which $\overline{\mathbf{V}}^{*\mathrm{T}}(\{\mathbf{z}\})\mathbf{1}$ is the vector of total sector outputs after disaggregation, $\overline{\mathbf{x}}^*(\{\mathbf{z}\})$, and all matrices are known except for $\overline{\mathbf{A}}^*(\{\mathbf{z}\})$. $\mathbf{1}$ denotes a vector of all 1's; multiplication by $\mathbf{1}$ produces a vector of row sums. The quantity $\overline{\mathbf{V}}^{*\mathrm{T}}(\{\mathbf{z}\})\mathbf{1}$ is then a vector of column sums of $\overline{\mathbf{V}}^*$. The solutions to Eqs. 39 and 40 are equivalent when the make and use matrices are square and for the same values of $(\{\mathbf{z}\})$.

The disaggregated value chain technology matrix $\underline{\mathbf{X}}^*(\{\mathbf{z}\})$ is calculated from the matrix difference of $\underline{\mathbf{V}}^*(\{\mathbf{z}\})$ and $\underline{\mathbf{U}}^*(\{\mathbf{z}\})$

Table 3. System Component Models to be Included in the P2P Modeling Framework

Scale	Component	Description
Economy	$\overline{\mathbf{A}}^*(\{\mathbf{z}\})$	Disaggregated direct requirements matrix
	$\overline{\mathbf{B}}^*(\{\mathbf{z}\})$	Disaggregated economy scale environmental interventions
	$\overline{\mathbf{f}}$	Final demand from economy (generally zero)
	$\overline{\mathbf{s}}$	Sector scaling vector (variable, analogous to throughput vector $\overline{\mathbf{x}}$)
Value chain	$\underline{\mathbf{X}}^*(\{\mathbf{z}\})$	Disaggregated value chain model
	$\underline{\mathbf{X}}_u(\{\mathbf{z}\})$	Value chain upstream cutoff matrix
	$\underline{\mathbf{A}}_d(\{\mathbf{z}\})$	Normalized value chain downstream cutoff matrix
	$\underline{\mathbf{B}}^*(\{\mathbf{z}\})$	Disaggregated value chain environmental interventions
	$\underline{\mathbf{f}}$	Final demand from value chain (generally zero)
	$\underline{\mathbf{s}}$	Value chain activity scaling vector (variable)
Process	$\mathbf{X}(\{\mathbf{z}\})$	Equipment model matrix
	$\mathbf{X}_u^E(\{\mathbf{z}\})$	Equipment-economy upstream cutoff matrix
	$\mathbf{X}_u^V(\{\mathbf{z}\})$	Equipment-value chain upstream cutoff matrix
	$\mathbf{A}_d^E(\{\mathbf{z}\})$	Normalized equipment-economy downstream cutoff matrix
	$\mathbf{X}_d^V(\{\mathbf{z}\})$	Equipment-value chain downstream cutoff matrix
	$\mathbf{B}(\{\mathbf{z}\})$	Equipment environmental interventions
	$\mathbf{f}$	Final demand from equipment scale process(es)
	$\mathbf{s}$	Equipment scale scaling vector (variable or fixed)
Unit operation	$\mathbf{H}(\{\mathbf{z}\})$	Unit operation models external to $\mathbf{X}(\{\mathbf{z}\})$

$$\underline{\mathbf{X}}^*(\{\mathbf{z}\}) = \underline{\mathbf{V}}^{*\mathrm{T}}(\{\mathbf{z}\}) - \underline{\mathbf{U}}^*(\{\mathbf{z}\}) \tag{41}$$

Integrating component models

Following disaggregation, the component models, listed and defined in Table 3, are integrated into a single P2P transactions matrix $\overline{\underline{\mathbf{X}}}(\{\mathbf{z}\})$ and a P2P environmental interventions matrix $\overline{\underline{\mathbf{B}}}(\{\mathbf{z}\})$, both shown in Table 4. $\overline{\underline{\mathbf{X}}}(\{\mathbf{z}\})$ captures flows within and between the sectors, activities, and processes. Each row corresponds to a particular commodity or product that is produced and consumed within the system, and each column corresponds to one system component and includes upstream cutoff, downstream cutoff, and intrascale exchanges. $\overline{\underline{\mathbf{B}}}(\{\mathbf{z}\})$ captures exchanges between the P2P system and the environment; each row corresponds to one environmental intervention such as a particular type of emission or a natural resource, and each column corresponds to one system component.

The P2P transactions matrix functions analogously to the direct requirements matrix of input–output analysis or the technology matrix of process life cycle assessment, with some key differences. Both $\overline{\mathbf{A}}$ and $\underline{\mathbf{X}}$ represented systems that were assumed to scale linearly, and both system models were multiplied by a vector of scaling factors ($\overline{\mathbf{x}}$ and $\underline{\mathbf{s}}$, respectively) determined from the final demand or functional unit vector, in order to calculate system-wide environmental interventions. $\overline{\underline{\mathbf{X}}}(\{\mathbf{z}\})$ will also be multiplied by a scaling vector, although because the equipment scale models represent individual processes, they cannot be assumed to scale linearly. The P2P scaling vector is defined as

$$\overline{\underline{\mathbf{s}}} = \begin{bmatrix} \overline{\mathbf{s}} \\ \underline{\mathbf{s}} \\ \mathbf{s} \end{bmatrix} \tag{42}$$

and consists of three subvectors, each of which correspond to the models at one scale of the system. $\overline{\mathbf{s}}$ has the same interpretation as the throughput vector $\overline{\mathbf{x}}$ of input–output analysis and scales the economic sector models as well as the value chain and equipment-economy downstream cutoff flows. $\underline{\mathbf{s}}$ scales the value chain activities, the value chain upstream cutoffs and the equipment-value chain downstream cutoffs. Both $\overline{\mathbf{s}}$ and $\underline{\mathbf{s}}$ are standard, linear scaling vectors because the economic sector and activity models are assumed to scale linearly. The last subvector of $\overline{\underline{\mathbf{s}}}$ is $\mathbf{s}$, which scales the process models. Due to the presence of economies of scale, the process models *cannot* be assumed to scale linearly; accordingly, the elements of $\mathbf{s}$ will in general be nonlinear, for instance $s^{0.7}$. To avoid finding the exact form of each element of $\mathbf{s}$, $\mathbf{s}$ can also be fixed in order to fix the scale of the process models at whatever scale is represented in the process models $\mathbf{H}(\{\mathbf{z}\})$.

The complete multiscale P2P modeling framework consists of a set of mass, energy, and monetary balance equations on the system's commodities and products

$$\begin{bmatrix} \overline{\mathbf{I}} - \overline{\mathbf{A}}^*(\{\mathbf{z}\}) & -\underline{\mathbf{X}}_u(\{\mathbf{z}\}) & -\mathbf{X}_u^E(\{\mathbf{z}\}) \\ -\underline{\mathbf{A}}_d(\{\mathbf{z}\}) & \underline{\mathbf{X}}^*(\{\mathbf{z}\}) & -\mathbf{X}_u^V(\{\mathbf{z}\}) \\ -\mathbf{A}_d^E(\{\mathbf{z}\}) & -\mathbf{X}_d^V(\{\mathbf{z}\}) & \mathbf{X}(\{\mathbf{z}\}) \end{bmatrix} \begin{bmatrix} \overline{\mathbf{s}} \\ \underline{\mathbf{s}} \\ \mathbf{s} \end{bmatrix} = \begin{bmatrix} \overline{\mathbf{f}} \\ \underline{\mathbf{f}} \\ \mathbf{f} \end{bmatrix} \tag{43}$$

which is more compactly written as

$$\overline{\underline{\mathbf{X}}}(\{\mathbf{z}\})\overline{\underline{\mathbf{s}}} = \overline{\underline{\mathbf{f}}} \tag{44}$$

and a set of fundamental models for processes at the equipment scale

$$\mathbf{H}(\{\mathbf{z}\}) \geq 0 \tag{45}$$

that are specified externally to $\overline{\underline{\mathbf{X}}}(\{\mathbf{z}\})$ as discussed previously. Equation 44 constrains the variable elements of $\overline{\underline{\mathbf{s}}}$ such that net

Table 4. P2P Transactions Matrix $\overline{\underline{\mathbf{X}}}(\{\mathbf{z}\})$ and Environmental Interventions Matrix $\overline{\underline{\mathbf{B}}}(\{\mathbf{z}\})$

	$\overline{\underline{\mathbf{X}}}(\{\mathbf{z}\})$	
$\overline{\mathbf{I}} - \overline{\mathbf{A}}^*(\{\mathbf{z}\})$	$-\underline{\mathbf{X}}_u(\{\mathbf{z}\})$	$-\mathbf{X}_u^E(\{\mathbf{z}\})$
$-\underline{\mathbf{A}}_d(\{\mathbf{z}\})$	$\underline{\mathbf{X}}^*(\{\mathbf{z}\})$	$-\mathbf{X}_u^V(\{\mathbf{z}\})$
$-\mathbf{A}_d^E(\{\mathbf{z}\})$	$-\mathbf{X}_d^V(\{\mathbf{z}\})$	$\mathbf{X}(\{\mathbf{z}\})$
	$\overline{\underline{\mathbf{B}}}(\{\mathbf{z}\})$	
$\overline{\mathbf{B}}^*(\{\mathbf{z}\})$	$\underline{\mathbf{B}}^*(\{\mathbf{z}\})$	$\mathbf{B}(\{\mathbf{z}\})$

Table 5. Submatrices Required to Assemble the P2P Transactions and Interventions Matrices

P2P transactions submatrices		
(100)	(59)	(82)
(61)	(54), (55)	(81)
(84)	(83)	(78), (77)
P2P interventions submatrices		
(98)	(56)	(79)

production of each commodity, value chain product and equipment scale product is equal to the final demand placed on the entire system. Equation 44 also forms one set of constraints on the design variables $\{\mathbf{z}\}$, which are further constrained by the fundamental models in Equation 45.

Demonstration of the P2P Modeling Framework with a Toy Example

In this section, a toy system is used to demonstrate the data and calculations involved in representing a system using the P2P modeling framework. As each component model used to represent the toy system is presented, the use of the model in conventional sustainability analysis and design methodologies such as EEIO analysis, life cycle assessment, and sustainable process design is discussed. The objective of the comparison is to demonstrate that the P2P framework relies on the same data and models as these conventional approaches. The framework establishes a rigorous, systematic method for integrating already established models, and available data into one cohesive model.

The toy P2P system consists of a two-sector economy, two value chain activities, and two processes. Each process involves two unit operation variables and several fundamental model equations. Both sectors are parent sectors; one sector has a constituent activity and the other has a constituent process. Neither of the value chain activities are parent activities, thus only the economy scale needs to be disaggregated. The structure of the system, including all exchanges between components and all parent–constituent relationships, is shown in Figure 7.

Economy model

Sectors 1 and 2, $\bar{S}_1$ and $\bar{S}_2$ in Figure 7, are modeled with an EIO model. Commodity exchanges between $\bar{S}_1$ and $\bar{S}_2$ are captured in monetary units by the following make and use matrices

$$\overline{\mathbf{V}} = \begin{bmatrix} \$500 & 0 \\ 0 & \$700 \end{bmatrix} \tag{46}$$

$$\overline{\mathbf{U}} = \begin{bmatrix} \$150 & \$200 \\ \$300 & \$100 \end{bmatrix} \tag{47}$$

For this example, $\overline{\mathbf{U}}$ and $\overline{\mathbf{V}}$ are given in dollars; note that input–output tables are commonly specified in millions of dollars. The elements of $\overline{\mathbf{V}}$ are interpreted as commodity flows from producing sectors; the elements of $\overline{\mathbf{U}}$ are interpreted as commodity flows to consuming sectors. For instance, the (1,1)th element of $\overline{\mathbf{V}}$ is \$500, indicating that Sector 1 produces \$500 worth of Commodity 1. The (1,1)th element of $\overline{\mathbf{U}}$ is \$150 and the (1,2)th element is \$200, indicating that of the \$500 worth of Commodity 1 that Sector 1 produced, \$150 worth was consumed by Sector 1 and \$200 worth was consumed by Sector 2. These flows are indicated by the arrows in Figure 7 that originate at $\bar{S}_1$ and terminate at $\bar{S}_1$ and $\bar{S}_2$, respectively.

Environmental data for the economy is given in the environmental interventions matrix $\overline{\mathbf{B}}$

$$\overline{\mathbf{B}} = [0.40 \quad 0.20] \tag{48}$$

which captures the exchange of flows between the economic sectors and the environment. In this system, only one environmental intervention is considered. The elements of $\overline{\mathbf{B}}$ have units of mass per dollar and are interpreted as the mass of some flow emitted to the environment per dollar of economic activity in each sector.

In order to perform the disaggregation procedure, data on total environmental interventions, the matrix $\overline{\mathbf{R}}$, is required. Unlike the data in $\overline{\mathbf{B}}$, which is normalized by each sector's total output, $\overline{\mathbf{R}}$ gives unnormalized flows of environmental interventions for each sector. For this economic system, $\overline{\mathbf{R}}$ is as follows

$$\overline{\mathbf{R}} = [200 \quad 140] \tag{49}$$

The elements of $\overline{\mathbf{R}}$ are interpreted as the total amount of environmental intervention generated by each sector during the time period represented in $\overline{\mathbf{U}}$ and $\overline{\mathbf{V}}$. Note that dividing each element of $\overline{\mathbf{R}}$ by the total sector output (diagonal elements of $\overline{\mathbf{V}}$) returns the original environmental interventions matrix, $\overline{\mathbf{B}}$

$$\overline{\mathbf{R}}\hat{\overline{\mathbf{x}}}^{-1} = [200 \quad 140] \begin{bmatrix} 500 & 0 \\ 0 & 700 \end{bmatrix}^{-1} = [0.40 \quad 0.20] \tag{50}$$

If only one of $\overline{\mathbf{R}}$ and $\overline{\mathbf{B}}$ is known, Eq. 50 can be used to obtain the other.

EEIO model

Given the data in Eqs. 46–48, an EEIO model can be derived. The direct requirements matrix is obtained from the make and use matrices according to Eq. 5

$$\overline{\mathbf{A}} = \overline{\mathbf{U}}(\overline{\mathbf{V}}^{\mathrm{T}})^{-1} = \begin{bmatrix} 0.30 & 0.29 \\ 0.60 & 0.14 \end{bmatrix} \tag{51}$$

$\overline{\mathbf{A}}$ is used to derive the Leontief inverse $(\overline{\mathbf{I}}-\overline{\mathbf{A}})^{-1}$ and calculate the total economic activity $\overline{\mathbf{x}}$ required to produce an arbitrary final demand $\overline{\mathbf{f}}$

$$\overline{\mathbf{x}} = (\overline{\mathbf{I}}-\overline{\mathbf{A}})^{-1}\overline{\mathbf{f}} = \begin{bmatrix} 0.70 & -0.29 \\ -0.60 & 0.86 \end{bmatrix}^{-1} \overline{\mathbf{f}} \tag{52}$$

$\overline{\mathbf{B}}$ and the Leontief inverse of Eq. 52 are used to calculate the total environmental interventions $\overline{\mathbf{g}}$ generated as a consequence of producing $\overline{\mathbf{f}}$

$$\overline{\mathbf{g}} = \overline{\mathbf{B}}(\overline{\mathbf{I}}-\overline{\mathbf{A}})^{-1}\overline{\mathbf{f}} = [0.40 \quad 0.20] \begin{bmatrix} 0.70 & -0.29 \\ -0.60 & 0.86 \end{bmatrix}^{-1} \overline{\mathbf{f}} \tag{53}$$

This EEIO model is used in macroscale or top-down analyses such as policy analysis and input–output LCA. It is also used in combination with process life cycle models in hybrid LCA.

Table 6. Symbol Definitions

Symbol	Description and Units
Input–output analysis	
$\overline{\mathbf{X}}$	Transactions matrix used to derive EIO model ($)
$\overline{\mathbf{v}}$	Value added vector ($)
$\overline{\mathbf{f}}$	Final demand vector ($)
$\overline{\mathbf{A}}$	Industry-industry direct requirements matrix (Input-output analysis section); Commodity-commodity direct requirements matrix (elsewhere)
$\overline{\mathbf{x}}$	Vector of total sector outputs ($)
$\overline{\mathbf{I}}$	Identity matrix with the same dimensions as $\overline{\mathbf{A}}$
$\left(\overline{\mathbf{I}}-\overline{\mathbf{A}}\right)^{-1}$	Total requirements matrix or Leontief inverse, before disaggregation
$\overline{\mathbf{B}}$	Environmental interventions matrix containing data on R environmental interventions (physical units)
$\overline{\mathbf{g}}$	Inventory vector of R total environmental interventions per sector
$\overline{\mathbf{U}}$	Economy scale use table before disaggregation ($)
$\overline{\mathbf{V}}$	Economy scale make table before disaggregation ($)
$\overline{\mathbf{A}}_c$	Commodity-commodity direct requirements matrix
$\overline{\mathbf{g}}$	Vector of total commodity outputs ($)
$\overline{\mathbf{e}}$	Commodity final demand vector ($)
Process to planet (P2P) modeling framework	
$\bar{S}$	Economy scale component (sector) of a P2P system
$\underline{S}$	Value chain scale component (activity) of a P2P system
S	Equipment scale component (process) of a P2P system
System component models	
$\underline{\mathbf{x}}_l$	Value chain activity model (physical units)
$\underline{\mathbf{X}}$	Value chain technology matrix (physical units)
$\underline{\mathbf{B}}$	Value chain scale interventions matrix containing data on R environmental interventions (physical units)
$\mathbf{h}_n(\mathbf{z}_n)$	One fundamental (unit operation) model associated with process n
$\mathbf{z}_n$	Vector of unit operation variables in process n
$\mathbf{x}_n(\mathbf{z}_n)$	Process input–output vector
$\{\mathbf{z}\}$	Set of unit operation variables for processes $1,\ldots,N$
$\mathbf{X}(\{\mathbf{z}\})$	Equipment scale technology matrix
$\mathbf{H}(\{\mathbf{z}\})$	Set of all fundamental models for processes $1,\ldots,N$
$\mathbf{B}(\{\mathbf{z}\})$	Equipment scale environmental interventions matrix containing models for R interventions
Interactions between scales	
$\underline{\mathbf{X}}_u$	Value chain upstream cutoff matrix containing product flows from the economy to the value chain ($)
$\underline{\mathbf{A}}_d$	Value chain downstream cutoff matrix containing product flows from the value chain to sectors (physical units, normalized by total output of destination sector)
$\underline{\mathbf{X}}_d$	Value chain downstream cutoff matrix (physical units, not normalized)
$\mathbf{X}_u^E(\{\mathbf{z}\})$	Equipment-economy upstream cutoff matrix containing product flows from the economy to processes ($)
$\mathbf{X}_u^V(\{\mathbf{z}\})$	Equipment-value chain upstream cutoff matrix: product flows from the value chain to processes (physical units)
$\mathbf{A}_d^E(\{\mathbf{z}\})$	Equipment-economy downstream cutoff matrix: product flows from processes to sectors (physical units, normalized by total output of destination sector)
$\mathbf{X}_d^E(\{\mathbf{z}\})$	Equipment-economy downstream cutoff matrix: products flows from processes to sectors, (physical units, not normalized)
$\mathbf{X}_d^V(\{\mathbf{z}\})$	Equipment-value chain downstream cutoff matrix containing product flows from processes to the value chain (physical units, not normalized)
Model disaggregation	
$\underline{\mathbf{U}}$	Value chain scale use matrix before disaggregation (physical units)
$\mathbf{U}$	Equipment scale use matrix (physical units)
$\underline{\mathbf{V}}$	Value chain scale make matrix before disaggregation (physical units)
$\mathbf{V}$	Equipment scale make matrix (physical units)
$\overline{\mathbf{V}}^*(\{\mathbf{z}\})$	Economy scale make matrix after disaggregation ($)
$\overline{\mathbf{U}}^*(\{\mathbf{z}\})$	Economy scale use matrix after disaggregation ($)
$\underline{\mathbf{P}}_F$	Value chain function permutation matrix relating value chain products to commodities (unitless)
$\underline{\mathbf{P}}_P$	Value chain activity permutation matrix relating constituent value chain activities to parent sectors (unitless)
$\mathbf{P}_F^E$	Equipment-economy function permutation matrix relating equipment scale products to commodities (unitless)
$\mathbf{P}_P^E$	Equipment-economy process permutation matrix relating constituent processes to parent sectors (unitless)
$\underline{\mathbf{p}}$	Vector of value chain product prices
$\mathbf{p}$	Vector of equipment scale product prices
$\underline{\mathbf{V}}^*(\{\mathbf{z}\})$	Value chain scale make matrix after disaggregation (physical units)
$\underline{\mathbf{U}}^*(\{\mathbf{z}\})$	Value chain use matrix after disaggregation (physical units)
$\mathbf{P}_P^V$	Equipment-value chain process permutation matrix relating constituent processes to parent value chain activities (unitless)
$\mathbf{P}_F^V$	Equipment-value chain function permutation matrix relating equipment scale products to value chain products (unitless)
$\overline{\mathbf{A}}^*(\{\mathbf{z}\})$	Direct requirements matrix after disaggregation
$\underline{\mathbf{X}}^*(\{\mathbf{z}\})$	Value chain technology matrix after disaggregation (physical units)
$\overline{\mathbf{R}}$	Economy scale total interventions matrix containing data on R environmental interventions (physical units)
$\overline{\mathbf{B}}^*(\{\mathbf{z}\})$	Economy scale interventions matrix after disaggregation (physical units)
$\overline{\mathbf{R}}^*(\{\mathbf{z}\})$	Economy scale total interventions matrix after disaggregation (physical units)
$\underline{\mathbf{B}}^*(\{\mathbf{z}\})$	Value chain scale interventions matrix after disaggregation (physical units)

Table 6. *Continued*

Symbol	Description and Units
Integrating component models	
$\bar{\mathbf{f}}$	Final demand from economy scale of P2P system (generally zero, \$)
$\bar{\mathbf{s}}$	Economy scale scaling vector
$\underline{\mathbf{f}}$	Final demand from value chain scale of P2P system (generally zero, physical units)
$\underline{\mathbf{s}}$	Value chain scale scaling vector
$\mathbf{f}$	Final demand from equipment scale of P2P system (physical units)
$\mathbf{s}$	Equipment scale scaling vector (elements may be non-linear or fixed)
$\overline{\underline{\mathbf{X}}}(\{\mathbf{z}\})$	Multiscale P2P transactions matrix
$\overline{\underline{\mathbf{B}}}(\{\mathbf{z}\})$	Multiscale P2P environmental interventions matrix
$\overline{\underline{\mathbf{s}}}$	P2P scaling vector
$\overline{\underline{\mathbf{f}}}$	Final demand from P2P system

Value chain model

Product exchanges at the value chain scale are typically in mixed physical units and of smaller magnitude than economy scale exchanges. Although the value chain products may be represented in different units, the exchanges of a particular product are always in consistent units. The value chain scale of the toy system, $\underline{S}_1$ and $\underline{S}_2$ in Figure 7, is represented by the make and use matrices $\underline{\mathbf{V}}$ and $\underline{\mathbf{U}}$

$$\underline{\mathbf{V}} = \begin{bmatrix} 35 & 0 \\ 0 & 50 \end{bmatrix} \tag{54}$$

$$\underline{\mathbf{U}} = \begin{bmatrix} 15 & 8 \\ 5 & 10 \end{bmatrix} \tag{55}$$

The value chain environmental interventions matrix $\underline{\mathbf{B}}$ for this system is defined as

$$\underline{\mathbf{B}} = [8 \quad 5] \tag{56}$$

Unlike the economic system, the value chain has only one interventions matrix that is not normalized.

Process LCA

In process LCA, Eqs. 54 and 55 are used to derive the technology matrix $\underline{\mathbf{X}}$, as follows

$$\underline{\mathbf{X}} = \underline{\mathbf{V}}^{\mathrm{T}} - \underline{\mathbf{U}} = \begin{bmatrix} 35 & 0 \\ 0 & 50 \end{bmatrix} - \begin{bmatrix} 15 & 8 \\ 5 & 10 \end{bmatrix} = \begin{bmatrix} 20 & -8 \\ -5 & 40 \end{bmatrix} \tag{57}$$

Columns of $\underline{\mathbf{X}}$ are models of the individual activities: activity 1 (Column 1 of $\underline{\mathbf{X}}$) consumes 5 units of Product 2 and 15 units of Product 1 for every 35 units of Product 1 it produces.

The inventory vector $\underline{\mathbf{g}}$ for the production of the functional unit $\underline{\mathbf{f}}$ is then calculated by applying Eq. 9

$$\underline{\mathbf{g}} = \underline{\mathbf{B}}\underline{\mathbf{X}}^{-1}\underline{\mathbf{f}} = [8 \quad 5] \begin{bmatrix} 20 & -8 \\ -5 & 40 \end{bmatrix}^{-1} \underline{\mathbf{f}} \tag{58}$$

Value chain cutoff flows

As seen in Figure 7, both value chain activities have inputs that are modeled as upstream cutoff flows rather than exchanges at the value chain scale. The upstream cutoff flows are defined for the toy system as

$$\underline{\mathbf{X}}_u = \begin{bmatrix} 0 & \$20 \\ \$12 & 0 \end{bmatrix} \tag{59}$$

Note that these cutoff flows are in monetary units rather than the physical units of the make and use matrices. In practice, the upstream cutoff flows must be converted to monetary units using the market prices of each input.

In addition to drawing inputs from the economy, Activity 1 provides a product to Sector 1. This output is a value chain downstream cutoff flow defined for the system in Figure 7 as

$$\underline{\mathbf{X}}_d = \begin{bmatrix} 8 & 0 \\ 0 & 0 \end{bmatrix} \tag{60}$$

After normalization by the total output of the destination sector, Eq. 60 becomes

$$\underline{\mathbf{A}}_d = \begin{bmatrix} \frac{8}{\$500} & 0 \\ 0 & 0 \end{bmatrix} \tag{61}$$

In Figure 7, the arrow originating at $\underline{S}_1$ and terminating at $\bar{S}_1$ represents this downstream cutoff flow.

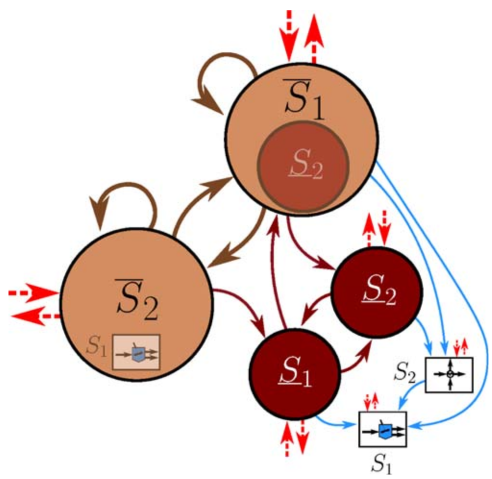

Figure 7. The toy system modeled in demonstration of the P2P modeling framework with a toy example consists of two parent sectors, two nonparent value chain activities and two processes.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Tiered hybrid LCA

Hybrid life cycle inventories are compiled from data on value chain upstream cutoffs, along with economy and value chain make, use and interventions matrices. The functional unit for a hybrid inventory is defined at the value chain scale ($\underline{\mathbf{f}}$), and contributions from the economy scale are calculated by treating the upstream cutoff flows as final demand on the economic system. For a basic or tiered hybrid LCA, the hybrid inventory vector $\mathbf{g}_t$ is calculated by adding the value chain inventory vector and the economy inventory vector, as follows[32,34,36]

$$\underline{\bar{\mathbf{g}}}_t = \underline{\mathbf{g}} + \bar{\mathbf{g}} = \underline{\mathbf{B}}\underline{\mathbf{X}}^{-1}\underline{\mathbf{f}} + \bar{\mathbf{B}}(\bar{\mathbf{I}} - \bar{\mathbf{A}})^{-1}\bar{\mathbf{f}}$$

$$= [8 \quad 5]\begin{bmatrix} 20 & -8 \\ -5 & 40 \end{bmatrix}^{-1}\underline{\mathbf{f}} + [0.40 \quad 0.20]\begin{bmatrix} 0.70 & -0.29 \\ -0.60 & 0.86 \end{bmatrix}^{-1}\bar{\mathbf{f}} \tag{62}$$

where

$$\bar{\mathbf{f}} = \begin{bmatrix} \$20 \\ \$12 \end{bmatrix} \tag{63}$$

Note that the data in Eq. 59 and in Eq. 63 is the same. The interpretation is largely the same as well. Equation 59 says that Activity 1 draws \$12 worth of input from Sector 2 and that Activity 2 draws \$20 worth of input from Sector 1. Equation 63 says only that \$20 worth of input to the value chain is drawn from Sector 1 and \$12 worth of input to the value chain is drawn from Sector 2; the exact destination of the inputs is not specified.

Integrated hybrid LCA

While tiered hybrid LCA accounts only for upstream cutoffs, the more advanced hybrid LCA methods such as integrated hybrid LCA include downstream cutoffs as well.[35] This is accomplished using the economy and value chain models to construct a hybrid transaction matrix $\underline{\bar{\mathbf{X}}}_i$ and a hybrid interventions matrix $\underline{\bar{\mathbf{B}}}_i$ analogous to those in Table 4

$$\underline{\bar{\mathbf{X}}}_i = \begin{bmatrix} \bar{\mathbf{I}} - \bar{\mathbf{A}}^* & -\underline{\mathbf{X}}_u \\ -\underline{\mathbf{A}}_d & \underline{\mathbf{X}} \end{bmatrix} \tag{64}$$

$$\underline{\bar{\mathbf{B}}}_i = \begin{bmatrix} \bar{\mathbf{B}}^* & \underline{\mathbf{B}} \end{bmatrix} \tag{65}$$

in which $\bar{\mathbf{A}}^*$ has been disaggregated according to Eqs. 26 and 27, and $\bar{\mathbf{B}}^*$ has been calculated from the disaggregated total interventions matrix according to Eqs. 36 and 37, with the equipment scale terms neglected in both calculations. Because the equipment scale is neglected, both matrices contain only constant terms and, assuming $\underline{\bar{\mathbf{X}}}_i$ to be square, Eq. 9 is used to calculate the integrated hybrid inventory vector

$$\underline{\bar{\mathbf{g}}}_i = \underline{\bar{\mathbf{B}}}_i \underline{\bar{\mathbf{X}}}_i^{-1} \underline{\bar{\mathbf{f}}}_i \tag{66}$$

Equipment scale models

Each process at the equipment scale represents a unit operation; Process 1 is a reactor and Process 2 is a heat exchanger. Process 2 heats the stream that enters Process 1 to be reacted, thus the two sets of process models are dependent on one another. Each process is controlled by two unit operation variables. In Process 1, z_{11} is the initial concentration of the reactive component in the stream entering Process 1, and z_{12} is the volumetric flow rate of that stream. In Process 2, z_{21} is the mass flow rate of the stream entering Process 1 and z_{22} is the final temperature of that stream. z_{12} and z_{21} are related to each other proportionally. Models $\mathbf{h}_1(z_{11}, z_{12}, z_{21})$ for process 1 impose constraints on z_{11}, z_{12}, and z_{21} and are defined as

$$h_{11}(z_{12}, z_{21}): \; z_{12} - 0.129 z_{21} = 0 \tag{67}$$

$$h_{12}(z_{11}, z_{12}): \; \frac{z_{11}z_{12}}{7}\left(1 - \frac{z_{12}}{7}\right) - 0.12 \le 0 \tag{68}$$

$$h_{13}(z_{11}, z_{12}): \; -\frac{z_{11}z_{12}}{7}\left(1 - \frac{z_{12}}{7}\right) \le 0 \tag{69}$$

$$h_{14}(z_{11}): \; z_{11} - 0.8 \le 0 \tag{70}$$

$$h_{15}(z_{11}): \; 0.3 - z_{11} \le 0 \tag{71}$$

For Process 2, models $\mathbf{h}_2(z_{21}, z_{22})$ impose constraints on z_{21} and z_{22} and are defined as

$$h_{21}(z_{21}, z_{22}): \; 4.2 z_{21}(z_{22} - 104) - 3000.0 \le 0 \tag{72}$$

$$h_{22}(z_{21}): \; 14 - z_{21} \le 0 \tag{73}$$

$$h_{23}(z_{21}): \; z_{21} - 50 \le 0 \tag{74}$$

$$h_{24}(z_{22}): \; 120 - z_{22} \le 0 \tag{75}$$

$$h_{25}(z_{22}): \; z_{22} - 140 \le 0 \tag{76}$$

To incorporate the equipment scale models into the P2P framework, the inputs and outputs of Processes 1 and 2 must be represented in make, use, and interventions matrices. While these matrices are derived from the process model equations, the process models $\mathbf{h}_1(z_{11}, z_{12}, z_{21})$ and $\mathbf{h}_2(z_{21}, z_{22})$ *are not duplicated verbatim*. The process models contain information on how unit operations within each process function. In contrast, the make, use and interventions matrices contain information on exchanges between the processes and between the processes and the environment, as follows

$$\mathbf{U}(\{\mathbf{z}\}) = \begin{bmatrix} z_{12} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \tag{77}$$

$$\mathbf{V}(\{\mathbf{z}\}) = \begin{bmatrix} 0 & z_{12}\left(z_{11} - \frac{z_{11}z_{12}}{7}\left(1 - \frac{z_{12}}{7}\right)\right) & z_{12}\left(\frac{z_{11}z_{12}}{7}\left(1 - \frac{z_{12}}{7}\right)\right) \\ 0.129 z_{21} & 0 & 0 \end{bmatrix} \tag{78}$$

The elements of $\mathbf{U}(\{\mathbf{z}\})$ and $\mathbf{V}(\{\mathbf{z}\})$ are obtained from knowledge of how S_1 and S_2 are connected by process streams. z_{12} is the (1,1)th element of $\mathbf{U}(\{\mathbf{z}\})$ because, as described above, z_{12} is the volumetric flow rate of the stream entering S_1 from S_2, shown in Figure 7. Its placement in the 1st row indicates that this stream consists of Product 1. In a similar manner, the (1,2)th and (1,3)th elements of $\mathbf{V}(\{\mathbf{z}\})$ are the flow rates of the streams out of S_2 (not shown in Figure 7, as they do not terminate at another system component). These two quantities are kept separate rather than being summed into one matrix element because they consist of different products.

Environmental interventions data is combined with the information in Eqs. 67–76 to produce the equipment scale environmental interventions matrix

$$\mathbf{B}(\{\mathbf{z}\}) = \left[\, 1.78 z_{12}\left(\frac{z_{11}z_{12}}{7}\left(1 - \frac{z_{12}}{7}\right)\right) \quad 1.4 z_{12} + 2.0 z_{22} \,\right] \tag{79}$$

The first element of $\mathbf{B}(\{\mathbf{z}\})$ specifies that 1.78 units of environmental intervention are generated for each unit of the stream leaving S_2. This could be due to disposal activities, or the stream could simply be emitted to the environment. The quantity, 1.78 units, is the data used to obtain equipment scale environmental interventions models. Similarly, the second term of $\mathbf{B}(\{\mathbf{z}\})$ is the scaled sum of z_{12}, a volumetric flow rate, and z_{22}, a temperature. The factors that scale the variables could represent environmental interventions due to energy required to pump liquid (z_{12}) and to heat the stream (z_{22}).

Process, product, and supply chain design

Equations 67–76, with the addition of cost data, would be used in traditional process, supply chain, and product design. The process models would be optimized on one or more of the unit operation design variables to maximize some economic objective function, as follows

$$\begin{aligned}
&\text{maximize} \\
&\qquad \$0.65z_{12}\left(\frac{z_{11}z_{12}}{7}\left(1-\frac{z_{12}}{7}\right)\right) \\
&\qquad -\$0.45z_{12}+\$0.074z_{21}(z_{22}-104) \\
&\text{subject to} \\
&\qquad z_{12}-0.129z_{21}=0 \\
&\qquad \frac{z_{11}z_{12}}{7}\left(1-\frac{z_{12}}{7}\right)-0.12\leq 0 \\
&\qquad -\frac{z_{11}z_{12}}{7}\left(1-\frac{z_{12}}{7}\right)\leq 0 \\
&\qquad z_{11}-0.8\leq 0 \\
&\qquad 0.3-z_{11}\leq 0 \\
&\qquad 4.2z_{21}(z_{22}-104)-3000.0\leq 0 \\
&\qquad 14-z_{21}\leq 0 \\
&\qquad z_{21}-50\leq 0 \\
&\qquad 120-z_{22}\leq 0 \\
&\qquad z_{22}-140\leq 0
\end{aligned} \tag{80}$$

The exact form of the objective function could represent annualized profits, NPV, or another process economics-related quantity.

Equipment scale cutoff flows

The production of several inputs to Processes 1 and 2 are modeled at the value chain or economy scales rather than the equipment scale. Just as value chain upstream cutoffs could alternatively be represented as exchanges within the value chain scale, equipment scale upstream cutoffs could be modeled as exchanges within the equipment scale. However, doing so would require that fundamental engineering models be available for the production of each product, which in general is not the case and additionally leads to a complex and possibly intractable model. Modeling the production of some inputs at larger, coarser scales reduces the amount of information required to build the P2P model and also reduces the model size, at the cost of decreased accuracy and specificity.

The equipment-value chain upstream cutoff matrix is defined as

$$\mathbf{X}_u^V(\{\mathbf{z}\})=\begin{bmatrix}0.79z_{12} & 0\\ 0 & 0.129z_{21}\end{bmatrix} \tag{81}$$

and the equipment-economy upstream cutoff matrix is defined as

$$\mathbf{X}_u^E(\{\mathbf{z}\})=\begin{bmatrix}\$0.45z_{12} & \$0.074z_{21}(z_{22}-104)\\ 0 & 0\end{bmatrix} \tag{82}$$

The flows in Eq. 81 are in mixed physical units and the flows in Eq. 82 are in monetary units. Although both processes receive inputs from the two larger scales as indicated by Eqs. 81 and 82, no equipment scale products are sold back to the system, thus both downstream process cutoff matrices consist of all zeros

$$\mathbf{X}_d^V=\begin{bmatrix}0 & 0\\ 0 & 0\end{bmatrix} \tag{83}$$

$$\mathbf{X}_d^E=\begin{bmatrix}0 & 0\\ 0 & 0\end{bmatrix} \tag{84}$$

P2P model

All flows shown in Figure 7 between the system components have now been defined. The value chain and economy scales must now be disaggregated. Further information on the relationship between parent and constituent components as well as price data is needed to perform the disaggregation. In the toy system, both economic sectors are parent sectors. $\bar{S}_1$ has one constituent activity, and $\bar{S}_2$ has one constituent process. The remaining activity and process are both standalone. From this information, the economy scale flows can be disaggregated to remove the flows corresponding to the constituents. The value chain flows need not be disaggregated, because neither value chain activity has a constituent process. Equations 85 and 86 define the permutation matrices that relate the constituent activity $\underline{S}_2$ to its parent sector $\bar{S}_1$

$$\underline{\mathbf{P}}_F=\begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix} \tag{85}$$

$$\underline{\mathbf{P}}_P=\begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix} \tag{86}$$

The location of the 1 in Eq. 85 indicates that value chain Product 2 (1 is in the second column) belongs to commodity 1 (1 is in the first row). Equation 86 indicates that $\underline{S}_2$ (1 is in the second row) is constituent to $\bar{S}_1$ (1 is in the first column).

Just as there were two sets of upstream and downstream process cutoff matrices, there are also two sets of equipment scale permutation matrices. In this system, products at the equipment scale do not correspond to value chain products, thus the equipment-value chain product permutation matrix consists of all zeros

$$\mathbf{P}_F^V=\begin{bmatrix}0 & 0\\ 0 & 0\\ 0 & 0\end{bmatrix} \tag{87}$$

Equipment scale Product 1 belongs to Commodity 2, as indicated by

$$\mathbf{P}_F^E = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \tag{88}$$

Finally, S_1 is constituent to $\bar{S}_2$

$$\mathbf{P}_P^E = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \tag{89}$$

but is not constituent to either $\underline{S}_1$ or $\underline{S}_2$

$$\mathbf{P}_P^V = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \tag{90}$$

Equations 47–89 contain most of the information necessary for the disaggregation procedure. However, the value chain and equipment scale models are in physical units, while the economy scale model is in monetary units. Price data at both the value chain and equipment scales are required in order to translate flows from one scale to another. This price data is given for the value chain products in Eq. 91 and for the equipment scale products in Eq. 92

$$\underline{\mathbf{p}} = [\$4 \quad \$6] \tag{91}$$

$$\mathbf{p} = [\$9 \quad \$5] \tag{92}$$

The adjusted use matrix $\overline{\mathbf{U}}^*$ is calculated from Eq. 27

$$\begin{aligned}\overline{\mathbf{U}}^*(\{\mathbf{z}\}) &= \overline{\mathbf{U}} - (\hat{\underline{\mathbf{p}}}\,\underline{\mathbf{P}}_F\underline{\mathbf{U}}\underline{\mathbf{P}}_P + \hat{\underline{\mathbf{p}}}\underline{\mathbf{P}}_F\underline{\mathbf{X}}_d + \underline{\mathbf{X}}_u\underline{\mathbf{P}}_P) - \left(\hat{\mathbf{p}}\mathbf{P}_F^E\mathbf{U}(\{\mathbf{z}\})\mathbf{P}_P^E + \hat{\mathbf{p}}\mathbf{P}_F^E\mathbf{X}_d^E(\{\mathbf{z}\}) + \mathbf{X}_u^E(\{\mathbf{z}\})\mathbf{P}_P^E\right) \\ &= \begin{bmatrix} \$150 & \$200 \\ \$300 & \$100 \end{bmatrix} - \left(\begin{bmatrix} \$4 & 0 \\ 0 & \$6 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 15 & 8 \\ 5 & 10 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} + \begin{bmatrix} \$4 & 0 \\ 0 & \$6 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 8 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & \$20 \\ \$12 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \right) \\ &- \left(\begin{bmatrix} \$9 & 0 \\ 0 & \$5 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} z_{12} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} \$9 & 0 \\ 0 & \$5 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} \$0.45z_{12} & \$0.074z_{21}(z_{22}-104) \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \right)\end{aligned} \tag{93}$$

$$\overline{\mathbf{U}}^* = \begin{bmatrix} \$90 & \$200-0.45z_{12} \\ \$300 & \$100-5z_{12} \end{bmatrix} \tag{94}$$

$\overline{\mathbf{U}}^*$ represents the use of commodities that are both produced and consumed at the economy scale.

The adjusted make matrix $\overline{\mathbf{V}}^*$ is calculated from Eq. 26

$$\begin{aligned}\overline{\mathbf{V}}^*(\{\mathbf{z}\}) &= \overline{\mathbf{V}} - \hat{\underline{\mathbf{p}}}\,(\underline{\mathbf{P}}_P)^{\mathrm{T}}\underline{\mathbf{V}}(\underline{\mathbf{P}}_F)^{\mathrm{T}} - \hat{\mathbf{p}}(\mathbf{P}_P^E)^{\mathrm{T}}\mathbf{V}(\{\mathbf{z}\})(\mathbf{P}_F^E)^{\mathrm{T}} \\ &= \begin{bmatrix} \$500 & 0 \\ 0 & \$700 \end{bmatrix} - \begin{bmatrix} \$4 & 0 \\ 0 & \$y6 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 35 & 0 \\ 0 & 50 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \\ &- \begin{bmatrix} \$9 & 0 \\ 0 & \$5 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & z_{12}\left(z_{11} - \frac{z_{11}z_{12}}{7}\left(1 - \frac{z_{12}}{7}\right)\right) & 0 \\ 0.129z_{21} & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}\end{aligned} \tag{95}$$

$$\overline{\mathbf{V}}^* = \begin{bmatrix} \$300 & 0 \\ 0 & \$700 \end{bmatrix} \tag{96}$$

The matrix subtracted from $\overline{\mathbf{V}}$ in Eq. 94 represents products produced by value chain activities in monetary units, thus $\overline{\mathbf{V}}^*$ in Eq. 95 represents the total output of the economic sectors less the output of their constituent activities and processes.

As seen by comparing Eq. 46 with Eq. 95, the disaggregated economic sectors have a lower total output. This reduction in total output is also applied to the total interventions matrix $\overline{\mathbf{R}}$, as follows

$$\begin{aligned}\overline{\mathbf{R}}^* &= [200 \quad 140] - [8 \quad 5] \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ &= [192 \quad 135]\end{aligned} \tag{97}$$

$\overline{\mathbf{R}}^*$ is then normalized to the level of sector output given in $\overline{\mathbf{V}}^*$ to calculate the adjusted economy scale interventions matrix $\overline{\mathbf{B}}^*$, as shown in Eq. 97

$$\begin{aligned}\overline{\mathbf{B}}^* &= \begin{bmatrix} \frac{192}{300} & \frac{135}{700} \end{bmatrix} \\ &= [0.64 \quad 0.19]\end{aligned} \tag{98}$$

The final calculation before combining the three models is calculating the adjusted total requirements matrix. $\overline{\mathbf{A}}^*$, the adjusted direct requirements matrix, is calculated from $\overline{\mathbf{U}}^*$ and $\overline{\mathbf{V}}^*$ according to Eq. 39 (restated as Eq. 98), as follows

$$\overline{\mathbf{A}}^* = \overline{\mathbf{U}}^* \left(\overline{\mathbf{V}}^{*\mathrm{T}}\right)^{-1}$$

$$= \begin{bmatrix} \$90 & \$200-0.45z_{12} \\ \$300 & \$100-5z_{12} \end{bmatrix} \begin{bmatrix} \frac{1}{300} & 0 \\ 0 & \frac{1}{700} \end{bmatrix} \quad (99)$$

$$\overline{\mathbf{A}}^* = \begin{bmatrix} 0.30 & 0.29-6.43\times10^{-4}z_{12} \\ 1.00 & 0.14-7.1\times10^{-3}z_{12} \end{bmatrix} \quad (100)$$

The effects of disaggregation can be seen by comparing Eq. 51 with Eq. 99.

The P2P transactions and interventions matrices shown in Table 4 can now be assembled from the equations given in Table 5

$$\underline{\overline{\mathbf{X}}}(\{\mathbf{z}\}) = \begin{bmatrix} 0.70 & 6.43\times10^{-4}z_{12}-0.29 & 0 & -\$20 & -\$0.45z_{12} & -\$0.074z_{21}(z_{22}-104) \\ -1.00 & 7.1\times10^{-3}z_{12}-0.14 & -\$12 & 0 & 0 & 0 \\ -\frac{8}{300} & 0 & 20 & -8 & -0.79z_{12} & 0 \\ 0 & 0 & -5 & 40 & 0 & -0.129z_{21} \\ 0 & 0 & 0 & 0 & -z_{12} & 0.129z_{21} \\ 0 & 0 & 0 & 0 & z_{12}(z_{11}-\frac{z_{11}z_{12}}{7}\left(1-\frac{z_{12}}{7}\right)) & 0 \\ 0 & 0 & 0 & 0 & z_{12}(\frac{z_{11}z_{12}}{7}\left(1-\frac{z_{12}}{7}\right)) & 0 \end{bmatrix} \quad (101)$$

$$\underline{\overline{\mathbf{B}}}(\{\mathbf{z}\}) = \begin{bmatrix} 0.64 & 0.19 & 8 & 5 & 1.78z_{12}(\frac{z_{11}z_{12}}{7}\left(1-\frac{z_{12}}{7}\right)) & 1.4z_{12}+2.0z_{22} \end{bmatrix} \quad (102)$$

The final component of the P2P model is the set of constraints on the unit operation variables, given in Eqs. 67–76.

Discussion and Conclusions

The P2P modeling framework is both detailed, containing fundamental models of individual processes and unit operations, and comprehensive, using a coarse EEIO model to capture national or planetary economic systems. It addresses the shortcomings of both conventional bottom up sustainable engineering methods, which fail to capture a sufficiently large system boundary, and top down sustainability analysis methods, which cannot capture the effects of small-scale decisions on the system. The P2P framework is suitable for a wide variety of sustainable engineering applications, including product design and supply chain design and analysis. Applications outside of engineering include economic policy analysis; because the P2P framework contains detailed models at the small scale, it can be used to model the effects of policies on individual plants and supply chains, and vice versa. The framework can also be used for advanced hybrid life cycle assessment with nonlinear and fundamental models. Life cycle optimization can be accomplished by including production technology alternatives at the value chain scale and optimizing the entire system. Applications of the framework currently in progress include sustainable chemical process design using an ethanol production system as a case study,[41] and life cycle design of a renewable energy production system considering decision variables in both the biomass conversion and land use stages.[63]

There are many extensions and alterations possible for the P2P framework, most of which involve replacing one type of model with another at one or more scales. In this work, the economy scale of the P2P system was represented by an EEIO model of a national economy; a MRIO model could be used instead to capture the global economy and account for the environmental effects of imported and exported goods and services. Similarly, the EEIO model could be replaced with the more flexible general equilibrium or partial equilibrium models to capture the effects of price changes and elasticities on the P2P system. The use of equilibrium models at the economy scale would also allow the P2P framework to be used more effectively for economic policy design and analysis.[64] Another economy scale option is the replacement of the EEIO model with a rectangular choice-of-technology (RCOT) model that contains alternative technologies for one or more industrial sectors.[65] At the value chain scale, the standard model that contains one activity per primary value chain product can also be replaced by an RCOT model to allow choosing between alternative production technologies at a smaller regional scale. Optimization can then be used to find the optimal P2P structure at the equipment scale, the value chain scale or the economy scale, or any combination of scales.

The basic concept behind the P2P framework, that of an input–output-based framework with some nonlinear elements, can be applied to ecological models as well. Current work with the P2P framework is integrating the existing framework, which represents technological and economic systems, with the framework for technoecological synergy.[66] The resulting technoeconomic-ecological framework will model ecosystems and their interactions with the technoeconomic system at relevant scales, and can be used to design industrial systems simultaneously with supporting ecological processes.

Notation

Annotations

A hat ̂ over a vector denotes diagonalization

A bar over a symbol indicates economy scale: $\bar{X}$

A bar under a symbol indicates value chain scale: $\underline{X}$

No bars indicates equipment and unit operation scale: X

Bars over and under a symbol indicates a multiscale model: $\underline{\overline{X}}$

Bold lower-case symbols indicate vectors

Bold upper-case symbols indicate matrices

A superscript star * on a component index indicates the remainder of a parent component after disaggregation; the same symbol on a vector or matrix of component models indicates that all parent components in the model have been disaggregated

Indexes

i = producing sector (Input–output analysis) or Commodity (elsewhere)
j = consuming sector (Input–output analysis) or Sector (elsewhere)
k = value chain product
l = value chain activity
m = equipment scale product
n = equipment scale process

A capital index (I, J, M and so on) indicates the number of system components of that type.

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